

**DESIGN AND USE OF IONIC LIQUIDS IN SEPARATION PROCESSES
FOR AZEOTROPIC MIXTURES**

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A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science
The Petroleum and Petrochemical College, Chulalongkorn University
in Academic Partnership with
The University of Michigan, The University of Oklahoma,
Case Western Reserve University, and Institut Français du Pétrole
2015

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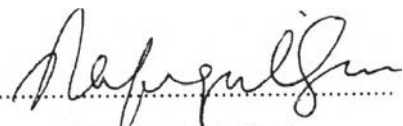
Thesis Title: Design and Use of Ionic Liquids in Separation Processes
for Azeotropic Mixtures
By: Worawit Peng-noo
Program: Petroleum Technology
Thesis Advisors: Dr. Uthaiporn Suriyaphadilok
Prof. Rafiqul Gani

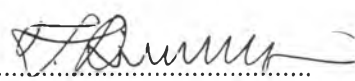
Accepted by The Petroleum and Petrochemical College, Chulalongkorn
University, in partial fulfillment of the requirements for the Degree of Master of
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ABSTRACT

5673036063: Petroleum Technology Program

Worawit Peng-noo: Design and Use of Ionic Liquids in
Separation Processes for Azeotropic Mixtures

Thesis Advisors: Dr. Uthaiporn Suriyaphadilok, and
Prof. Rafiqul Gani 432 pp.

Keywords: Separation / Azeotrope / Ionic liquids / Extractive distillation

Separation of azeotrope and close-boiling mixtures is a challenge in several industries. Ionic liquids (ILs) have been recently determined as alternative entrainers in the extractive distillation (ED) owing to the flexibility in their tailor-made molecular structures and properties for a specific work. A systematic methodology of selection and design of the best IL-based separation process was developed to investigate the viability of the azeotropic separation process using ILs through five different mixtures as case studies including the mixtures of ethanol + water, ethanol + hexane, benzene + hexane, toluene + methylcyclohexane (MCH), and ethylbenzene (EB) + p-xylene (PX). The Hildebrand solubility Group Contribution parameter along with the capacity and selectivity of ILs are the key parameters for selecting the suitable ILs as entrainers. All first four azeotropic mixtures were successfully demonstrated and four best ILs were identified, i.e. [MMIM][DMP] from ethanol + water, [EMIM][BTI] from ethanol + hexane mixture, [EMIM][EtSO₄] from benzene + hexane mixture, and [HMIM][TCB] from toluene + methylcyclohexane (MCH) mixture. However, the proposed screening criteria cannot effectively demonstrate the isomer mixture, i.e. EB + PX mixture, due to the similarity of these isomers causing no differences in the calculated Hildebrand solubility parameter, selectivity and capacity. A simulation process of ILs was carried out successfully, which a minimum energy requirement and a solvent usage were determined and compared with the conventional solvent process. In order to get a supported decision-making in an investment, economic evaluation was determined and compared between the IL and conventional solvent processes.

บทคัดย่อ

วรวิทย์ เฟื่องหนู : การออกแบบการเลือกใช้ไอออนิกลิควิดในกระบวนการแยกสำหรับของผสมอะซีโอโทรป (Design and Use of Ionic Liquids in Separation Processes for Azeotropic Mixtures) อ. ที่ปรึกษา: ดร. อุทัยพร สุริยประภาติลล และ ศ.ดร. ราฟีก กานี 432 หน้า

การจัดการกับปัญหาที่เกี่ยวข้องกับกระบวนการแยกของผสมอะซีโอโทรป (Azeotrope) และของผสมที่มีจุดเดือดใกล้เคียงกัน (Close-boiling) เป็นปัญหาที่ท้าทายในหลากหลายอุตสาหกรรมนั้น ทำให้ไม่นานมานี้ของเหลวไอออนิก (Ionic liquids) ได้ถูกพิจารณานำมาเลือกใช้เป็นสารช่วยกลั่น (Entrainers) ในหอกลั่นแบบสกัด (Extractive distillation) อันเนื่องมาจากการยืดหยุ่นปรับแต่งได้ในตัวโครงสร้าง โมเลกุลและคุณสมบัติเฉพาะของของเหลวไอออนิก ดังนั้นระบบวิธีการสำหรับการคัดเลือกและการออกแบบกระบวนการแยกโดยใช้ของเหลวไอออนิกที่ดีที่สุดถูกพัฒนาขึ้นมาโดยผ่านการตรวจสอบการนำไปใช้งานได้จริงในทุกๆระบบจากของผสมห้าชนิดซึ่งเป็นกรณีศึกษาในครั้งนี้ ได้แก่ของผสมเอทานอลกับน้ำ เอทานอลกับเฮกเซน เบนซีนกับเฮกเซน โทลูอีนกับเมทิลไซโคลเฮกเซน และ เอทิลเบนซีนกับพาราไซลีน พารามิเตอร์หลักที่เสนอใช้ในการคัดเลือกของเหลวไอออนิกที่ดีที่สุดของแต่ละระบบในงานวิจัยนี้มีดังนี้ พารามิเตอร์ของการละลายของฮิลเดบรอนด์ (Hildebrand solubility Group Contribution parameter) พร้อมด้วยพารามิเตอร์ของความสามารถในการละลายได้ (Capacity) และความสามารถในการเลือกการละลาย (Selectivity) ของของเหลวไอออนิก ซึ่งของเหลวไอออนิกที่ดีที่สุดที่ผ่านการคัดเลือกคือ [MMIM][DMP] จากของผสมเอทานอลกับน้ำ [EMIM][BTI] จากของผสมเอทานอลกับเฮกเซน [EMIM][EtSO₄] จากของผสมเบนซีนกับเฮกเซน และ [HMIM][TCB] จากของผสมโทลูอีนกับเมทิลไซโคลเฮกเซน อันเนื่องด้วยหลักการคัดเลือกนี้ยังไม่สามารถตอบสนองการทำงานอย่างมีประสิทธิภาพกับของผสมไอโซเมอร์ (Isomer) ได้ ทำให้ของผสมเอทิลเบนซีนกับพาราไซลีนไม่ถูกนำไปวิเคราะห์ต่อจนจบในท้ายที่สุด จากความคล้ายกันของสารไอโซเมอร์ทำให้ไม่มีความแตกต่างในค่าพารามิเตอร์ Hildebrand ค่าพารามิเตอร์ Capacity และ ค่าพารามิเตอร์ Selectivity แบบจำลอง (Simulation) กระบวนการของของเหลวไอออนิกได้ถูกสร้างขึ้นใหม่และคำนวณค่าการใช้พลังงานและการใช้สารละลายที่น้อยที่สุด เพื่อนำไปเปรียบเทียบกับกระบวนการที่ใช้ตัวทำละลายอินทรีย์ (Conventional solvent) แต่เพื่อให้ได้ข้อมูลประกอบการตัดสินใจในการลงทุน การประเมินเชิงธุรกิจได้ถูกจัดทำขึ้นเพื่อเสนอเปรียบเทียบกระบวนการแยกด้วยของเหลวไอออนิกและตัวทำละลายอินทรีย์ในขั้นตอนสุดท้าย

ACKNOWLEDGEMENTS

This master thesis would not have been completely finished without the assistance and kind support of the following individuals and organizations:

First of all, I am very appreciated to Dr. Uthaiporn Suriyapraphadilok, my advisor, for providing invaluable guidance, creative suggestions and kind support throughout this research work.

I would like to express my sincere gratitude to Prof. Rafiqul Gani for giving me the best opportunity and priceless experience to visit Computer Aided Process Engineering Center (CAPEC), Technical University of Denmark. Absolutely, he offered the warmest welcome, untouchable knowledge, and also kind support throughout this research work.

I would like to especially thank Assoc. Prof. Thirasak Rirksomboon and Asst. Prof. Bunyaphat Suphanit for participating on behalf of my thesis committee. Their comments are very beneficial for accomplishing this research work.

I would like to extend my thanks to all members and staffs of the Petroleum and Petrochemical College, Chulalongkorn University, Thailand, and also all my graduate friends for their cheering and encouragement. I am grateful for the partial scholarship and partial funding of the thesis work provided by the Petroleum and Petrochemical College.

Finally, I am deeply indebted to my family for their love, understanding, encouragement, and support me at all time.

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ABBREVIATIONS

Nomenclature of the Ionic Liquids

Cations

[MMIM] ⁺	1-Methyl-3-Methylimidazolium
[EMIM] ⁺	1-Ethyl-3-Methylimidazolium
[EM2IM] ⁺	1,2-Dimethyl-3-Methylimidazolium
[PMIM] ⁺	1-Propyl-3-Methylimidazolium
[BMIM] ⁺	1-Butyl-3-Methylimidazolium
[HMIM] ⁺	1-Hexyl-3-Methylimidazolium
[OMIM] ⁺	1-Methyl-3-Octylimidazolium
[DMIM] ⁺	1-Decyl-3-Methylimidazolium
[PDMIM] ⁺	1-Propyl-2,3-Dimethylimidazolium
[16MIM] ⁺	1-Hexadecyl-3-Methylimidazolium
[OHDMIM] ⁺	1-(2-Hydroxyethyl)-3-Methylimidazolium
[C6H13OCH2MIM] ⁺	1-Hexyloxymethyl-3-Methylimidazolium
[(C6H13OCH2)2IM] ⁺	1,3-Dihexyloxymethylimidazolium
[EMPY] ⁺	1-Ethyl-3-methylpyridinium
[BMPY] ⁺	1-Butyl-3-methylpyridinium
[EMPYR] ⁺	1-Ethyl-1-methylpyrrolidinium
[BMPYR] ⁺	1-Butyl-1-methylpyrrolidinium
[PMPIP] ⁺	1-Propyl-1-Methylpiperidinium
[PeMPIP] ⁺	1-Pentyl-1-Methylpiperidinium
[HMPIP] ⁺	1-Hexyl-1-Methylpiperidinium
[3C6C14P] ⁺	Trihexyltetradecylphosphonium
[3BMP] ⁺	Tributylmethylphosphonium
[P1444] ⁺	Triisobutylmethylphosphonium
[E3S] ⁺	Triethylsulphonium
[OMA] ⁺	Trioctylmethylammonium
[TMHA] ⁺	Trimethylhexylammonium

Anions

[Br] ⁻	Bromide
[Cl] ⁻	Chloride
[PF ₆] ⁻	Hexafluorophosphate
[BF ₄] ⁻	Tetrafluoroborate
[CF ₃ SO ₃] ⁻ or [OTf] ⁻	Trifluoromethanesulfonate
[NTf ₂] ⁻ or [BTf] ⁻	Bis(trifluoromethylsulfonyl)imide
[PF ₃ (C ₂ F ₅) ₃] ⁻ or [FAP] ⁻	Tris(pentafluoroethyl)trifluorophosphate
[Ac] ⁻	Acetate
[CF ₃ CO ₂] ⁻ or [TFA] ⁻	Trifluoroacetate
[NO ₃] ⁻	Nitrate
[TOS] ⁻	Tosylate
[SCN] ⁻	Thiocyanate
[N(CN) ₂] ⁻ or [DCA] ⁻	Dicyanamide
[TCAM] ⁻	Tricyanomethanide
[B(CN) ₄] ⁻ or [TCB] ⁻	Tetracyanoborate
[BOB] ⁻	Bis[oxalato(2-)]-borate
[EtSO ₄] ⁻	Ethylsulfate
[MeSO ₄] ⁻	Methylsulfate
[OcSO ₄] ⁻	Octylsulfate
[Me(EtO) ₂ SO ₄] ⁻ or [MDEGSO ₄] ⁻	Diethylglycol monomethyl ether sulfate or 2-(2-methoxyethoxy)ethylsulfate
[HSO ₄] ⁻	Hydrogensulfate
[MeSO ₃] ⁻	Methanesulfonate
[ToSO ₃] ⁻	P-Toluenesulfonate
[MePO ₃] ⁻	Methylphosphonate
[DMP] ⁻	Dimethylphosphate

LIST OF SYMBOLS

c_{ii}	= cohesive energy density
C_i	= contribution of group i
g_{ij}	= energy parameter characteristic of the i-j interaction
g_{ij}	= energy parameter characteristic of the i-j interaction
Δg_{ij}	= binary interaction parameter between component i and j
Δh_{vap}	= enthalpy of vaporization
K_1	= K-factor for component 1
K_2	= K-factor for component 2
M	= the molecular mass
n_i	= the number of groups of type i
n_i	= the number of times that a group appears in the molecule
N	= number of stages
N_F	= feed stage location
P_1^s	= vapor pressures of component 1
P_2^s	= vapor pressures of component 2
R	= gas constant
T	= absolute temperature
T_b	= normal boiling temperature
T_c	= critical temperature
v_i	= molar volume of component i
V_i	= volume/mole fraction of component i
V_C	= critical volume
x_1	= mole fraction for component 1 in the liquid phase
x_2	= mole fraction for component 2 in the liquid phase
y_1	= mole fraction for component 1 in the vapor phase
y_2	= mole fraction for component 2 in the vapor phase

Greek Symbols

α_{12} = separation factor or relative volatility

α_{ij} = non-randomness parameter in the NRTL equation

γ_1 = activity coefficient of component 1

γ_2 = activity coefficient of component 2

γ_i^C = combination part of the activity coefficient of component i

γ_i^R = residual part of the activity coefficient of component i

δ_i = solubility parameter of component i

ω = acentric factor

ρ_L = liquid densities of the ionic liquids