CHAPTER 5

RESULTS AND DISCUSSIONS

To gain familiarity with the diffusion model concentration profiles were generated for several values of the Peclet number for both phases and several values of the number of transfer units. The physical system simulated was the transfer of iodine from an aqueous solution to a carbon tetrachloride phase with a distribution coefficient for this particular system being very high, namely 89.9. As values of Peclet numbers (P_x and P_y) were increased, indicating a flow pattern approaching piston flow, efficiencies of extraction showed a high rate of increase for P_x and P_y lesser than 10 and a slow rate of increase after a value of 10 (Figures 3 - 28, 3 - 29). The value 10 probably has no specific significance because for another system this value would probably change. However the shape of the efficiency curve as a function of Peclet numbers would probably not change. In other words there exists a value of Peclet numbers beyond which increase in efficiency would be minimal.

During utilization of the diffusion model by the design Engineer for scaling up a given extraction process from laboratory scale to industrial scale, the three parameters of the model must be either known or measured on the laboratory unit before being used to design the industrial equipment. The Peclet numbers for both phases are best measured from experiments using tracer and optimization techniques and

use may also be made of several references published in the past thirty years. Determination of the Peclet numbers should be no major problem. However the determination of the number of transfer units is a little bit more complicated to obtain experimentally and little relevent data may be found. One method is to take concentration profiles of the solute in both phases so as to obtain a fairly complete concentration profile along the length of contactor resulting in something like 20 or so experimental points, then optimizing for the number of transfer units using numerical or other methods. This method is highly accurate but suffers from a major deficiency, namely that the measurement of 20 or so concentrations is a tedious endeavor to obtain only one parameter. It was therefore proposed to study the determination of this parameter using concentration data at the extremities of the column. In this study concentration profiles were generated through known values of P_x , P_y and R_x. From the concentration profiles, the concentrations at the extremities yielded jump ratios as defined in an earlier chapter. The next task was to find a correlation in the form $R_x = f(P_x, P_y, \text{jump ratio})$ which would enable an accurate identification of R_x. The results as indicated in Chapter 3 were not satisfactory. The problem stems perhaps from the fact that the choice of correlation was inappropriate and additional search for an appropriate correlation may prove successful. The success of such an endeavor would greatly simplify the problem of parameter identification for scale up of extraction column. Another method not attempted in this study would be a numerical optimization based on concentrations at the extremities and not concentrations along

the entire profile. This second method however would still be more complex and time consuming to use than the first method described in this study.

For many years Engineers building extraction columns had used the H.E.T.P. concept to scale up columns. The concept is as follows, a laboratory scale column of length (L) operating on a particular process yields an equivalent of n theoretical plates. The H.E.T.P. is therefore L/n. Once this value known an industrial column using the same process and requiring m equilibrium stages would require an overall height of m X (H.E.T.P.) of column. Earlier users discovered that this method of design resulted in the construction of columns which were too small for the job. In an attempt at explaining this non-linear phenomena evidenced experimentally the following set of simulations were made. Instead of making experiments on a real column, the diffusion model was used as an idealized model of an extraction columns of lengths from one to ten meters and to calculate the H.E.T.P. for each column based on the extraction of iodine from water to carbon tetrachloride as before. The details of this particular experiment are presented in chapter 3 but the important result obtained was that H.E.T.P. varied with column height as discovered by extraction column builders several years ago at great investment cost. From this initial concept of H.E.T.P. which proved inaccurate for design purposes evolved the piston flow concept as described thoroughly in the textbook by Robert E. Treybal on liquid-liquid extraction. Then from that approach evolved the more accurate Miyauchi's diffusion model based on a combination between piston flow and a dispersion

concept worked out by P.V. Danckwerts and T. Miyauchi separately in the early 1950's.

The diffusion model may be used to represent mass transfer in an extraction column only if several assumptions are satisfied[5]. One of these assumption is dispersed phase homogencity. Several researchers[12,14,15,16] subsequently made discoveries that the dispersed phase is not homogeneous because of a phenomena called forward mixing and described earlier in chapter 4. The design Engineer is thus faced with the dilema of using the diffusion model with no considerations of forward mixing whatsoever or developing a wholy new extraction model. In an attempt at making such a decision this study was aimed at determining the extent of forward mixing influence on the overall extraction efficiency of the extraction column. Based on previous recorded experimental evidence of forward mixing[15] in which drops of carbon tetrachloride moved along a pulsed perforated plate column at valocities which varied along the height of the column, simulations using a modified diffusion model were made. In each of four sets of comparisons representing four experimental conditions a comparison of concentration profiles is made (Figures 4 - 5 to 4 - 8). The dashed line represents the simulation in which forward mixing is taken into account through variation in the velocity of the dispersed phase as a function of height (as u changes with height z so does P_x and R_x). The solid line represents the simulation with an average velocity for the dispersed phase also obtained experimentally in the same earlier reference, and for exact same experimental conditions so that both simulations may be compared in a meaningful

manner. The results indicate very clearly that the influence of forward mixing upon the overall extraction efficiency of an extraction column is minimal for this set of experimental conditions. It is to be noted that extraction of iodine from water to carbon tetrachloride was the system simulated in this study.

The major conclusion from this last study would be that it appears that forward mixing may not be a major factor influencing efficiencies of liquid-liquid extraction columns. This result directly enhances the value of the diffusion model as an Engineer's tool to design industrial columns. However a cautions note must be sounded that additional checks of this result should be attempted on other systems whereever possible as all the tools for such an attempt have been developped and presented in this study.

This study looked at forward mixing on the point of view of velocity of drops profile as a function of length. Another effect as yet unaccounted for is the variation in drop sizes from droplet distributor to the middle of the extractor where the drops finally become an average size, and the variation in surface area for mass transfer accompanying this variation in drop size. A detailed study into this influence would be indeed interesting but indeed very difficult to implement experimentally. Some experimental data does exist on this aspect and could be processed by a future researcher.