CHAPTER II

DEVELOPMENT OF THE MATHEMATICAL ANALYSIS

The mathematical analysis to be developed involves the measurement of axial dispersion coefficients in the continuous phase of an extraction column using tracer analysis.

The schematic representation of the system is shown in figure 2.1

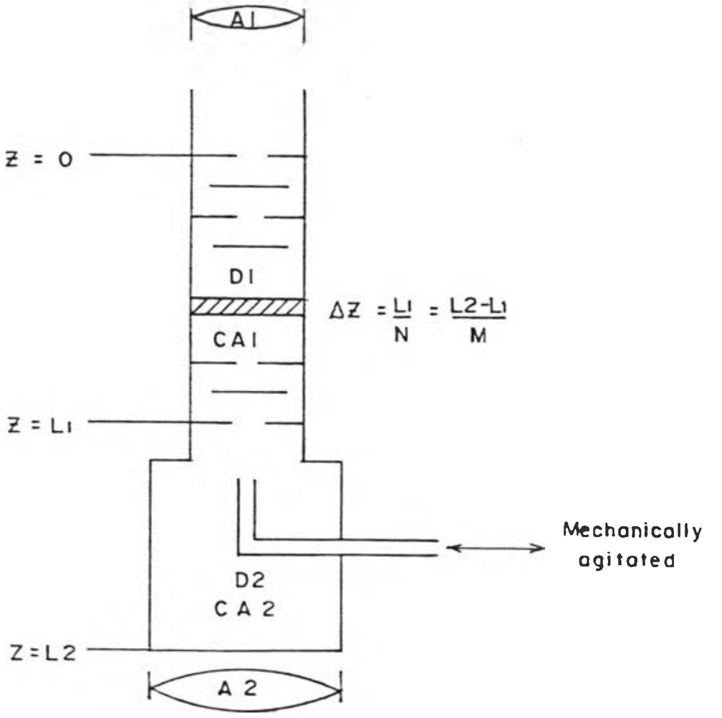

Fig. 2.1 Schematic representation of the extraction column system. The column rests on top of a support base of larger diameter and the column is mechanically agitated. The column agitation is represented by a dispersion coefficient D1 in cm2/s, and the support by a dispersion coefficient D2. The continuous phase does not flow and if there are solid particles or liquid droplets these will be in suspension in the system.

The parameter sought will be D1 whereas parameter D2 representing dispersion in the support section will be estimated as explained later. The column may contain perforated plates, or disks and rings and may be pulsed, or it may contain rotating disks, and parameter D1 will depend on inside geometry and intensity of mechanical agitation. Parameter D1 will represent agitation in the continuous phase present with or without the presence of a dispersed phase such as solid particles or liquid droplets. The methodology in principle enables D1 for an extraction column to be measured without having to build the entire column. And in addition it is unnecessary to have the continuous phase flow through the system, and if solid particles or liquid droplets are present they must have densities similar to the continuous phase and must be suspended. Parameter D2 represents the agitation in the support section.

The measurement of parameter D1 is done by pouring a quantity of tracer in the liquid at the top of the column. Then due to mechanical agitation the tracer diffuses downward towards the support zone and at the bottom of the column a concentration measurement of the tracer is made as a function of time which is a curve similar to the response to a step function in a linear system.

The actual measurement of parameter D1 is done by assuming an axial dispersion model under a non-flow situation for the continuous phase with the appropriate boundary conditions and use numerical optimization to obtain the desired parameter D1 based on a known value of D2.

The derivation of the model equations and the optimization criteria used is described as follows.

2.1 Derivation of the Equations

The equation governing the behavior of the continuous phase may be written as

$$D1 \frac{\partial Ca1}{\partial z} = \frac{\partial Ca1}{\partial t} \tag{2.1}$$

$$D2 \frac{\partial Ca2}{\partial z} = \frac{\partial Ca2}{\partial t} \tag{2.2}$$

initial conditions may be expressed as

$$Ca1(z>0,t=0) = 0 \tag{2.3}$$

$$Ca2(z>0,t=0) = 0 \tag{2.4}$$

boundary conditions may be expressed as

at Z = 0

$$Cin\delta(t)w = D1 \frac{\partial Ca1}{\partial z} A1 \tag{2.5}$$

and at t=0 $\quad Ca1(z=0,t=0) = \text{constant} \qquad (2.6)$

at t>0 $\quad \dfrac{\partial Ca1(z=0,t)}{\partial z} = 0 \qquad (2.7)$

at z=L1 $\quad A1D1 \dfrac{\partial Ca1}{\partial z} = A2D2 \dfrac{\partial Ca2}{\partial z} \qquad (2.8)$

at t>0 $\quad \dfrac{\partial Ca1(z=L1,t)}{\partial z} = 0 \qquad (2.9)$

2.2 Application of Numerical Analysis to the Equations

Equations 2.1 and 2.2 become

$$D1\left[\frac{Ca1(i+1,j)-2Ca1(i,j)+Ca1(i-1,j)}{\Delta z^2}\right] = \frac{Ca1(i,j+1)-Ca1(i,j))}{\Delta t} \quad (2.10a)$$

$$D2\left[\frac{Ca2(k+1,j)-2Ca2(k,j)+Ca2(k-1,j)}{\Delta z^2}\right] = \frac{Ca2(k,j+1)-Ca2(k,j)}{\Delta t} \quad (2.11a)$$

then

$$Ca1(i,j+1) = \frac{D1\Delta t}{\Delta z^2}[Ca1(i+1,j)+Ca1(i-1,j)]+Ca1(i,j)(1-\frac{2D1\Delta t}{\Delta z^2}) \quad (2.10b)$$

$$Ca2(k,j+1) = \frac{D2\Delta t}{\Delta z^2}[Ca2(k+1,j)+Ca2(k-1,j)]+Ca2(k,j)(1-\frac{2D2\Delta t}{\Delta z^2}) \quad (2.11b)$$

from equation 8

$$A1D1\left[\frac{Ca1(N,j)-Ca1(N-1,j)}{\Delta z}\right] = A2D2\left[\frac{Ca2(2,j)-Ca2(1,j)}{\Delta z}\right] \quad (2.12)$$

at z=L1 we assume that

$$A1\ Ca1(N,j) = A2\ Ca2(1,j) \quad (2.13)$$

and finally

$$Ca1(N,j) = \frac{[A1D1/A2D2]Ca1(N-1,j) + Ca2(2,j)}{[A1D1/A2D2] + A1/A2} \quad (2.14)$$

at z=L2 we assume that

$$Ca2(M-1,j) = Ca2(M,j) \quad (2.15)$$

at Z = 0 where equation 6 is applicable we may either use the equality

$$CA1(1,j) = CA1(2,j) \quad (2.16a)$$

or we can make use of the Taylor's series and derive that

$$CA1(1,j) = [4CA1(2,j) - CA1(3,j)]/3 \quad j > 1 \qquad (2.16b)$$

a more flexible boundary condition and the one used in this study for that boundary condition.

The vector sought is CA1(N,j) where N represents the bottom of the column section where the measurement probe is located.

The computer program is presented in the ANNEX I

2.3 The Optimization Criteria

The measurement of parameter D1 is made by optimizing the vector CA1(N,j) obtained from theoretical analysis with CA1exp(N,j) obtained from experiments. The criteria Epsilon is defined as

$$\text{Epsilon} = \sum_{i=1}^{n} [Ca1_i(N,j) - Ca1_i exp(N,j)]^2 \qquad (2.17)$$

where $CA1_i(N,j)$, $CA1_i exp(N,j)$ must be normalized prior to calculation of criteria Epsilon. Thus by varying D1 one can obtain an optimal criteria Epsilon which yields the corresponding value of parameter D1 sought.