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A systematic visual methodology to design ionic liquids and ionic liquid mixtures: Green solvent alternative for carbon capture

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ABSTRACT

Ionic liquids (ILs) have gained great interest recently to substitute volatile organic compounds (VOCs), since their properties can be tuned to match certain targets and applications. Further to this, another possibility to optimise ILs for their specific application is through IL mixtures. In this work, an insightful and yet simple systematic approach to design pure ILs and their mixtures is presented. This newly presented approach allows the visualisation of IL mixture design problem, and hence provides insights and allows users to solve the problem visually. The visualisation of problem and solutions is achieved by applying property integration framework in this proposed methodology. In property integration framework, IL products design problem is mapped from property domain into cluster domain through property clustering technique. Therefore, the proposed methodology provides a property based platform to visualise the overall performance of the designed IL products with graphical tools. A feasible IL product is always designed to fit a purpose based on consideration of multiple target properties, but these properties can be contradicting one another. The presented approach allows multiple target properties consideration during the design process, by portraying these properties and target of each clearly on a single graphical tool. To date, the study of properties of pure ILs and IL mixtures is still in the infant phase, and these data are still scarce. Hence, some of the prediction models do not cover all available ILs. To overcome this problem, the proposed approach is developed to adapt property data of pure ILs directly, together with existing property prediction models to predict the properties of the designed IL mixtures. The presented approach is able to generate a list of potential solutions to users, and the final decision can be made by users accordingly, through further screening and experimental validations. An illustrative case study, which focuses on the design of carbon capture solvents, is solved to demonstrate the proposed approach.

1. Introduction

Volatile organic compounds (VOCs) have been widely used for various industrial applications. However, the VOCs can easily escape into the atmosphere with detrimental effects on environmental and human health (Blanchard et al., 1999). Literature studies reported that the effects of VOCs range from nauseous to carcinogens (Muñoz et al., 2007), and even to global warming agents (Rocha-Rios et al., 2009). These problems occur mainly due to high volatility of the compounds, which can be avoided using low volatility compounds. Besides, using solvent with low volatility is more cost effective as solvent loss will be minimal. Recently, a new class of compounds, namely ionic liquids (ILs) has been introduced as a potential replacement of VOCs. ILs, which refer to organic salts that remain in liquid form at room temperature, exhibit no measurable vapour pressure at room temperature and remain stable over their wide temperature range (Marsh et al., 2004) due to Coulombic attraction between cations and anions (Bates et al., 2002). These suggest that ILs are more environmental friendly compared to VOCs for not releasing harmful compounds during process. Another key feature of ILs is that their thermophysical properties can be tuned through choosing proper cation-anion combinations (Plechkova and Seddon 2008). Hence, pure ILs can be designed to possess the most adequate characteristics and suit various industrial applications, such as electrochemical solvents, lubricants, heat transfer fluids, and entrainers (Brennecke and Maginn 2001).

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Nomenclature

Abbreviations

AUP	Augmented property index
CAMD	Computer-aided molecular design
CCS	Carbon capture and storage
GC	Group contribution
IL	Ionic liquid
MEA	Monoethanolamine
MINLP	Mixed integer non-linear programming
VBI	Viscosity blending index
VOC	Volatile organic compounds

Ionic liquids

$[MIm]^+$	Methylimidazolium cation
$[Py]^+$	Pyridinium cation
$[MPyr]^+$	Methylpyrrolidinium cation
$[N_{4111}]^+$	Butyltrimethylammonium cation
$[N_{1888}]^+$	Methyltrioctylammonium cation
$[BF_4]^-$	Tetrafluoroborate anion
$[PF_6]^-$	Hexafluorophosphate anion
$[NTf_2]^-$	Bis(trifluoromethylsulfonyl)imide anion

Indices

d	Property (d = 1, 2, . . ., N_p)
i	Component (i = 1, 2, . . ., p)
k	Groups (k = 1, 2, . . ., q)

Parameters

a_{mn}	UNIFAC group interaction parameter between group m and n
a_i	Constant for group i in Antoine equation
$A_{k,\mu}$	Contribution of group k to parameter A_μ
b_i	Constant for group i in Antoine equation
$B_{k,\mu}$	Contribution of group k to parameter B_μ
c_i	Constant for group i in Antoine equation
C_i	Solvent cost of IL i (USD/mol)
$c_{p,k}$	Specific heat capacity contribution of group k (J/mol.K)
$\Delta H_{vap,k}$	Heat of vaporisation contribution of group k (kJ/mol)
N	Avogadro constant
n_k	Free bond number of group k
P_k	Contribution of group k to the overall Hildebrand solubility parameter ($MPa^{1/2}$)
Q_k, Q_m, Q_n	Group surface area parameter in the UNIFAC model
R	Universal gas constant (J/mol.K)
R_k	Group volume parameter in the UNIFAC model

Variables

A_μ	Coefficient in the model equation for the viscosity
A_κ	Coefficient in the model equation for the electrical conductivity
A_λ	Coefficient in the model equation for the thermal conductivity
AUP_i	Augmented property index for component i
AUP_k	Augmented property index for group k
B_μ	Coefficient in the model equation for the viscosity
B_κ	Coefficient in the model equation for the electrical conductivity
B_λ	Coefficient in the model equation for the thermal conductivity
C	Solvent cost of IL mixture (USD/mol)
C_{di}	property cluster for property d of component i
C_{dk}	Property cluster for property d of group k
$c_{P,i}$	Specific heat capacity of component i (J/mol.K)
F_i	Auxiliary property for component i (surface fraction/mole fraction)
g^{CH_3}	Number of CH_3 groups in the selected cation
$\Delta H_{vap,i}$	Heat of vaporisation of component i (kJ/mol)
M	Molecular weight (g/mol)
P_i^S	Saturated vapour pressure of component i (MPa)
q_i	Parameter relative to the molecular van der Waals surface areas of pure component i
r_i	Parameter relative to the molecular van der Waals volumes of pure component i
S	CO_2 solubility in mixture (kmol CO_2/kg solvent)
S_i	CO_2 solubility in component i within mixture (kmol CO_2 /kg solvent)
V	Molecular volume ($Å^3$)
V_i	Auxiliary property of component i
VBI_i	Viscosity blending index of component i
v_k, v_m	Number of group k or m
$vk^{(i)}$, $vm^{(i)}$	Number of group k or m in component i
x_i	Mole fraction of component i in liquid phase
x_j	Mole fraction of group j in the mixture
X_m, X_n	Fraction of group m or n in the mixture
y_i	Mole fraction of component i in gas phase

Greek Symbols

μ_i	Dynamic viscosity of component i (Pa.s)
κ	Electrical conductivity (S/m)
λ	Thermal conductivity (W/m.K)
ρ	Density (g/cm^3)
ρ_c	Critical density (g/cm^3)
ρ_i	Density of component i (g/cm^3)
ρ_k	Density contribution of group k (g/cm^3)
ρ_0	Adjustable parameter for density (g/cm^3)
σ	Reduced density
ϕ^r	Reduced dimensionless Helmholtz function
ϕ_δ^r	Derivative of reduced dimensionless Helmholtz function
ϕ_i	Gas-phase fugacity coefficient of component i
γ_i	Activity coefficient of component i
γ_i^C	Combinatorial contribution to the activity coefficient of component i
γ_i^R	Residual contribution to the activity coefficient of component i
Γ_K	Residual activity coefficient of group k
$\Gamma_K^{(i)}$	Residual activity coefficient of group k in pure component i
θ_m	Fraction of group m in a mixture of the liquid phase
Ψ_{nm}	Group interaction parameter
τ_d	d^{th} property
τ_d^{min}	Lower bound of d^{th} property
τ_d^{max}	Upper bound of d^{th} property
$\Psi_d(\tau_{di})$	Property operator of d^{th} property of component i
$\Psi_d(\tau_{dk})$	Molecular property operator of d^{th} property of functional group k
$\psi_d^{ref}(\tau_d)$	Reference value for molecular property operator of d^{th} property
$\Psi_d(\tau_d)_M$	Property operator of d^{th} property of mixture M

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