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Performance simulation of the absorption chiller using water and ionic liquid 1-ethyl-3-methylimidazolium dimethylphosphate as the working pair

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ABSTRACT

The thermodynamic performance of the absorption chiller using water and ionic liquid 1-ethyl-3-methylimidazolium dimethylphosphate ([EMIM][DMP]) as the working pair was simulated. In addition, the effects of evaporation temperature on the performance coefficient, COP, generation temperature, concentration of strong solution and flow rate ratio were also analyzed. At the same condensing and absorbing temperature, the simulating results indicated that the performance coefficient for the water + [EMIM][DMP] was lower than that for aqueous solution of lithium bromide (H_2O + LiBr) but still higher than 0.7, while the generation temperature was lower than that for H_2O + LiBr, which indicated that the working pair, water + [EMIM][DMP], was capable of being used as a novel working pair for the absorption chiller driven by lower temperature level waste heat or hot water generated by common solar collector.

1. Introduction

With rapid economic growth, human beings have to face more and more serious environmental and energy issues. The ways to solve these problems are developing and utilizing renewable energy resources, enhancing energy utilization efficiency and so on. Absorption chillers or absorption heat pumps are both important energy-saving devices which can be driven by a lot of low-grade thermal energy, such as solar energy and industrial waste heat from industrial process, so the devices will play an important role in improving energy utilization efficiency and reducing environmental pollution and carbon dioxide emissions.

The performance of absorption cycles depends on the thermodynamic properties of working pairs consisted of refrigerant and absorbent. Up to now, the commonly-used working pairs are ammonia + water solution (NH_3 + H_2O) and aqueous solution of lithium bromide (H_2O + LiBr). However, the corrosion, crystallization and toxicity are their inevitable weakness in industrial application. Therefore, seeking more advantageous working pairs with good thermal stability, no corrosion and no crystallization, has become a research focus in recent years.

Ionic liquids (ILs) are room-temperature melting salts that can remain liquid state at near or below room temperature [1]. In the last few decades, ILs have attracted considerable attentions due to their unique properties, e.g. negligible vapor pressure [2], non-flammability, thermal stability [3], low melting points, liquid state over a wide temperature range from room temperature to about 300 °C, good solubility and so on [4].

Up to now, extensive researches are focusing on the properties of ILs used as the reaction solvent in reaction process, or extraction agent in separation process [5–8]. Because of excellent properties of ILs, it is possible that ILs are used as a new type of absorbent of coolants for absorption chiller or absorption heat pump. However, the reports on ILs used as absorbent in absorption heat pump or absorption chiller are very limited. The pressure and heat capacity of binary solution of 2,2,2-trifluoroethnol (TFE) + 1-butyl-3-methyl imidazolium tetrafluoroborate ([bmim][BF_4]), were studied and the negative deviation from Raoult's Law of these binary solution were found [9]. The solubility and diffusivity of Hydrofluorocarbon (HFCs) in [bmim][BF_4] and 1-butyl-3-methyl imidazolium hexafluoroborate ([bmim][BF_6]) were also predicted qualitatively, and the excess properties G^E, H^E and S^E of solution of R-134a and [bmim][BF_6] predicted by Non-Random Two Liquid (NRTL) active coefficients models were given [10]. The solubility of ammonia, NH_3, in 1-ethyl-3-methylimidazolium acetate ([emim][Ac]), 1-ethyl-3-methylimidazolium ethylsulfate ([emim][$EtOSO_3$]), 1-ethyl-3-methylimidazolium thiocyanate ([emim][SCN]), and dimethylethanolamine acetate ([DMEA][Ac]), were further studied, respectively [11]. The vapor pressure and specific heat capacity of binary solution, [emim][$EtOSO_3$] and water were studied as a new working pair [12]. Moreover, the vapor pressure, excess enthalpy and specific heat capacity of binary solution 1-ethyl-3-methylimidazolium dimethylphosphate ([EMIM][DMP]) with water,

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Nomenclature

COP	coefficient of performance
C_P	specific heat capacity (kJ/kg K)
F	flow rate ratio
H	enthalpy (KJ/mol)
H^E	excess enthalpy (KJ/mol)
m	mass flow rate (kg s^{-1})
p	pressure (MPa)
Q	heat load (kW)
T	temperature (K)
x_2	molar fraction of [EMIM][DMP] in solution
x_1	molar fraction of water in solution
x_d	molar fraction of [EMIM][DMP] in dilute solution
x_s	molar fraction of [EMIM][DMP] in strong solution

Subscripts

A	absorber
C	condenser
E	evaporator
G	generator

ethanol or methanol were also studied respectively and these binary systems presented negative deviation from Raoult's Law and negative excess enthalpies [13], which made it possible to be used as the working pair for absorption chiller or absorption heat pump.

Up to now, the research article published on the performance simulation of absorption chiller with ionic liquid working pair are very limited and only few articles can be found in recent years. A. Yokozeki and M.B. Shiflett [14] calculated the coefficient of performance with water and some ILs, including [EMIM][DMP] when condensing, absorption and evaporation temperatures were 40 °C, 30 °C and10 °C respectively based on their established thermodynamic properties. In this article 0.690 of COP for H_2O + [EMIM][DMP] was found. A. Martín and M. D. Bermejo [15] simulated the performance of absorption refrigeration cycles using ionic liquid + supercritical CO2 pairs. Shiqiang Liang et al. [16] simulated the performance of absorption refrigeration cycle with methanol and 1,3-methylimidazolium dimethylphosphate, CH_3OH + [MMIM][DMP], and the predicted COP of 0.82 was found in this article when condensing, absorption and evaporation temperatures were 40 °C, 30 °C and5°C respectively.

By now the detailed research report on the thermodynamic performance of absorption refrigeration cycle with working pair H_2O + [EMIM][DMP] has not been found. So it is necessary to determine whether the binary solution H_2O + [EMIM][DMP] could be used as a new working pair for absorption chiller or absorption heat pump, in which the ionic liquid [EMIM][DMP] was used as an absorbent while the water as a refrigerant, it was necessary to simulate the thermodynamic performance of absorption refrigeration cycle based on the thermodynamic data of binary solution H_2O + [EMIM][DMP] presented in our previous study [13].

2. The thermodynamic properties of [EMIM][DMP] + water, water and water steam

The thermodynamic properties of binary solution water + [EMIM][DMP] have been reported in our previous studies [13], here some thermodynamic properties related to the performance simulation are given as follows.

2.1. The pressure of solution

Because of non-volatilization of ionic liquid, [EMIM][DMP], the vapor phase is consisted of only water, the pressure of this system is

$$p = \gamma_1 x_1 p_1^s \tag{1}$$

where, γ_1 is the activity coefficient of water, x_1 is the mole fraction of water in solution, $p_1{}^s$ is the saturation vapor pressure of pure water.

The activity coefficients of water in the solution [EMIM][DMP](2) + H_2O(1) are given in the form of NRTL model as follows:

$$\ln \gamma_1 = x_2^2\left[\tau_{21}\left(\frac{G_{21}}{x_1 + x_2 G_{21}}\right)^2 + \frac{\tau_{12}G_{12}}{(x_2 + x_1 G_{12})^2}\right] \tag{2}$$

$$\ln \gamma_2 = x_1^2\left[\tau_{12}\left(\frac{G_{12}}{x_2 + x_1 G_{12}}\right)^2 + \frac{\tau_{21}G_{21}}{(x_1 + x_2 G_{21})^2}\right] \tag{3}$$

$$G_{12} = \exp(-\alpha\tau_{12}), G_{21} = \exp(-\alpha\tau_{21}) \tag{4}$$

$$\tau_{12} = \frac{\Delta g_1}{RT}, \tau_{21} = \frac{\Delta g_2}{RT} \tag{5}$$

where, $\alpha = 0.6004$ is the non-random parameter of the NRTL model. Δg_1 and Δg_2 are both binary interaction parameters and expressed as follows:

$$\Delta g_i = a_i + b_i T + c_i T^2 (i = 1, 2) \tag{6}$$

where a_i, b_i, and c_i are all regression parameters and are given in Table 1.

The saturated vapor pressure of pure water $p_1{}^s$, can be calculated by Antoine equation (7).

$$\ln(p^s/\mathrm{kPa}) = 16.28837 + 3816.4/[-46.13 + (T/\mathrm{K})] \tag{7}$$

2.2. Enthalpy of solution

Enthalpy of the solution [EMIM][DMP] + H_2O at T and at IL mole fraction x_2 can be calculated by Eq. (8).

$$H = H_{298} + \int_{298}^{T} C_P \mathrm{d}T \tag{8}$$

where, H_{298} (kJ/kmol) is the specific enthalpy of solution with IL mole fraction x_2 at 298 K, and is shown in Eq. (9).

$$H_{298} = H_{298}^E + x_2 \int_{273}^{298} C_{P,[\mathrm{EMIM}][\mathrm{DMP}]}\mathrm{d}T + x_1 \int_{273}^{298} C_{P,[H_2O]}\mathrm{d}T \tag{9}$$

where, H_{298}^E is the excess enthalpy of solution, in kJ/kmol and calculated by Eq. (10), $C_{P,[\mathrm{EMIM}][\mathrm{DMP}]}$ and C_{P,H_2O} are the specific heat capacities of [EMIM][DMP] and H_2O, in kJ/kmol K, respectively.

$$H_{298}^E/x_1x_2 = \sum_{1}^{4} A_i(1 - 2x_2)^{i-1} \tag{10}$$

Table 1
Parameters in Eq. (6).

a_1	b_1	c_1	a_2	b_2	c_2
-4.0495×10^5	2.1839×10^3	−2.810	-7.5891×10^3	10.215	−0.0356