ANALYSIS AND EVALUATION OF 2,2,2-TRIFLUOROETHANOL/IONIC LIQUIDS AS NEW WORKING PAIRS FOR HEAT TRANSFORMERS

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ABSTRACT

In this work, the performance of new proposed 2,2,2-trifluoroethanol/ionic liquid mixtures for absorption heat transformer applications is studied. The 1-ethyl-3-methylimidazolium tetrafluoroborate ([emim][BF_4]) and 1-butyl-3-methylimidazolium tetrafluoroborate ([bmim][BF_4] have been selected as new absorbent for absorption heat transformer systems with 2,2,2-trifluoroethanol (TFE) as refrigerant. The selection of these ionic liquids is based on a computational-experimental study to select suitable ionic liquids with optimized properties for TFE absorption applications.

The performance of these two TFE/ionic liquid mixtures is analysed and evaluated. The solution concentration (i.e. refrigerant in ionic liquids) in absorber and generator are predicted based on experimental vapour-liquid equilibrium data. The experimental data of both vapor liquid equilibrium and excess enthalpy of the mixture are correlated using Non-Random Two Liquid (NRTL) method available in Aspen Plus software.

The performance indicators, such as coefficient of performance and solution mass flow rate are studied and analyzed. The simulation results show that the new proposed working fluid of TFE/[bmim][BF_4] and TFE-[emim][BF_4] are suitable for absorption heat transformer applications. The COP of new proposed TFE-ionic liquid working pairs is slightly lower than conventional water-lithium bromide working fluid. However solution mass flow ratio of the new proposed working fluids gives better values as compared to conventional water-lithium bromide working pair. The TFE/[bmim][BF_4] working pair gives better performances as compare to the TFE/[emim][BF_4] working pair.

Keywords: Heat transformer, ionic liquid, 2,2,2-trifluoroethanol, performance.

1. Introduction

In absorption heat transformer systems, the most used working fluid is water/lithium bromide (H_2O/LiBr) as it has many advantages such as non toxic, no rectification process needed, etc. However, the water/lithium bromide has disadvantages such as crystallization problem and necessity of corrosion inhibitors [1]. Several variations of the working fluid pairs have been studied to gain wider application area than conventional water/LiBr working fluids. One of the working fluids have been investigated for absorption refrigeration cycle is 2,2,2-trifluoroethanol/ionic liquid. The use of ionic liquid (IL) as an alternative absorbent in the absorption heat transformer systems may give some advantages such as eliminate the necessity of corrosion inhibitors due to its non-corrosive characteristic and avoid crystallization because they are soluble in all the composition range

In this work, the performance new proposed 2,2,2-trifluoroethanol/ionic liquid mixtures for absorption heat transformer applications is studied. The 1-ethyl-3-methylimidazolium tetrafluoroborate ([emim][BF_4]) and 1-butyl-3-methylimidazolium tetrafluoroborate ([bmim][BF_4] have been selected as new absorbents for absorption heat transformer systems with 2,2,2-trifluoroethanol (TFE) as refrigerant. The selection of these ionic liquids is based on a computational-experimental study to select suitable ionic liquids with optimized properties for TFE absorption applications [2].

The simulation is carried out in two main steps. The first step is to calculate and to regress the thermodynamic properties of TFE-ionic liquid mixture, and the second is to build and to perform the simulation of the absorption heat transformer in ASPEN Plus.

The performance of the absorption system is analysed using parameters useful for evaluating working fluid pairs in absorption systems. These performance indicating parameters studied in this work are coefficient of performance and solution circulation ratio.

The coefficient of performance (*COP*) of the absorption heat transformer is defined as the ratio of available useful heat output of the system (Q_{abs}) to the driving external heat inputs of the system (evaporator and generator heat inputs: Q_{evap} and Q_{gen}, respectively). Mathematically, the COP can be expressed as follows:

$$COP = \frac{Q_{abs}}{Q_{evap} + Q_{gen}} \tag{1}$$

Furthermore, solution circulation ratio (*f*) is defined as the ratio of the mass flow rate of the basic solution per unit mass of vapour generated in the generator is also used to evaluate the cycle performance. Mathematically, the solution circulation ratio can be described as follows:

$$f = \frac{\dot{m}_s}{\dot{m}_r} \tag{2}$$

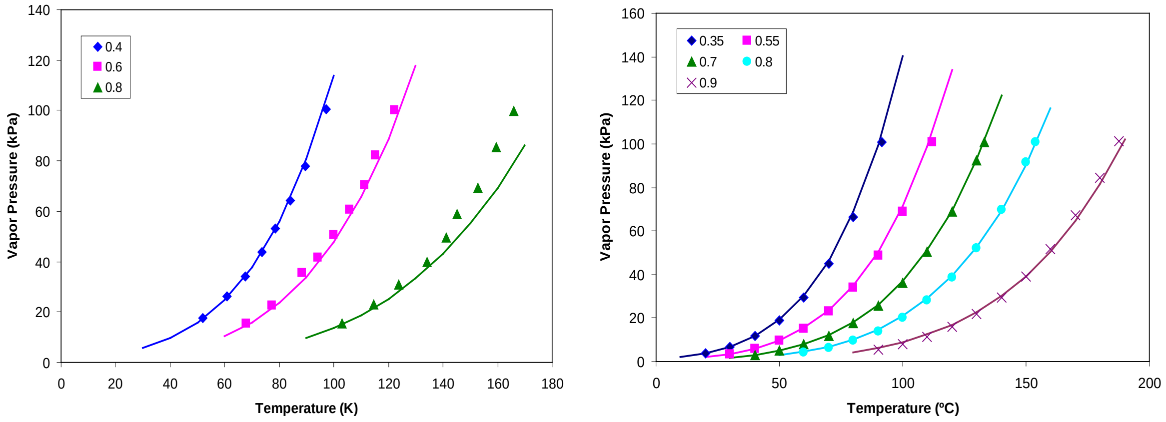
where $\dot{m}_s$ is strong solution mass flow rate and $\dot{m}_r$ is refrigerant mass flow rate.

2. Thermodynamic Modelling

The most important step in the simulation process is to model the thermodynamic properties of the working fluid mixture. To carry out the thermodynamic properties of the working fluids model, the Non-Random Two Liquids (NRTL) property method is chosen. The NRTL property method is available in ASPEN Plus software.

The experimental data of vapour-liquid equilibrium of refrigerant and ionic liquid mixtures are extracted from literature [3-4]. In addition, to obtain better result in thermodynamic calculations, particularly in specific enthalpy of the mixtures, it is necessary to include the experimental data of excess enthalpy of the TFE and ionic liquid mixture [5].

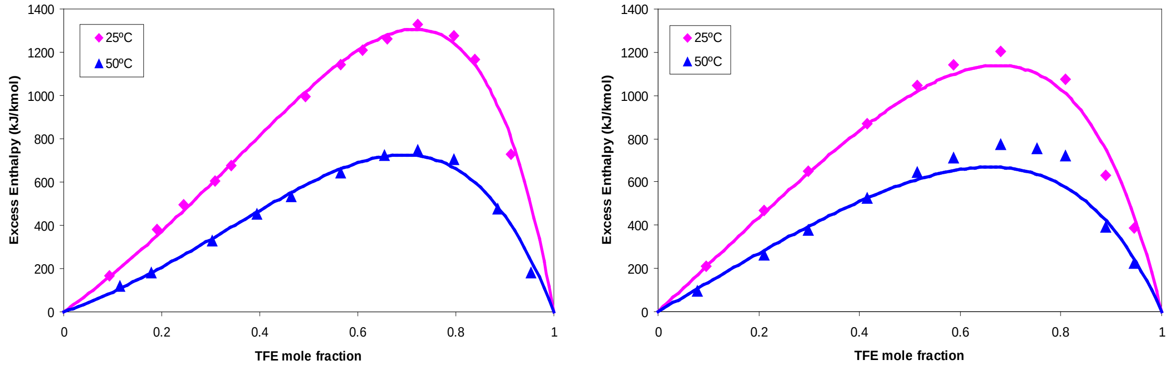
The comparison of the regressed and measured vapour-liquid equilibrium data for the investigated working mixture is shown on figure 1. From these figures it can be seen that the regression VLE lines are well agreed as compared with the measured VLE data. The higher discrepancy appears for TFE/[bmim][BF_4] mixture at IL mass fraction of 0.8 and at temperature above 150ºC. This discrepancy can be ignored as in this work the maximum operation temperature is 130ºC.



(a) TFE/[bmim][BF_4] (b) TFE/[emim][BF_4]

Figure 1: Comparison of the calculated and measured vapour pressures of TFE/ionic liquid mixtures. Symbols represent experimental data (ionic liquid mass fraction) and lines represent regressed results.

In addition, figure 2 shows the comparison of the regressed and measured excess enthalpy data for the investigated working mixture at temperature of 25ºC and 50ºC. From these figures it also can be seen that the regression excess enthalpy lines are in good agreement as compared with the measured excess enthalpy data from literatures.



(a) TFE/[bmim][BF_4] (b) TFE/[emim][BF_4]

Figure 2: Comparison of the calculated and measured enthalpy of mixing of TFE/ionic liquid mixtures at 25ºC and 50ºC. Symbols represent experimental data and lines represent regressed results.

3. Absorption Heat Transformers Simulation

The absorption heat transformer cycle is modeled in ASPEN Plus based on basic single effect absorption heat transformer cycle configuration. The flowsheet diagram of the TFE-ionic liquid absorption heat transformer cycle is shown in figure 3.

Because ASPEN Plus uses a sequential solver, it is necessary to model a “break” in closed cycles to give inputs to the model [6]. In the present work the outlet of the absorber is not connected to the, therefore the stream at absorber outlet and stream at hot stream inlet of the heat exchanger are defined as stream 1A and stream 1, respectively. The model is considered to be well converged if these two fluid streams give the same results. The break in stream 1 allows for inputs to be given for the model. These inputs were the absorber temperature, a vapour fraction of zero, the solution mass flow rate, and the mass fraction of refrigerant and ionic liquid.

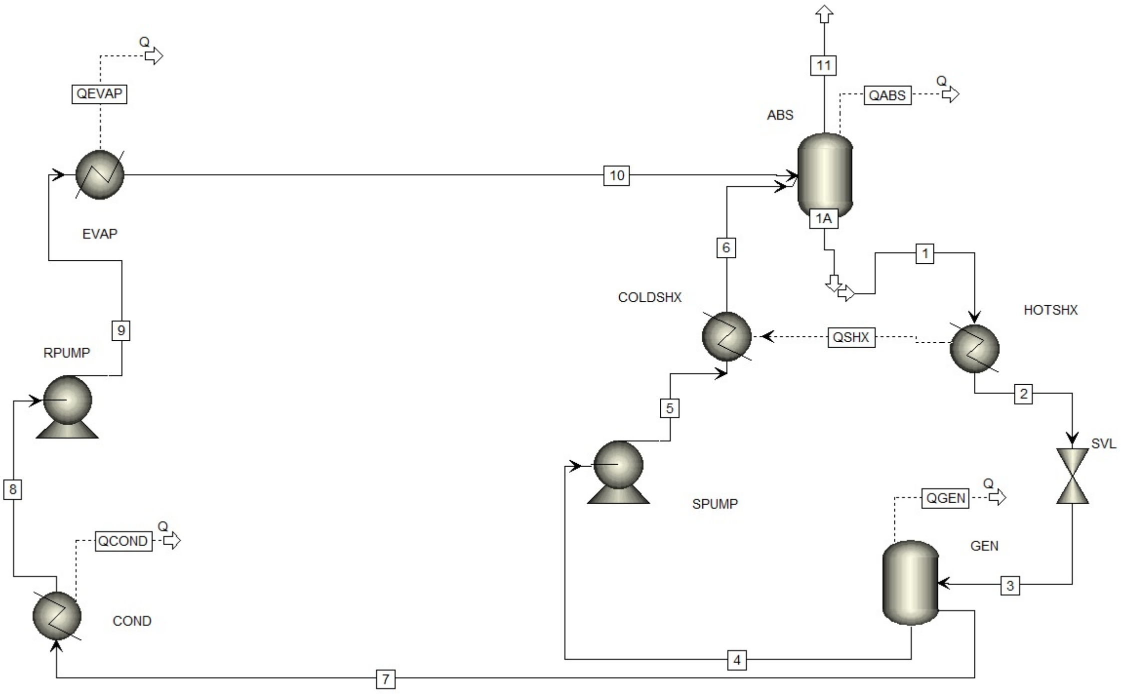


Figure 3: Flowsheet diagram of absorption heat transformer cycle in ASPEN Plus

The cycle components and the assumptions given in each component are specified below:

- Absorber (ABS): for simplification model, the absorber consist of ASPEN model ‘flash’ for vapor-liquid phase. The vapor refigerant is absorbed by producing useful heat at high temperature. In this model, the stream 11 must gives zero mass flow. The solution exit the absorber is assumed at saturated liquid condition.
- Generator (GEN): consist of ASPEN model ‘flash’ for vapor-liquid phase. The vapor refigerant is generated by supplying heat at medium temperature.
- Condenser (COND): consist of ASPEN model ‘heater’. The refrigerant at the condenser outlet is at saturated-liquid condition. Hence the lower working pressure is equal to the vapor pressure of the refrigerant at condenser temperature
- Evaporator (EVAP): consist of ASPEN model ‘heater’. The refrigerant at the condenser outlet is at saturated-vapor condition. Therefore the higher working pressure of the heat transformer is equal to the vapor pressure of the refrigerant at evaporator temperature
- Solution heat exchanger: consist of two ASPEN models ‘heater’ (COLDSHX and HOTSHX). The heat is transferred from stream 1 (hot side inlet) to stream 5 (cold side inlet), resulting in stream 2 (hot side outlet) and stream 6 (cold side outlet). The heat exchanger effectiveness is set to 0.8. The correlation between heat exchanger effectiveness and each stream temperature is implemented in ASPEN Plus using calculator block.
- Solution pump (SPUMP) and refrigerant pump (RPUMP): consist of ASPEN model ‘pump’. The discharge pressure of the solution pump is equal to the higher working pressure level.
- Solution valve(SVL): consist of ASPEN model ‘valve’. The discharge pressure of the valves is equal to the lower working pressure.

4. Results and Discussions

4.1. Validation

The simulation results of the absorption heat transformer are compared with the simulation data published in open literature [7] to validate the thermodynamic model and the simulation built in ASPEN Plus. The comparison is done with water-lithium bromide working fluid at similar operation condition. In this validation, instead of using heat exchanger effectiveness of 0.8, the hot-stream outlet temperature (T_6) is set at 120ºC. The comparison result is shown in table 1.

Table 1: Comparison between present work and literature [7]

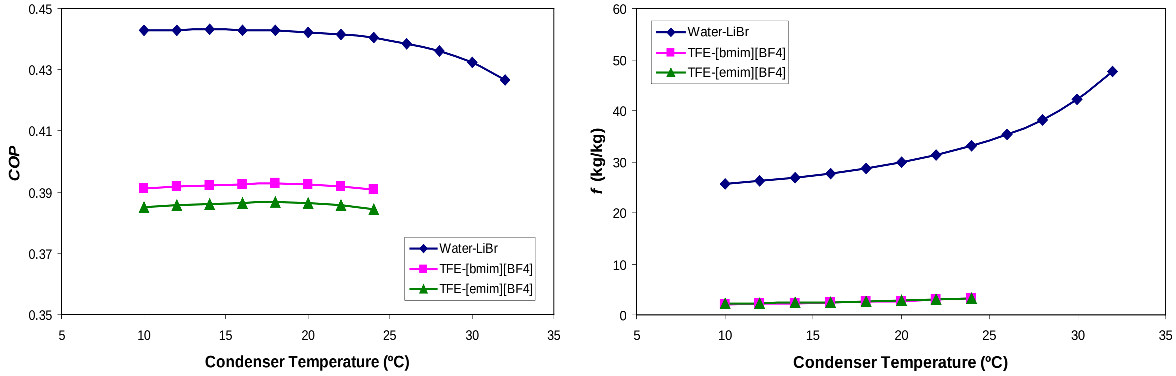
Variable	Unit	Present work	Ref. [7]
T_{abs}	ºC	130	130
T_{cond}	ºC	25	25
T_{gen}	ºC	80	80
T_{evap}	ºC	80	80
T_6	ºC	120	120
f		11.93	9.51
COP		0.475	0.48
Weak Solution Concentration		0.5994	0.5926
Strong Solution Concentration		0.6496	0.6549

From table 1 it can be seen that the results of present work are well agree as compared to the simulation result from literature [7]. The slightly higher discrepancy is observed on solution circulation ratio. However, if the deviations at weak and strong solution concentration are considered, the present work is in good agreement with the literature [7].

4.2. Effect of Condenser Temperature

This paper presents the performances of new proposed 2,2,2-trifluoroethanol/ionic liquid mixtures for absorption applications. Two ionic liquids, [bmim][BF_4] and [emim][BF_4], are studied in this work. For analytical purpose, the results of the simulation are compared with conventional working fluid of water-lithium bromide.

Figure 4 shows the effect of condenser temperature to the performance of absorption heat transformer. In this simulation, the absorber temperature (T_{abs}) is set to 130ºC, and the generator temperature and evaporator temperature are set to 80ºC.



(a) (b)

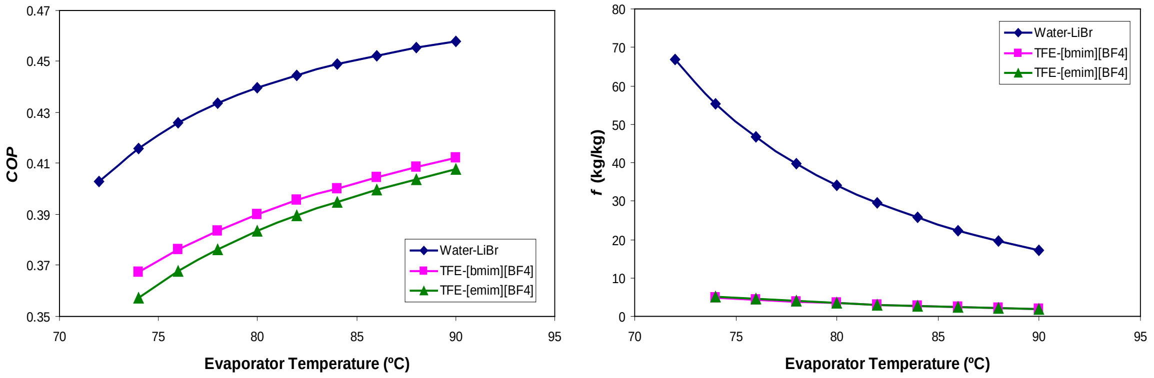
Figure 4: Effect of condenser temperature to (a) COP and (b) circulation ratio

The results show that the COP of new proposed TFE/ionic liquid working pairs is slightly lower than conventional Water/Lithium Bromide working fluid. The COP of Water/Lithium Bromide is about 0.43–0.45 at condenser temperature between 10ºC and 32ºC. The COP of TFE/[bmim][BF_4] working pair is slightly higher as compared to the COP of TFE/[emim][BF_4] working pair. At condenser temperature between 10ºC and 25ºC, the COP of TFE/[bmim][BF_4] working pair lays around 0.39 and the COP of TFE/[emim][BF_4] working pair lays around 0.385.

For the solution mass flow ratio, the result show that the new proposed working fluids gives better values as compared to conventional water/lithium bromide working pair. At condenser temperature between 10ºC and 25ºC, the solution mass flow ratio of TFE/[bmim][BF_4] and TFE/[emim][BF_4] working pairs lay around 2–3.6, and at condenser temperature between 10ºC and 34ºC, the solution mass flow ratio of water/lithium bromide working pair lays around 25.6–47.3.

4.3. Effect of Evaporator Temperature

Figure 4 shows the effect of condenser temperature to the performance of absorption heat transformer. Similarly to the study above, in this simulation, the absorber temperature (T_{abs}) is set to 130ºC, and the generator temperature is set to 80ºC, and the condenser temperature is set to 25ºC.



(a) (b)

Figure 5: Effect of evaporator temperature to (a) COP and (b) circulation ratio

Similarly with the study of the effect of the condenser temperature, The results show that the COP of conventional water-lithium bromide working fluid is higher than those new proposed TFE/ionic liquid working pairs. The COP of water-lithium bromide increases from 0.40 to 0.46 when the evaporator temperature is increased from 72ºC and 90ºC. The COP of TFE/[bmim][BF_4] working pair is slightly higher as compared to the COP of TFE/[emim][BF_4] working pair. When the evaporator temperature is increased from 74ºC to 90ºC, the COP of TFE/[bmim][BF_4] working pair increases from 0.36 to 0.41 and the COP of TFE/[emim][BF_4] working pair increases from 0.35 to 0.40.

For the solution mass flow ratio, the result show that the new proposed working fluids gives better values as compared to conventional water-lithium bromide working pair. At evaporator temperature between 74ºC and 90ºC, the solution mass flow ratio of TFE/[bmim][BF_4] and TFE/[emim][BF_4] working pairs lay around 1.9–5.4, and at evaporator temperature between 72ºC and 90ºC, the solution mass flow ratio of water-lithium bromide working pair lays around 17.2–66.7.

5. Conclusions

The performances of new proposed 2,2,2-trifluoroethanol/ionic liquid mixtures for absorption applications. Two ionic liquids, [bmim][BF_4] and [emim][BF_4], are studied in this work. The performance indicators, such as coefficient of performance and solution mass flow rate are studied and analyzed. The simulation results show that the new proposed working fluid of TFE/[bmim][BF_4] and TFE/[emim][BF_4] are suitable for absorption heat transformer applications.

The COP of new proposed TFE/ionic liquid working pairs is slightly lower than conventional water-lithium bromide working fluid. However solution mass flow ratio of the new proposed working fluids gives better values as compared to conventional water/lithium bromide working pair. The TFE/[bmim}[BF_4] working pair gives better performances as compare to the TFE/[emim][BF_4] working pair.

6. Acknowledgment

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