CHAPTER V
CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

A methodology for the screening of ILs as entrainers and for the design of ILs-based separation processes in various homogeneous binary aqueous azeotropic systems was highlighted through two case studies: ethanol + water and isopropanol + water. The use of environmental friendly entrainers clearly showed a higher energy savings and provided better separation performance than the conventional entrainers (EG). Additionally, an extended Hildebrand solubility parameter group contribution for ILs has been developed to screen the miscibility of the ILs with the target solute component which was considered as main criteria. The best candidates for aqueous systems were selected for final evaluation as follows: [C_1MIM][DMP] (δ_{IL}= 27.08 $MPa^{1/2}$), [C_2MIM][N(CN)$_2$] (δ_{IL}= 25.84 $MPa^{1/2}$), [C2MIM][Ac] (δ_{IL}= 25.16 $MPa^{1/2}$), and [C_2MIM][EtSO$_4$] (δ_{IL}= 24.45 $MPa^{1/2}$). According to the ranking of the solubility parameter, the overall energy consumption of the whole process for ethanol + water separation can be ranked as [C_1MIM][DMP] (3.16 MW) < [C_2MIM][N(CN)$_2$] (3.3 MW) < [C_2MIM][EtSO$_4$] (3.44 MW). This confirms that the solubility parameter is one important criterion for screening ILs as entrainer. The [C_1MIM][DMP] was chosen as the final candidate, as it performed the best ILs for the separation of ethanol + water azeotrope based on minimum energy requirement, giving an energy savings of 21.55% compared to the EG. In addition, the use of [C_2MIM][Ac] as entrainer was unfeasible due to the extremely low operating pressure and its relatively low degradation temperature.

Considering the design flexibility for the isopropanol + water azeotropic separation process with the same ILs entrainer, product purity, and designed parameters, [C_1MIM][DMP] was excluded since the extraction with [C_1MIM][DMP] could not give 99.8%mol purity of the alcohol with a reasonable number of theoretical stages. The [C_2MIM][N(CN)$_2$] was selected to study the design flexibility of the azeotropic separation process with the same IL entrainer and product purity. It is aimed to study the effect of the size of the alcohol to other designed parameters in the extractive distillation and separation processes. From the final analysis, an increase of the size of the alcohol (ethanol [CH_3CH_2OH] to isopropanol [$CH_3CH_2CH_2OH$]) resulted in an increase of the reflux ratio, the ILs flowrate, and the flash heat duty; however, it gave a reduction of the reboiler heat requirements and the operating temperature of the flash. As a result, the overall energy consumption of the whole process showed a decrease of 11.3 % as compared to that of the ethanol + water system because the isopropanol + water had a weaker interaction than the ethanol + water leading to the easier to extract water from isopropanol than extracting of water from ethanol.

Though the cost of ionic liquids may appear prohibitive, costs can be reduced by recycling the ionic liquid to reduce the material and energy inputs. As more data becomes available, ionic liquid property models will become more accurate and the design of ionic liquids and IL-based processes will become more reliable and useful.

5.2 Recommendations

So far, the physical, corrosive and toxicological properties of the ILs, predictive thermodynamic (binary interaction parameters) as well as phase equilibrium properties of azeotropic mixtures containing ILs have been insufficient. Therefore, more research experiment is needed to be done in each of these fields to determine the practical suitability of the ILs in industrial scale applications.

The pilot plant experiments for the separation of alcohol + water in extractive distillation processes are recommended to test the actual behaviour and performance of the best ILs.

For future work, the proposed methodology should be tested and applied for other non-aqueous systems, for instance, aromatics/aliphatic systems, or alcoholic/aliphatic systems. It is recommended to perform heat integration, estimate the capital expenditures (CAPEX) and operating expenditures (OPEX), and perform a detailed economic evaluation in order to fully evaluate the application of ILs in extractive distillation processes.