CHAPTER 10

CONCLUSIONS

1. This study set out to characterize and identify suitable solvents for separating 1-octene and 2-hexanone. Virtually all studies on solvents considered non polar mixtures and found that solvents with high polar cohesive energies could separate components with differences in molar volume. In the system studied here there are also marked differences in polarity and other bonding abilities between the components to be separated. For this "new" system it was found that effective solvents are those having strong abilities to interact with solutes and so discriminate between them. These abilities are reflected in properties such as high dielectric constants, high polarities, high polar and hydrogen part solubility parameters and low molar volumes. Four specific identified solvents were also shown to be of practical value.

2. The experimental results (of which there are more than in any of the studies referred to) and conclusions are in agreement with theoretical considerations and postulated models. The fundamental concept is that a strongly interacting solvent is able to interact with 2-hexanone to a greater extend than it does with 1-octene, thus decreasing the relative volatility of the former. The practical value of many of these models is confirmed.

3. This study clearly showed that UNIFAC and infinite dilution selectivities are not the best indicators of actual solvent performance under typical plant solvent concentrations. Specific solvent properties are almost twice more accurate. The literature contains many objections to the use of infinite dilution coefficients because these are determined under conditions far from actual operating conditions. The results from this study indicate that this objection has factual merit.

4. The ASEEK program described earlier is a useful and effective tool for identifying potential solvents. In its present form it selects according to infinite dilution selectivities and UNIFAC predictions. While the solvents identified may not perform in the precise order as they appear in the lists generated, the agreement is good. The program can be made even more effective by allowing the user to indicate selection based on certain solvent properties such as those listed under point 1. Implementing this will be easy since all these parameters are calculated by ASEEK in any case as intermediate quantities during the calculation of the selectivities. The program can also be extended to cater better for two liquid phases and include some measure of artificial intelligence.

5. While the benefits of experimental solvent evaluation can never be discounted, it is believed that a thorough consideration of the various factors which govern solvent selectivity will almost invariably result in an accurate characterisation of effective solvents before any experimental work is done. Available models and correlations can be used with great success.