CHAPTER III
METHODOLOGY

3.1 Equipment and Software

Equipment:

- Desktop computer (Intel® Core™ 2 Duo CPU T5900 2.20 GHz, 2 GB of RAM, Windows 7 and Microsoft Office 2010).

Software:

1. ICAS version 16
2. Pro II version 9.1

3.2 Methodology

3.2.1 Literature Survey Study

a. Study the "Separation of azeotropic mixtures with ionic liquids"
   - List out the important steps of design separation processes with ionic liquids.
   - List out the properties of ionic liquids and what are key properties that help identify which ionic liquids can be used for azeotropic separation.
   - Collect the predictive property models of ionic liquids
   - Collect the experimental data related to necessary properties of ionic liquids.
   - Study the vapor–liquid equilibrium (VLE) for azeotropic systems with ionic liquids.

b. Study the method proposed by (Roughton *et al.*, 2012), which is shown in Figure 2.10.
   - Study the Hildebrand solubility parameter group contribution (GC) model—how to obtain relevant parameters to calculate the solubility parameter.

- Study UNIFAC-IL and/or NRTL to predict the VLE of ternary systems containing ionic liquids.
- List all data and variables needed for the design of azeotropic separation with ionic liquid
- Analyst the needed data to calculate for each step

c. List out the homogeneous aqueous and the non-aqueous binary azeotropes and classify binary azeotropes based on boiling point temperature and functional group.

3.2.2 Designing and Screening Ionic Liquid Candidates

a. Test the Hildebrand solubility parameter group contribution model and UNIFAC-IL to design ionic liquid entrainers in azeotropic separation.
b. Calculate the target property to screen the designed candidates
c. Examine Roughton's method whether it can be applied to both aqueous and non-aqueous binary azeotropic mixtures and improve the method if needed.

3.2.3 Conceptual Process Design and Simulate Process

a. Study IL-based separation processes that have been used successfully in the design and simulation of ionic liquid-based separation processes (Seiler et al., 2004, Roughton et al., 2012).
b. Select case studies based on Section 3.2.2 .
c. Design extractive distillation column and ionic liquid recovery, and then simulate the azeotropic separation process based on the minimum overall heat duty for the entire process.

3.2.4 Validation

Apply the improved method to case studies of azeotropic separation—ethanol/water, isopropanol/water azeotrope.