CHAPTER V
CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

A systematic methodology of selection and design of the best IL-based separation process has been accomplished through the demonstration of four homogeneous binary mixtures as case studies; one aqueous system i.e. ethanol + water mixture and three non-aqueous systems i.e. ethanol + hexane, benzene + hexane, and toluene + methylcyclohexane (MCH) mixtures. In fact, there are five case studies in the beginning but a special case (i.e. ethylbenzene + p-xylene mixture) has not been further discussed at the end since the screening criteria of IL pre-selection step has not effectively supported in the case of isomer mixture. Hence, only four best ILs were expressed; i.e. [MMIM][DMP] from ethanol + water mixture in an aqueous system; furthermore, in three non-aqueous systems, [EMIM][BTI] from ethanol + hexane mixture, [EMIM][EtSO4] from benzene + hexane mixture, and [HMIM][TCB] from toluene + MCH mixture. In addition, all results of each step were in agreement, for example, the best ILs presented the most perfect separation capability to break azeotrope or increase the relative volatility of mixture, the lowest energy requirement and solvent usage, and also the most economical process as compared to other ILs and conventional solvents.

In a case of other two ILs (i.e. [EMIM][DCA] and [EMIM][EtSO4]) in water + ethanol mixture, they could be the alternative choices using as entrainers since both ILs showed the lower energy requirement and solvent usage in the simulation process but have not further discussed in economic comparison as same as another one IL (i.e. [BMIM][BTI]) in ethanol + hexane mixture. Nevertheless, the best ILs in this contribution could be confirmed with the available IL data from literature database at the moment. IL data should be updated continuously to obtain the best ILs to cover all recent ILs that have been recently studied.

This proposed methodology was divided into three main stages; selection stage including 3 major steps (i.e. mixture selection, separation process selection and IL pre-selection), verification stage including 2 major steps (i.e. verification of

mixture and verification of IL), and comparison stage including 3 major steps (i.e. VLE comparison, simulation comparison and economic comparison). The Hildebrand solubility Group Contribution parameter along with the capacity and selectivity of ILs are the key parameters for screening criteria in this proposed methodology. Thus, this part should be comprehensive and carefully follow the instruction step-by-step. A simulation process of ILs and economic evaluation could be the preliminary process for further applications and a supported decision-making for investment. The programs in this work such as ProPred, ICAS, Pro II, and Econsoftware were nominated for running. In summary, the methodology is guaranteed for viability in generic systems and the most suitable for selection and design of the best IL-based separation process.

5.2 Recommendations

Due to the previous scope of work and time limitation, ethanol + water mixture was only a representative for an aqueous system and the last case study. Thus, there might not be enough supported information to set the initial default range of target window in aqueous system due to the effects of hydrogen-bond interaction and polarity of ILs such as a hydrophilic property. Furthermore, the experimental data of extensive and intensive properties of ILs such as physical property, corrosion, toxicity, NRTL binary parameters as well as behavior phase equilibrium of azeotropic mixture containing ILs have been insufficient that make unfortunately a lot of ILs missed to further demonstrate in verification of IL step. In addition, Hildebrand solubility Group Contribution parameter along with the capacity and selectivity of ILs as key parameter in the screening criteria of IL pre-selection step should be updated continuously for highest efficiency of the methodology. In part of simulation process, IL process has been preliminary process using a simple flash evaporator in the recovery technology for a comparison in each mixture. The last step of economic comparison would be more efficient and feasible for being a supported decision-making in an investment if the industrial IL prices will be available in the future. If it is possible, the pilot plant experiments of all case studies are recommended to test after getting the best ILs from this proposed methodology.