CHAPTER 5

CONCLUSIONS

Isobaric VLE data have been measured for the binary system tert-butanol (1) + water (2) and for the ternary systems tert-butanol (1) + water (2) + TRIS (3) with different concentrations of TRIS \( w_3 = 0.05, 0.10, 0.20 \), 2-propanol (1) + water (2) + EPPS (3) and 1-propanol (1) + water (2) + EPPS (3) with different concentrations of EPPS \( w_3 = 0.05, 0.10, 0.20, 0.30 \) at 101.32 kPa by using a modified recirculating type of Othmer equilibrium still. All the experimental data were passed the thermodynamic consistency test. The binary system tert-butanol (1) + water (2) was measured and compared with the literature values in order to validate the experimental method. The ternary systems were studied in order to investigate the effect of biological buffer TRIS and EPPS on the VLE behavior.

The equilibrium temperature increases as TRIS was added in the aqueous tert-butanol mixtures. The vapor phase composition of tert-butanol significantly moved toward the organic end. The shifting effect was enhanced by increasing TRIS concentration. In the presence of EPPS in aqueous propanol mixtures, the shifting effect was also found significantly from the aqueous 2-propanol system, while only minor shifting effect was found from aqueous 1-propanol system.

The NRTL model was used to correlate the experimental data of binary system and the new ternary VLE data. Satisfactory results were obtained and the optimal values of the binary interaction parameters for tert-butanol (1) + water (2), water (1) + TRIS (3), tert-butanol (1) + TRIS (3), water (1) + EPPS (2), 2-propanol (1) + EPPS (3), and 1-propanol (1) + EPPS (3) were determined through the data correlations.

The validity of the binary interaction parameters determined from the LLE data correlation using for predicting the VLE phase boundaries have been tested for the ternary systems 2-propanol (1) + water (2) + EPPS (3) and 1-propanol (1) + water (2) + EPPS (3). The calculation results indicate that the binary interaction
parameters obtained from LLE data correlation are unable to predict accurately the VLE properties of the aqueous 1-propanol and the aqueous 2-propanol systems in the presence of biological buffer EPPS. In the process simulation, we need to use the parameters determined from LLE data for the decanter and those from VLE data for the buffer-recovery distillation column.