Mass transfer in droplets with turbulent internal circulation - Mathematical description

Jayantilal Mohanbhai Patel

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MASS TRANSFER IN DROPLETS
WITH TURBULENT INTERNAL CIRCULATION-
MATHEMATICAL DESCRIPTION

BY
JAYANTILAL MOHANBHAI PATEL

A
THESIS
submitted to the faculty of
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ABSTRACT

This investigation was carried out to check the accuracy of the eigenvalues, $\lambda_n$, calculated by Wellek and Skelland, using some method other than the Rayleigh-Ritz technique and also, to determine the coefficients, $B_n$ in series solution, which were not calculated before.

The eigenvalues were obtained by trial and error procedure using the standard Runge-Kutta method. The coefficients $B_n$ were obtained by using eigenvalues. By using this information the fractional extraction was calculated as a function of droplet contact time.

The Wellek-Skelland modification was also solved by finite difference technique to compute fraction extracted as a function of contact time.

The eigenvalues, $\lambda_n$, and coefficients, $B_n$, were also obtained by Hamming's method, and the values agreed with those obtained by the Runge-Kutta method to within 2%. The first eigenvalues obtained by Wellek and Skelland and the values obtained by the author were in agreement to within 5%. The family of curves of $E_m$ versus $bt$, obtained using finite difference method, is in agreement with the physical situation. Therefore, at the higher values of $bt$ (> 0.5) results observed using Runge-Kutta method should be used, and at lower values of $bt$ (< 0.5) the results obtained using finite difference should be considered to be more accurate.
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NOMENCLATURE

\[ A_f, A_r, A_c \] = total interfacial area between two consecutive plates for the respective stages of drop formation, free rise (or fall) and coalescence, (cm²).

\[ A_n \] = coefficient in series solution

\[ a \] = radius of droplet, (cm)

\[ B_n \] = coefficients in series solution, dimensionless

\[ b = \frac{u}{128 (1 + \mu_d/\mu_c)d_e} \]

\[ C, c \] = concentration of solute in disperse phase, (g mole/liter)

\[ C_o \] = initial concentration (g mole/liter)

\[ D \] = molecular diffusivity (cm²/sec)

\[ D_2 \] = molar flow rate of disperse phase entering the column (lb. mole/hr.)

\[ D_n, D_{n+1} \] = molar flow rate of disperse phase at plates n and n+1 respectively in stagewise column (lb. mole/hr.)

\[ d_e \] = droplet diameter (cm)

\[ E \] = eddy diffusivity

\[ E_m \] = fraction extracted, \[ \frac{C_o - C}{C_o} \]

\[ e(\text{exp}) \] = base of natural logarithm

\[ h \] = modified continuous phase resistance \[ \frac{512 k_c (1 + \mu_d/\mu_c)}{\mu u} \]

\[ h_o \] = heat transfer coefficient

\[ h_\mu \] = unit vector in \( \mu \) direction

\[ h_\eta \] = unit vector in \( \eta \) direction

\[ h_\phi \] = unit vector in \( \phi \) direction
\[ K_{df}, K_{dr}, K_{dc} = \text{overall coefficients of mass transfer in terms of disperse phase concentration during droplet formation, free rise (or fall) and coalescence, (cm/sec)} \]

\[ k = \text{thermal conductivity} \]

\[ k_c, k_d = \text{individual mass transfer coefficient, continuous and dispersed phase, respectively (cm/sec)} \]

\[ M = \text{molecular weight of phase under consideration} \]

\[ M(t) = \text{mass of the solute in dispersed phase at time } t \]

\[ m = \text{distribution coefficient, dispersed phase concentration/continuous phase concentration at equilibrium} \]

\[ n = \text{an integer number} \]

\[ N_{Re} = \text{Reynolds number, } \frac{d_c u \rho_c}{\mu_c} \]

\[ (N_{Sc})_c = \text{continuous phase Schmit number, } \frac{\mu_c}{\rho_c D} \]

\[ N_{Nu} = \text{Nusselt number, } \frac{h_0 d_e}{k} \]

\[ N_{Pe} = \text{Peclet number, } \frac{d_c u}{D} \]

\[ N_{Sh} = \text{Sharewood number, } \frac{k_c d_e}{D} \]

\[ q = \text{rate of mass transfer (lb. mole/hr)} \]

\[ r = \frac{4\rho}{d_e}, \text{ torus radius} \]

\[ R = \Delta r / \Delta x^2 \]

\[ t = \text{time during free fall (or rise) period (sec)} \]

\[ \bar{t} = \text{average circulation time in droplet (sec)} \]

\[ U, u = \text{droplet free fall (or rise) velocity (cm/sec)} \]

\[ X = \text{dimensionless cylindrical coordinates (radial)} \]

\[ x = \text{solute concentration in dispersed phase, mole fraction} \]
\[ y = \text{solute concentration in dispersed phase in Chapter 2, radial direction in remaining chapters, } (1-r) \]

\[ y^* = \text{solute concentration in dispersed phase in equilibrium with continuous phase, mole fraction} \]

\[ \bar{Z} = \text{average displacement of fluid} \]

\[ \lambda_n = \text{an eigenvalue} \]

\[ \mu_d, \mu_c = \text{viscosity of dispersed phase and continuous phase respectively, centipoise} \]

\[ \rho_d, \rho_c = \text{density of dispersed phase and continuous phase, respectively } (g/cm^3, \text{ lb/ft}^3) \]

\[ \rho = \text{torus radius} \]

\[ \theta = \text{polar angle, spherical coordinate system} \]

\[ \tau = \text{dimensionless time, } Dt/a^2 \]

\[ \phi = \text{polar angle, toroidal coordinate system} \]

\[ \eta = \text{polar angle, toroidal coordinate system} \]

\[ \mu = \text{parameter, toroidal coordinate system} \]

\[ \psi_n = \text{an eigenvalue} \]

\[ \xi = \text{radial direction for Hadamard type circulation} \]

**Subscripts**

- \( ab \): solute a is diffusing in continuous phase b
- \( c \): continuous phase
- \( d \): dispersed phase
- \( f \): drop formation
- \( n \): integer number
- \( r \): step size in \( y \) direction
- \( s \): step size in \( t \) direction
INTRODUCTION

To formulate a procedure for the design of liquid extraction columns from rate equations and in order to avoid the need for experimental determination of stage efficiencies (which are frequently obtained at substantial cost in time, effort and money), it is essential to be able to predict the rate of mass transfer in liquid extraction columns under various conditions. One such procedure (24) is outlined below. The design procedure outlined below reduces, in essence, to the use of rate equations to locate a pseudo-equilibrium curve for the purposes of stepping off the desired number of stages between the pseudo-equilibrium and operating curves on the x-y diagram. This method considers mass transfer during drop formation, free rise (or fall), and coalescence on each plate.

It will be clear from this outline that the ability to predict mass transfer coefficients for dispersed phase systems is of utmost importance. The purpose of this investigation is to present theoretical relations for predicting the dispersed phase mass transfer coefficient of circulating and/or oscillating liquid droplets based on a modification of the Handlos and Baron model.

Location of the Pseudo-Equilibrium Curve

Consider the nth stage of a perforated plate column, as shown in the figure 1.1. For transfer into disperse phase and with $y^*$
Figure 1.1 - Plates $n+1$ and $n$ in a perforated plate extraction column.

Figure 1.2 - Location of the pseudo equilibrium curve and determination of the actual stages.
constant for a given stage due to agitation provided by the moving
droplets, the rate of mass transfer in the nth stage is:

\[ q = K_{dr} A_f (y^*_n - y_f)_m + K_{dr} A_r (y^*_n - y_r)_m + K_{dc} A_c (y^*_n - y_c)_m \]  \hspace{1cm} (1.1)

i.e., the sum of the transfer rates during droplet formation on
plate n, free rise, and coalescence beneath plate n + 1.

Now

\[(y^*_n - y_f)_m = (y^*_n - y_n) \]  \hspace{1cm} (1.2)

\[(y^*_n - y_c)_m = (y^*_n - y_{n+1}) \]  \hspace{1cm} (1.3)

and if D stays approximately constant over stage n, then

\[ (y^*_n - y_r)_m = \frac{(y^*_n - y_n) - (y^*_n - y_{n+1})}{\ln \left( \frac{y^*_n - y_n}{y^*_n - y_{n+1}} \right)} \]  \hspace{1cm} (1.4)

with this approximation, equation 1.1 becomes:

\[ q = K_{dr} A_f (y^*_n - y_n) + K_{dr} A_r \frac{(y^*_n - y_n) - (y^*_n - y_{n+1})}{\ln \left( \frac{y^*_n - y_n}{y^*_n - y_{n+1}} \right)} \]

\[ + K_{dc} A_c (y^*_n - y_{n+1}) \]  \hspace{1cm} (1.5)

*All symbols are defined in the Nomenclature Section, page vii.*
Making the usual simplifying assumption that only solute is transferred or that solute transfer is accompanied by equimolal countertransfer of solvents between phases,

\[ q = \frac{D_{n+1}y_{n+1} - D_n y_n}{1 - y_{n+1}} \]  

(1.6)

and from material balances:

\[ D_n = \frac{D_2(1 - y_2)}{(1 - y_n)} \]  

(1.7)

\[ D_{n+1} = \frac{D_2(1 - y_2)}{(1 - y_{n+1})} \]  

(1.8)

Suppose \( K_{df}, K_{dr}, K_{dc}, A_f, A_r, \) and \( A_c \) are all predictable. A trial and error procedure can then be used to estimate \( y_{n+1} \) corresponding to a given pair of \( y_n \) and \( y_n^* \) values as follows with reference to figure (1.2).

1. Assume value of \( y_{n+1} \) corresponding to a selected pair of \( y_n \) and \( y_n^* \) values in figure (1.2).

2. Calculate \( D_n \) and \( D_{n+1} \) corresponding to \( y_n \) and the assumed \( y_{n+1} \).

3. Calculate \( q \) from equations (1.5) and (1.6).

If these two estimates of \( q \) agree, the assumed value of \( y_{n+1} \) is correct; otherwise the process is repeated until the agreement between the \( q \) values is obtained. A graphical solution of equations
(1.5) and (1.6) for the correct value of \( y_{n+1} \) would probably abbreviate this procedure. In this manner the pseudo equilibrium curve of figure (1.2) is constructed and used with the operating curve to step off the required number of actual perforated plates.

**Evaluation of \( K_{dr} \).**

Attention in the literature has largely centered around the individual dispersed phase \( (k_{dr}) \) and continuous phase coefficients \( (k_{cr}) \) during the free fall (or rise), which are combined to give, \( K_{dr} \), overall mass transfer coefficients as follows - on the assumption of interfacial equilibrium:

\[
\frac{1}{K_{dr}} = \frac{1}{k_{dr}} + \frac{m}{k_{cr}} \quad (1.9)
\]

With this concept in mind many individuals working in the field of liquid extraction have developed mathematical and empirical models describing the hydrodynamic behaviour and mass transfer mechanism in and around the drop (15). Some of these mass transfer models are described in the next chapter.

Handlos and Baron (8) have developed a dispersed phase transfer mechanism to predict the resistance to mass transfer inside the circulating and/or oscillating droplets. They assumed that there was no resistance to mass transfer in the continuous phase. The model may be represented as:
\[
\frac{\partial c}{\partial t} = b \frac{1}{r} \frac{\partial}{\partial r} \left( (6r^2 - 8r + 3) r \frac{\partial c}{\partial r} \right) \tag{1.10}
\]

where \( b = \frac{U}{128 (1 + \mu_0/c) d_e} \) \tag{1.11}

The boundary conditions employed are:

\[ C = 0, \quad r = 1, \quad t > 0 \tag{1.12} \]
\[ C \text{ is finite,} \quad r = 0, \quad t = t \tag{1.13} \]
\[ C = C_0, \quad r = r, \quad t = 0 \tag{1.14} \]

The derivation of this model will be discussed later in this work.

Wellek and Skelland (25) modified this model by considering the additional effect of a finite continuous phase resistance in the boundary conditions of the original model. In the most practical applications resistance to mass transfer exists in both phases. Instead of boundary condition (1.12), the following relation (derived later in this work) is employed to consider the resistance outside the drop.

\[ \frac{\partial c}{\partial r} = hc, \quad r = 1, \quad t > 0 \tag{1.15} \]

A solution to the problem was obtained for various values of the continuous phase resistance by the Rayleigh-Ritz Variational technique, using a polynomial approximation for the concentration distribution inside the droplet. The solution consisted of the first three eigenvalues for various values of 'h'.

The purpose of this investigation is to use some method other than the Rayleigh-Ritz technique in order to check the accuracy of eigenvalues $\lambda_n$ calculated by Wellek and Skelland and, in addition, to determine the constants $B_n$ in the series solution, which were not calculated by Wellek and Skelland. The Rayleigh-Ritz variational technique gives good approximation for lower eigenvalues only. The eigenvalues will be obtained by trial and error procedure using standard Runge-Kutta and Hamming's method. After obtaining the eigenvalues, the coefficients $B_n$ will be computed. From this information the fractional extraction will be computed as a function of droplet contact time.

The Wellek-Skelland model will also be solved by a finite difference method to compute fraction extracted as a function of contact time. The results of these two methods will then be compared.

From the fractional extraction, the dispersed phase mass transfer coefficient can be calculated.

$$k_{dr} = - \frac{de}{6t} \ln(1 - E_m)$$ (1.16)

The dispersed phase mass transfer coefficient can then be used in the design procedure outlined above when oscillating droplets may be expected. The conditions under which droplet oscillation may be expected are discussed in reference (30).
II. LITERATURE REVIEW

This section includes the different mass transfer mechanisms for the inside of the droplets and a review of correlations for the continuous phase mass transfer coefficients.

Mass Transfer Mechanisms: Solute transfer between a drop and the field fluid in a spray column takes place in three stages. The first is during the period of drop formation, second is during free fall or rise of the drop and the third stage is the extraction at coalescent layer.

The mass transfer mechanism during the formation of the droplet and the extraction at the coalescent layer is discussed elsewhere (25).

In this section only the mechanisms postulated for the extraction process during rise (or fall) of the droplet are discussed.

Newman Model: Newman (18) derived a relation for mass transfer in a stagnant spherical drop, using the following partial differential equation obtained from Fick's second law.

\[
\frac{\partial c}{\partial t} = D \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c}{\partial r} \right)
\]

(2.1)

\[
C = C_0, \quad r = r, \quad t = 0
\]

(2.2)

\[
C \text{ is finite} \quad r = 0, \quad t = t
\]

(2.3)
\[ C = C_i, \quad r = a, \quad t = 0 \]  
\[ r = a, \quad t = 0 \]  
(No continuous phase resistance i.e. \( k_c \rightarrow \infty \))

The solution of the above equation may be expressed as:

\[
E_m = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp\left(-\frac{n^2 \pi^2 D t}{a^2}\right)
\]  
\[ \text{(2.5)} \]

where \( E_m \) is the fraction extracted.

\[
k_d = -\frac{dE}{6t} \ln(1 - E_m)
\]  
\[ \text{(1.16)} \]

It can be shown that as \( t \rightarrow \infty \)

\[
k_d = \frac{6.56 D}{d_e}
\]  
\[ \text{(2.5a)} \]

**Grober Modification**: Grober (7) modified the Newman model. He considered the case of finite continuous phase resistance. The solution to equation 2.1 was originally obtained for the case of heat transfer. Boundary condition 2.4 is replaced with the following boundary condition for mass transfer:

\[
k_c(C_i - C) = D \frac{\partial C}{\partial r}, \quad r = a, \quad t > 0
\]  
\[ \text{(2.6)} \]

The solution is:

\[
E_m = 1 - 6 \sum_{n=1}^{\infty} A_n \exp\left(-\frac{\psi_n^2 D t}{a^2}\right)
\]  
\[ \text{(2.7)} \]

where \( A_n \) and \( \psi_n \) are functions of \( k_c d/D \) and \( n \), and both of the above expressions are valid only if there are no circulation.
currents inside the droplets and the droplets are spherical. The values of $A_n$ and $\psi_n$ are tabulated in appendix (E).

**Kronig and Brink Model**: The extraction of a substance dissolved in spherical liquid droplets, falling (or rising) in another fluid under the influence of gravity was investigated by Kronig and Brink (12). Internal circulation currents, which exist in some droplets because of viscous flow between the fluids, modify the rate of extraction as compared with internally stagnant droplets. The rate of extraction is increased by internal circulation. Under certain simplifying assumptions (e.g., solute diffusion is only in a direction perpendicular to the internal streamlines and that continuous phase resistance is negligible), the following partial differential equation governing combined action of laminar convection and molecular diffusion was derived:

\[
\frac{\partial}{\partial \xi} \left( P(\xi) \frac{\partial c}{\partial t} \right) = \frac{a^2}{16 D} Q(\xi) \frac{\partial c}{\partial t} \tag{2.8}
\]

where $\xi = 4x^2(1 - x^2)\sin^2 \theta$, $r = 1$ at drop surface, and $P(\xi)$ and $Q(\xi)$ are complex integrals.

$\xi = 1$ is at the center of circulation currents. The circulation streamlines are shown in figure 2.1 The boundary conditions are:

\[
C = C_0, \quad \xi = \xi \quad t = 0 \tag{2.9}
\]

$C$ is finite $\xi = 1 \quad t = t \tag{2.10}$

$C = C_i \quad \xi = 0 \quad t > 0 \tag{2.11}$
Figure 2.1 Hadamard Streamlines
The solution of the above equation for \((k_c \to \infty)\) no resistance to transfer in continuous phase is:

\[
E_m = 1 - \frac{3}{8} \sum_{n=1}^{\infty} B_n^2 \exp \left(-16 \lambda_n \frac{D_t}{a^2}\right)
\]

(2.8a)

where \(B_n\) and \(\lambda_n\) are functions of \(n\) (and are tabulated in appendix E).

It can be shown that as \(t \to \infty\)

\[
k_d = \frac{17.9 D}{de}
\]

(2.5b)

**Elzinga and Banchero Modification:** While investigating the continuous phase film coefficients for heat transfer to liquid drops, Elzinga and Banchero (4) modified the Kronig and Brink model to include finite continuous phase resistance by replacing the boundary condition (2.11) to (2.12):

\[
\frac{3}{32} k_c \frac{\partial c}{\partial \xi} = D \frac{\partial c}{\partial \xi}, \quad \xi = 0, \quad t > 0
\]

(2.12)

The solution of equation (2.8) with above boundary condition is:

\[
E_m = 1 - \frac{3}{8} \sum_{n=1}^{\infty} B_n^2 \exp \left(-16 \lambda_n \frac{D_t}{a^2}\right)
\]

(2.13)

\(B_n\) and \(\lambda_n\) are functions of \(k_c d/D_d\) and \(n\), and values are tabulated in appendix E.

The Kronig and Brink model and the Elzinga-Banchero model hold only for Reynolds numbers less than one and Peclet numbers approaching infinity. In most industrial applications, the Reynolds numbers are greater than one.
Johns and Beckmann Model: Johns and Beckmann (10) have presented the solution to viscous flow model which reduces to the stagnant drop and the Kronig and Brink models in the respective limits, that is, $N_{Pe} = 0$ and $N_{Pe} = \infty$, and complements these models in the interval $0 < N_{Pe} < \infty$. The assumptions were similar to those used for Kronig and Brink model (12) except that the limitation $N_{Pe} = \infty$ was relaxed. The following equation was obtained by them:

$$\frac{\partial c}{\partial \tau} = \frac{1}{R^2} \frac{\partial}{\partial R} \left( R^2 \frac{\partial c}{\partial R} \right) + \frac{1}{R^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial c}{\partial \theta} \right)$$

$$+ N_{Pe} \left\{ (1 - R^2) \left( \cos \theta \frac{\partial c}{\partial R} \right) + \frac{2R^2 - 1}{R} \left( \sin \theta \frac{\partial c}{\partial \theta} \right) \right\}$$

$c(R, \theta, \tau) = 0$

$c(R, \theta, 0) = c_0(R, \theta)$

$$N_{NU} = \frac{h_d d e}{h}$$

The above equation was solved numerically.

The asymptotic Nusselt number and selected asymptotic concentration profiles are shown in figures (2.2) and (2.3). The dilute region in the neighborhood of the axis $\theta = 0$ results from the counterclockwise flow about the point $R = \frac{\sqrt{2}}{2}$, and $\theta = \frac{\pi}{2}$ and the boundary condition $c(1, \theta, \tau)$. The profile shown in figure 2.3 (for $N_{Pe} \to \infty$) represents the Kronig and Brink assumption, $c \to c(\xi, \tau)$ as $\tau \to \infty$.
and $N_{Pe} \to \infty$, and provides a logical limit to sequence of the profiles shown in figure 2.3. Qualitatively the asymptotic Nusselt number satisfies two independent conditions:

1. $N_{Nu} = 17.90$ (Kronig and Brink limit) as $N_{Pe} \to \infty$
2. $N_{Nu} = 6.56$ (Stagnant drop limit) as $N_{Pe} = 0$

The asymptotic Nusselt number also satisfies the form of Peclet number dependence prescribed by perturbation analysis of Kronig, Van Der Veen and Ijzerman (13) for small $N_{Pe}$.

The mechanism of viscous single drop extraction was analyzed in terms of transport by viscous convection and molecular diffusion. The solution of this model spans the transfer mechanism between the convection limited or stagnant drop model and diffusion limited or Kronig and Brink model (figure 2.2) and thereby extends and places in perspective models which commonly are applied in the analysis of experimental data (10).

Handlos and Baron Model: Handlos and Baron (8) considered the case of a completely turbulent drop with an internal circulation pattern of concentric circles and assumed that the liquid between two streamlines becomes radially mixed after one revolution as shown in the figure 3.1. The following partial differential equation was developed to describe the mechanism:

$$\frac{\partial c}{\partial t} = b \frac{1}{r} \frac{\partial}{\partial r} \left( (6r^2 - 8r + 3) r \frac{\partial c}{\partial r} \right)$$

(2.14)
Fig. 27: Asymptotic Nusselt number.

Fig. 23: Normalized asymptotic concentration profiles.
where

\[
b = \frac{U}{128 \left(1 + \frac{\mu d}{\mu c}\right)}
\]

\[
C = 0, \quad r = 1, \quad t > 0
\]  \hspace{1cm} (2.15)

\[
C \text{ is finite, } r = 0, \quad t = \text{t}
\]  \hspace{1cm} (2.16)

\[
C = C_0, \quad 0 \leq r \leq 1, \quad t = 0
\]  \hspace{1cm} (2.17)

The following solution may be obtained:

\[
E_m = 1 - 2 \sum_{n=1}^{\infty} B_n^2 \exp (-\lambda_n bt)
\]  \hspace{1cm} (2.18)

Handlos and Baron only calculated the lowest eigenvalue equation 2.18 using Ritz method. The value obtained for the lowest eigenvalue, \(\lambda_1\), was 2.88 for no continuous phase resistance (i.e. \(k_c \to \infty\)).

**Wellek-Skelland Modification:** Wellek and Skelland (16) modified the Handlos and Baron turbulence model for circulating and/or oscillating droplets by considering the effect of a finite continuous phase resistance in the boundary condition of the original partial differential equation. The boundary condition (2.15) was replaced by (2.18).

\[
\frac{\partial C}{\partial r} = h C \quad r = 1 \quad t > 0
\]

where

\[
h = \frac{512 k_c \left(1 + \frac{\mu d}{\mu c}\right)}{m U}
\]  \hspace{1cm} (2.19)
The solution of the Wellek and Skelland modification is:

\[ E_m = 1 - 2 \sum_{n=1}^{\infty} B_n^2 \exp (-b \lambda_n t) \]  \tag{2.20}

In order to determine \( \lambda_n \), the eigenfunction \( Y_n(y) \) is approximated by a fourth order polynomial

\[ Y_n(y) = a_0 + a_1 y + a_2 y^2 + a_3 y^3 + a_4 y^4 \]  \tag{2.21}

where \( a_0 = a_1 / h \).

Applying the Rayleigh-Ritz method, one solves for \( \lambda_n \) from the characteristic equation obtained from the determinant of the coefficients \( a_1, a_2, a_3 \) and \( a_4 \). The determinant is obtained by successive partial differentiation of

\[ 0 = K = \int_0^1 \frac{d}{dy} \left( (1 - 5y + 10y^2 - 6y^3) \frac{dY_n}{dy} \right) \]

\[ - \int_0^1 (1 - y) Y_n^2 dy \]  \tag{2.22}

with respect to \( a_1, a_2, a_3 \) and \( a_4 \). The characteristic equation was obtained using the Hessenberg algorithm (14).

The calculations for \( \lambda_n \) were performed for various values of the continuous phase resistance \( h \). Values of \( \lambda_n \) are tabulated in the appendix (E).

The dispersed phase mass transfer coefficient is defined as
\[ k_d = -\frac{d_e}{6t} \ln (1 - E_m) \]  

(1.16)

Considering equations 2.20 and 1.16 and limiting attention to the first eigenvalues, the mass transfer coefficient is

\[ k_d = \frac{\lambda_1 u}{768 (1 + \mu_d/\mu_c)} \]  

(1.16a)

where \( \lambda_1 \) is a function of \( k_c \). This value of the dispersed phase mass transfer coefficient is essentially the value of \( k_d \) as time approaches infinity. It should be noticed that the values of \( B_n \) in equation 2.20 were not calculated.

Correlations for the Continuous Phase Mass Transfer Coefficients:

Only a few of the many correlations will be presented here. For continuous phase transfer from a rigid (non-circulating) sphere, the following equation was derived by Frossling (5):

\[ k_c = \frac{D_p}{d_e M} \left( 2 + 0.55 (N_{Re_c})^{1/2} (N_{Sc_c})^{1/3} \right) \]  

(2.23)

The constant 0.55, however, was experimentally determined. The relationship is valid for \( 2 \leq N_{Re_c} \leq 1000 \).

For the droplets with circulating currents inside, Boussinesq (1) has shown that:

\[ k_c = \frac{D_p}{d M} \left( \frac{2}{\sqrt{\pi}} (N_{Re_c})^{1/2} (N_{Sc_c})^{1/2} \right) \]  

(2.24)
The above equation can also be obtained by using Higbie's penetration theory. *

For continuous phase transfer from droplets which are internally circulating but not oscillating, Garner and Tayeban (6) found experimentally:

\[ k_c = \frac{D_p}{dM} \left( 0.6 (N_{Re_c})^{1/2} (N_{Sc_c})^{1/2} \right) \quad (2.25) \]

When the droplets were both circulating and oscillating they correlated their experimental data for transfer in the continuous phase by:

\[ k_c = \frac{D_p}{dM} \left( 50 + 0.0085 (N_{Re_c})^{1.0} (N_{Sc_c})^{0.7} \right) \quad (2.26) \]

Nearly all of the above relationships assume the drops to be spherical. It is well known, however, that drops usually show large deformation, often to predictable oblate spheroidal shape (28). In the droplet Reynolds number range of commercial interest (100-1000) drag-coefficients for discs and some oblate spheroids are greater than those for spheres at the same Reynolds number by about 100% (19).

Skelland and Cornish correlated data on the rate of mass transfer from rigid oblate spheroids in an air stream as follows:

\[ k_c = 0.74 \frac{D_p}{d_p M} \left( \frac{d_p U \rho}{\mu_c} \right)^{0.5} \left( \frac{\mu_c}{\rho D_c} \right)^{1/3} \quad (2.27) \]

where \( d_p \) is the total surface area of the spheroid divided by its

* in which contact time is defined by \( d_e / U \).
perimeter normal to the flow (23). Wellek, Agrawal, and Skelland (28) have presented a method for predicting the distortion of droplets into oblate spheroidal shapes, and thus enabling the calculation of $d_p$ for non-spherical droplets.
III. THEORY

Handlos and Baron have proposed a dispersed phase transfer mechanism which shows promise in predicting the very low resistance to mass transfer inside circulating and/or oscillating droplets. The original solution presented by Handlos and Baron assumed that there was no resistance to transfer in continuous phase. It should be pointed out that the development of their eddy diffusion model is devoid of any constant or parameter which must be obtained from experimental measurements. However, it is assumed that the velocities of continuous and dispersed phase are known and the velocity of falling (or rising) droplets can be predicted.

The model is based on the assumption that internal circulation is fully developed. The circulation pattern within the spherical droplet is assumed to be a system of tori. For a cross-sectional view of the drop see figure (3.1). Handlos and Baron further assumed that "random radial vibrations" are superimposed upon the streamlines. Handlos and Baron do not specifically state the source of these vibrations, but oscillation of the droplets is one likely source. The mixing between streamlines is due to these vibrations which are the key to their eddy diffusion mechanism. The mechanism is independent of any molecular diffusion process.

Before discussing the eddy diffusion mechanism it should be emphasized that the entire transfer process is assumed to take place
Figure 3.1  Handlos and Baron Streamlines
within the outer surface of the torus. This in effect neglects any resistance to transfer in the volume of the droplet between the outer surface of the torus and the interfacial area of the sphere.

The eddy diffusion process is assumed to obey the following relation:

\[ \mathbf{\nabla} \cdot \mathbf{N} = - \overline{E} \nabla C \]  \hspace{1cm} (3.1)

where \( \mathbf{N} \) is the flux of solute, and \( C \) is the vector gradient of solute concentration. A differential mass balance on the system within the torus is expressed as:

\[ \frac{\partial c}{\partial t} = - \nabla \cdot \mathbf{N} = \nabla (\overline{E} \nabla C) \]  \hspace{1cm} (3.2)

Now the problem faced by Handlos and Baron was to devise a relation for the eddy mass diffusivity, \( \overline{E} \), which would enable the solution of equation (3.2).

Handlos and Baron suggest that "if the transfer process can be described by eddy diffusion, the transfer process is also represented by the Einstein equation, which connects the mean square deviation (of a particle in fluid) for a given time to the effective diffusivity."

\[ \overline{E} = \frac{\overline{Z}^2}{4t} \]  \hspace{1cm} (3.3)

This assumes that Einstein equation applies in two dimensions. In
order to determine the mean square deviation, $Z_r^2$ and the characteristic time, $t$, in equation (3.3) it is necessary to understand the mixing process as assumed by Handlos and Baron.

Elements of fluid circulate in one plane, in a path describing a circle of radius $\rho$. See figure (3.1). The average circulation time, $\bar{t}$, i.e. time for an element to complete one circuit, for paths ranging from zero to $d/4$, is taken to be characteristic time $t$ and is given as:

$$\bar{t} = \frac{16}{3} \frac{d_e}{U} \left(1 + \frac{\mu d}{\mu_c}\right)$$

(3.4)

Handlos and Baron state that equation (3.4) is the average circulation time for the Hadamard-type circulation patterns. It should be recalled that these streamlines are derived for the laminar situation ($N_{Re} < 1$).

Consider what happens to an element of fluid during the circulation process. Suppose the element is initially at radius $\rho$. After a time sufficient for one circuit along the streamline, the element is displaced to a point $\rho'$ as a result of the random radial motion. In the 'limiting' case of complete mixing in one circulation period, the probability that an element is found between $\rho'$ and $\rho + d\rho$ is, according to Handlos and Baron, the ratio of the differential element of volume $\rho'\text{ to the total volume of the torus.}$
\[ V_\rho = 2\pi^2 \left( \frac{d_e}{4} \right)^2 (\rho')^2 = \text{volume of torus, } \rho' \]  
(3.5a)
\[ V_{\text{total}} = 2\pi^2 \left( \frac{d_e}{4} \right)^3 = \text{total volume of torus, } d/4 \]  
(3.5b)
\[ dV_{\rho'} = 4\pi^2 \left( \frac{d_e}{4} \right)^2 (\rho')d\rho = \text{differential volume of torus at } \rho' \]  
(3.5c)

\[ P(\rho')d\rho' = \text{probability of finding element between } \rho' \text{ and } \rho' + d\rho' \]  
(3.6)

Therefore
\[ P(\rho')d\rho' = \frac{32\rho'd\rho'}{d^2} \]  
(3.7)

A dimensionless radius of torus \( r \) is defined as
\[ r = \frac{\rho}{d/4} \]  
(3.8)

Substituting in equation (3.7) we have,
\[ P(r')dr' = 2r'dr' \]  
(3.9)

The displacement, \( Z \), of an element of fluid during the circulating period is given by:
\[ Z = \rho' - \rho = \frac{d_e}{4} (r' - r) \]  
(3.10)

Or
\[ Z^2 = \frac{d_e^2}{16} (r' - r)^2 \]  
(3.11)

According to Handlos and Baron, the mean square displacement for many complete circuits is simply the expected value of \( Z^2 \),
which is

\[ Z^2 = \int_0^1 Z^2 \, P(r') \, dr' = \frac{d^2}{8} \int_0^1 (r' - x)^2 \, r' \, dr' \]

\[ = \frac{d_e^2}{96} (6x^2 - 8x + 3) \quad (3.12) \]

Substitution of equation (3.4) and (3.12) in (3.3) gives the relation for effective diffusivity.

\[ \bar{E}(r') = \frac{U(6r^2 - 8r + 3) d_e}{2048 \left( 1 + \frac{\mu d}{\mu_c} \right)} \quad (3.13) \]

Now it is possible to return to the problem of solving the differential mass balance:

\[ \frac{\partial c}{\partial t} = \nabla \cdot (\bar{E} \nabla c) \quad (3.2) \]

If mass transfer in the torus is only in the radial direction, equation (3.2) can be represented by the relation for an infinite cylinder:

\[ \frac{\partial c}{\partial t} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \bar{E} \rho \frac{\partial c}{\partial \rho} \right) \quad (3.14) \]

or

\[ \frac{\partial c}{\partial t} = \frac{16}{d_e^2} \frac{1}{r} \frac{\partial}{\partial r} \left( \bar{E} \cdot r \frac{\partial c}{\partial r} \right) \quad (3.15) \]
Substituting (3.12) into (3.14) we have,
\[ \frac{\partial c}{\partial t} = b \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{6r^2 - 8r + 3}{r} \frac{\partial c}{\partial r} \right) \] (3.16)

where
\[ b = \frac{U}{128 \left( 1 + \frac{\mu_d}{\mu_c} \right) d_e} \] (3.17)

Equation (3.16) may be considered to be the differential form of the Handlos and Baron model.

For convenience let, \( r = 1 - y \). (3.18)

Equation (3.16) is transformed to,
\[ \frac{\partial c}{\partial t} = \frac{b}{1-y} \frac{\partial}{\partial y} \left( 1 - 5y + 10y^2 - 6y^3 \right) \frac{\partial c}{\partial y} \] (3.19)

Handlos and Baron employed following boundary conditions with equation (3.19):

\[ C = 0, \quad y = 0, \quad t > 0 \] (3.20)
\[ C \text{ is finite}, \quad y = 1, \quad t = t \] (3.21)
\[ C = C_0, \quad 0 < y < 1, \quad t = 0 \] (3.22)

Equation (3.20) implies that there is no resistance to transfer in the continuous phase, and hence the continuous phase concentration is equal to the concentration at the surface of the torus. Equation (3.21) implies, due to symmetry:
\[ \frac{\partial c}{\partial y} = 0 \quad \text{at} \quad y = 1, \quad t = t \] (3.21a)
Equation (3.22) describes the initial condition of the drop, i.e. initially the concentration of drop is uniform.

Wellek-Skelland (26) replaced boundary condition (3.20) by the following boundary condition which assumes a finite continuous phase resistance:

\[- E(\rho) \frac{\partial c}{\partial \rho} = \frac{k_c}{m} C, \quad \rho = \frac{d_e}{4}, \quad t > 0\]

or in terms of y:

\[\frac{\partial c}{\partial y} = h_c, \quad y = 0, \quad t > 0\]

where \( h = \frac{512 k_c \left( \frac{\mu d}{\mu c} \right)}{m u} \) \hspace{1cm} (3.25)

Boundary condition (3.24) at the surface of the droplet is obtained as follows:

\[- E(\rho) \frac{\partial c}{\partial \rho} = \frac{k_c}{m} c, \quad \rho = \frac{d_e}{4}, \quad t > 0\] \hspace{1cm} (3.24a)

\[- E(r) \frac{d^4}{d y^2} \frac{\partial c}{\partial r} = \frac{k_c}{m} c, \quad r = 1, \quad t > 0\] \hspace{1cm} (3.24b)

\[- E(y) \frac{d^4}{d y^2} \left( - \frac{\partial c}{\partial y} \right) = \frac{k_c}{m} c, \quad y = 0, \quad t > 0\] \hspace{1cm} (3.24c)

\[\frac{\partial c}{\partial y} = \frac{k_c}{m} \frac{d_e}{4} \frac{2048 \left( \frac{\mu d}{\mu c} \right)}{u d_e} c, \quad y = 0, \quad t > 0\] \hspace{1cm} (3.24d)

\[\therefore \frac{\partial c}{\partial y} = h_c, \quad y = 0, \quad t > 0\] \hspace{1cm} (3.24)
Boundary condition (3.24) assumes that the continuous phase mass transfer coefficient, $k_c$, and the distribution coefficient, $m$, are uniform over the entire droplet interface. This may not be a precise physical description, but is good enough to describe many situations. These assumptions are also necessary for the Grober (7) and Elizinga and Banchero (4) modification. This boundary condition also assumes that the concentration of solute in the bulk of continuous phase is negligible during the contact period.

Mathematical Details of the Solution:

The partial differential equation to be solved and the relevant boundary conditions are:

$$\frac{\partial c}{\partial t} = \frac{b}{1-y} \cdot \frac{\partial}{\partial y} \left( (1 - 5y + 10y^2 - 6y^3) \frac{\partial c}{\partial y} \right)$$  \hspace{1cm} (3.19)

$$\frac{\partial c}{\partial y} = hc, \quad y = 0, \quad t > 0$$  \hspace{1cm} (3.24)

$C$ is finite, $\quad y = 1, \quad t = t$  \hspace{1cm} (3.21)

$C = C_0, \quad 0 \leq y \leq 1, \quad t = 0$  \hspace{1cm} (3.22)

By the method of separations of variables, the solution is assumed to take form:

$$C = T(t) \cdot Y(y)$$  \hspace{1cm} (3.26)

For the sake of convenience the function $T(t)$ and $Y(y)$ will often be referred as $T$ and $Y$, respectively. It is now possible to separate
equation (3.19) into two ordinary differential equations:

\[
\frac{dT}{dt} + b_\lambda T = 0
\]  

(3.27)

\[
\frac{d}{dy} \left( P(y) \cdot \frac{dY}{dy} \right) + \lambda \cdot Q(y) Y = 0
\]  

(3.28)

where:

\[
P(y) = 1 - 5y + 10y^2 - 6y^3
\]

\[
Q(y) = 1 - y
\]

\[
\lambda = \text{separation of variable constant}
\]

The solution of equation (3.27) is

\[
T(t) = B \exp(-b\lambda t)
\]  

(3.29)

where B is a constant to be determined. The boundary conditions for equation (3.28) can be shown to be:

\[
\frac{dY}{dy} = hY, \quad y = 0
\]  

(3.30)

\[
Y \text{ is finite, } y = 1
\]  

(3.31)

Equation (3.28), (3.30), and (3.31) represent a Sturm-Liouville system. Non-trivial solutions to that system exist in most cases only for a discrete set of values of \((\lambda_1, \lambda_2, \ldots)\) called eigenvalues \((2, 17, 27)\). While at the moment the function \(Y(y)\) is not known, from the theory of Sturm-Liouville problems it is known that it will
consist of series of orthogonal eigenfunctions, \( Y_1, Y_2, Y_3, \ldots, Y_n \).

In this work \( Y \) will also be considered normalized, with the normalizing factor included in \( B \). It can also be seen that equation (3.29) actually represents a set of solutions. Accordingly, the general solution of equation (3.26) is:

\[
C(y, t) = C_0 \sum_{n=1}^{\infty} B_n Y_n \cdot \exp(-b \lambda n t) \tag{3.32}
\]

Equation (3.32) represents the solute concentration at any value of \( y \) and \( t \). (The above general solution of equation (3.26) is outlined in appendix A.)

To get the average concentration in the drop at any time, consider the problem of transfer into the droplet where the initial mass of solute in the droplet is \( M(0) \) and the mass at any time is \( M(t) \).

\[
M(t) = \int_0^{V_t} C \, dV
\]

\[
dV_p' = 4\pi^2 \frac{d}{4} \rho dp \tag{3.5c}
\]

\[
dV_y = -\frac{\pi^2 d^3}{16} (1-y) \, dy \tag{3.34}
\]

\[
\therefore M(t) = \frac{C_0 \pi^2 d^3}{16} \sum_{n=1}^{\infty} B_n \exp(-b \lambda n t) \int_0^1 (1-y) Y_n \, dy \tag{3.35}
\]

Applying the initial condition (equation 3.22) to equation (3.32) leads to the following expression.
1 = \sum_{n=1}^{\infty} B_n Y_n \quad (3.36)

In order to obtain \( B_n \), the condition of orthogonality is applied to equation (3.36). Both sides of equation (3.36) are multiplied by \((1 - y)\), \(Y_n\) and \(dy\) and integrated over the interval of \(0 \leq y \leq 1\).

\[
\int_{0}^{1} (1 - y) Y_n dy = B_n \int_{0}^{1} (1 - y) Y_n^2 dy \quad (3.37)
\]

By the application of the theory of orthogonal functions equation (3.37) reduces to (2).

\[
B_n = \int_{0}^{1} (1 - y) Y_n dy \quad (3.38)
\]

Substituting equation (3.38) into (3.35) leads to the following expression:

\[
M(t) = \frac{C_o \pi^2 \sigma^3}{16} \sum_{n=1}^{\infty} B_n^2 \exp (-b \lambda_n t) \quad (3.39)
\]

Equation (3.39) may be expressed as

\[
\frac{M(t)}{M(0)} = 2 \sum_{n=1}^{\infty} B_n^2 \exp (-b \lambda_n t) \quad (3.40)
\]

Johnson and Hamielec (11) prefer to express equation (3.40) in terms of the functional extraction approach:

\[
E_m = 1 - 2 \sum_{n=1}^{\infty} B_n^2 \exp (-b \lambda_n t) \quad (3.41)
\]

In order to use equation (3.41), we will have to determine \( B_n \) and \( \lambda_n \).
Continuing with the problem of determining $B_n$, consider equation (3.38) with $q(y) = (1 - y)$

$$B_n = \int_0^1 q(y) Y_n \, dy$$  \hfill (3.42)

Through the use of equation (3.28), equation (3.42) can be shown to be equivalent to:

$$B_n = -\frac{1}{\lambda_n} \int_0^1 \frac{d}{dy} \left( P(y) \frac{dY_n}{dy} \right)$$  \hfill (3.43)

and carrying out the integration:

$$B_n = -\frac{1}{\lambda_n} \left( P(1) \frac{dY_n(1)}{dy} - P(0) \frac{dY_n(0)}{dy} \right)$$

$$= -\frac{1}{\lambda_n} \left( (0) \frac{dY_n(1)}{dy} - (1) \frac{dY_n(1)}{dy} \right)$$

$$\therefore B_n = \frac{1}{\lambda_n} \frac{dY_n(0)}{dy}$$  \hfill (3.44)

This equation will be used to calculate $B_n$ after calculating $\lambda_n$. The procedure(s) to obtain $\lambda_n$ and $dY(0)/dy$ will be discussed in next chapter.
IV. COMPUTATION TECHNIQUES

It is obvious from preceding section that the evaluation of $B_n$ and $\lambda_n$ is required to complete the solution of Handlos and Baron model.

Consider equation (3.28) with the relevant boundary conditions:

$$\frac{d}{dy}\left(P(y)\frac{dY}{dy}\right) + \lambda \cdot Q(y) \cdot Y = 0$$  \hspace{1cm} (3.28)

$$\frac{dY}{dy} = hY \quad y = 0$$  \hspace{1cm} (3.30)

$Y$ is finite \hspace{1cm} $y = 1$  \hspace{1cm} (3.31)

Rearranging equation (3.28)

$$\frac{d^2Y}{dy^2} = -\left(\frac{-5+20y-18y^2}{1-5y+10y^2-6y^3}\right) \frac{dY}{dy} - \frac{\lambda_n (1-y) \cdot Y}{(1-5y+10y^2-6y^3)}$$  \hspace{1cm} (4.1)

or

$$\frac{d^2Y}{dy^2} = -\frac{\lambda_n Y}{(6y^2-4y+1)} - \left(\frac{18y^2-20y+5}{(1-5y+10y^2-6y^3)}\right) \frac{dY}{dy}$$  \hspace{1cm} (4.1a)

Boundary condition (3.31) can be replaced by

$$\frac{dY}{dy} = 0 \quad y = 0$$  \hspace{1cm} (4.2)

For convenience (3) in the numerical calculation the following normalized boundary condition was used:
Thus, the differential equation to be solved and relevant boundary conditions are

$$\frac{d^2 Y}{dy^2} = -\frac{\lambda_n Y}{(6y^2-4y+1)} \left( \frac{18y^2-20y+5}{(1-5y+10y^2-6y^3)} \right) \frac{dY}{dy} \quad (4.1a)$$

$$\frac{dY}{dy} = hY, \quad y = 0 \quad (3.30)$$

$$\frac{dY}{dy} = 0, \quad y = 1 \quad (4.2)$$

$$Y = 1.0, \quad y = 1 \quad (4.3)$$

Equation 4.1a does not exist at $y = 1$, but using the power series solution it can be shown that,

$$\frac{d^2 Y}{dy^2} = -\frac{\lambda}{6}, \quad y = 1 \quad (4.4)$$

The above relationship is derived in appendix B.

**Numerical Methods to Solve Ordinary Differential Equations**

Many techniques are available for the approximate solution of an ordinary differential equation. The following two methods are used frequently:

1. Runge-Kutta Method

2. Hamming's Method
Runge-Kutta Method for Calculation of $\lambda_n$ and $B_n$

The Runge-Kutta method (with a trial and error procedure) was used to compute the value of $\lambda_n$ and $\frac{dY(0)}{dy}$, which was used in equation (3.44) to calculate $B_n$.

Equation 4.1a is of the type

$$\frac{d^2Y}{dy^2} = G(y, Y, Y')$$  \hspace{1cm} (4.5)

Runge-Kutta's formulae are (9):

$$Y_{n+1} = Y_n + h Y_n' + \frac{h}{6} (m_0 + m_1 + m_2)$$  \hspace{1cm} (4.6)

$$Y_n' = Y_n' + \frac{1}{6} (m_0 + 2m_1 + 2m_2 + m_3)$$

where:

$$m_0 = h G(y_n, Y_n, Y_n')$$

$$m_1 = h G(y_n + \frac{1}{2} h, Y_n + \frac{1}{2} h Y_n', Y_n' + \frac{1}{2} m_0)$$

$$m_2 = h G(y_n + h, Y_n + h Y_n' + \frac{1}{4} h m_0, Y_n' + \frac{1}{2} m_1)$$

$$m_3 = h G(y_n + h, Y_n + h Y_n' + \frac{1}{2} h m_1, Y_n' + m_2)$$

First approximations for $\lambda_n$ were obtained from Wellek and Skelland eigenvalues. Using the above equation (4.6) starting from $y = 1$ and integrating to $y = 0$, $Y_n(y)$ and $Y_n'(y)$ were calculated in the entire interval. For a starting value, the initial conditions equations (4.2) and (4.3) were used. If the resultant solution satisfied the boundary condition,
\[
\frac{dY}{dy} = hY, \quad y = 0
\]  

(3.30)

the assumed value of \( \lambda \) was considered to be the correct eigenvalue. If the above condition was not satisfied to the required test value, a new value was chosen for \( \lambda \) and the procedure was repeated. The following test equation was used:

\[
\frac{dY}{dy} - hY < 0.0005
\]

Successive estimates of \( \lambda \) are made by the Reguli-falsi procedure. Successive estimates were made according to the following formula (3).

\[
\lambda_{i+1} = \lambda_i - \left( \frac{F(0)}{m(i)} \right)^{(i)}
\]

(4.7)

where the superscript indicates the \( i \)th iteration.

\[
[F(0)]^{(i)} = [Y'(0)]^{(i)} - h[Y(0)]^{(i)}
\]

(4.8)

\[
m(i) = \frac{[F(0)]^{(i)} - [F(0)]^{(i-1)}}{\lambda_i - \lambda_{i-1}}
\]

(4.9)

The flow chart of the above procedure is given in the appendix G. The computer program is also presented in appendix G.

\( Y'(0) \) is calculated during the above calculations. Using equation (3.44), \( B_n \) was obtained (for \( n = 1, 2, 3, 4 \)).

Hamming's Method to Calculate \( B_n \) and \( \lambda_n \)

Hamming's method can be used instead of Runge-Kutta method.
to get better accuracy. Equation (4.1a) is a second order differential equation. It can be easily reduced to two first order ordinary differential equations by suitably defining new variables (21). This technique was applied as follows:

$$\frac{d^2 Y}{dy^2} = G(y, Y, Y')$$  \hspace{1cm} (4.5)

substituting \( Y' = V \) the equivalent equations are:

\[
Y' = V  \hspace{1cm} (4.10)
\]

\[
V' = G(y, Y, V)  \hspace{1cm} (4.11)
\]

In vector notation, Hamming's method is:

**Predictor:**

\[
\begin{pmatrix}
P_{Y_{n+1}} \\
P_{V_{n+1}}
\end{pmatrix} =
\begin{pmatrix}
Y_{n-3} \\
V_{n-3}
\end{pmatrix} + 4h \frac{3}{3} \left\{ 2 \begin{pmatrix}
Y'_n \\
V'_n
\end{pmatrix} - \begin{pmatrix}
Y'_{n-1} \\
V'_{n-1}
\end{pmatrix} + 2 \begin{pmatrix}
Y'_{n-2} \\
V'_{n-2}
\end{pmatrix} \right\}
\]

**Modifier:**

\[
\begin{pmatrix}
M_{Y_{n+1}} \\
M_{V_{n+1}}
\end{pmatrix} = \begin{pmatrix}
P_{Y_{n+1}} \\
P_{V_{n+1}}
\end{pmatrix} - \frac{112}{121} \left\{ \begin{pmatrix}
P_{Y_{n}} \\
P_{V_{n}}
\end{pmatrix} - \begin{pmatrix}
C_{Y_{n}} \\
C_{V_{n}}
\end{pmatrix} \right\}
\]

\[
\begin{pmatrix}
M'_{Y_{n+1}} \\
M'_{V_{n+1}}
\end{pmatrix} = \begin{pmatrix}
M_{V_{n+1}} \\
G(y_{n+1}, M_{Y_{n+1}}, M_{V_{n+1}})
\end{pmatrix}
\]
Corrector:
\[
\begin{pmatrix}
CY_{n+1} \\
CV_{n+1}
\end{pmatrix} = \frac{1}{8} \left[ 2 \left( \begin{pmatrix} Y_n \\ V_n \end{pmatrix} - \begin{pmatrix} Y_{n-2} \\ V_{n-2} \end{pmatrix} \right) + 3h \left( \begin{pmatrix} M'Y_{n+1} \\ M'V_{n+1} \end{pmatrix} + 2 \begin{pmatrix} Y'_n \\ V'_n \end{pmatrix} - \begin{pmatrix} Y'_{n-1} \\ V'_{n-1} \end{pmatrix} \right) \right]
\]

Final Value:
\[
\begin{pmatrix}
Y_{n+1} \\
V_{n+1}
\end{pmatrix} = \begin{pmatrix}
CY_{n+1} \\
CV_{n+1}
\end{pmatrix} + \frac{9}{121} \left( \begin{pmatrix} PY_{n+1} \\ PV_{n+1} \end{pmatrix} - \begin{pmatrix} CY_{n+1} \\
CV_{n+1} \end{pmatrix} \right)
\]

This method requires the first four starting points, which in this case were calculated using the Runge-Kutta method. The same trial and error procedure was applied as described in the previous section.

Using both the Runge-Kutta and Hamming's method, the first four eigenvalues were calculated for different values of \( h \). The values of \( B_n \) were calculated using equation (3.44). See tables 1 and 2 for the results. From these results, \( E_m \) was calculated using equation (3.41). \( E_m \) was plotted versus \( b_t \) in figures 5.2 and 5.3.

Both the methods discussed above, namely the Runge-Kutta method and Hamming's method, have certain advantages and disadvantages. The Runge-Kutta method is easy to program, requires less computer storage, is self starting, and is such that it is easy to change the step size. On the other hand neither truncation error nor estimates of them are obtained in the calculation procedure. Using Hamming's method, it is easy to estimate the
truncation error, it is difficult to program, requires more memory, and it is not self starting.

The calculations using the above methods were programmed in the Fortran language and performed on an IBM 1620 digital computer (Model II).

**Numerical Methods to Solve Parabolic Partial Differential Equation:**

The numerical approach to the solution of a partial differential equation is very similar to the method used in the numerical solution of an ordinary differential equation. The derivatives, appearing in the equation, are replaced by finite difference ratios with the result that the differential equation is replaced by a difference equation. The difference equation is then solved by an algebraic or arithmetic procedure (14).

A partial differential equation can be represented by explicit (forward difference) or implicit finite difference formulae. For convergence of the method, the explicit representation is restricted by the size of step. This minimizes the usefulness of explicit representation of partial differential equation. Several implicit formulae have been developed to avoid this difficulty. They are due to Lassonen, Crank and Nicholson and Douglas (14).
Solution of Handlos and Baron Model by Finite Difference Method

The equation to be solved is:

\[ \frac{\partial c}{\partial t} = \frac{b}{1-y} \frac{\partial}{\partial y} \left( 1 - 5y + 10y^2 - 6y^3 \right) \frac{\partial c}{\partial y} \]  
(3.19)

\[ \frac{\partial c}{\partial y} = h \cdot c, \quad y = 0, \quad t > 0 \]  
(3.24)

\[ c \text{ is finite,} \quad y = 1, \quad t = t \]  
(3.21)

\[ c = c_0, \quad 0 \leq y \leq 1, \quad t = 0 \]  
(3.22)

Boundary condition (3.21) can also be represented as:

\[ \frac{\partial c}{\partial y} = 0, \quad y = 1, \quad t = t \]  
(4.13)

For convenience, a new variable was defined:

\[ E = \frac{c_0 - c}{c_0} \]  
(4.14)

or

\[ c = c_0 (1 - E) \]  
(4.15)

Equation (3.19) is transformed to:

\[ \frac{\partial E}{\partial t} = \frac{b}{1-y} \frac{\partial}{\partial y} \left( 1 - 5y + 10y^2 - 6y^3 \right) \frac{\partial E}{\partial y} \]  
(4.16)

and relevant boundary conditions are:

\[ \frac{\partial E}{\partial y} = h (E - 1), \quad y = 0, \quad t > 0 \]  
(4.17)
\[
\frac{\partial E}{\partial y} = 0, \quad y = 1, \quad t = t \quad (4.18)
\]
\[
E = 0, \quad 0 \leq y \leq 1, \quad t = 0 \quad (4.19)
\]

Equation (4.17) on rearranging becomes:

\[
\frac{\partial E}{\partial t} = b (1 - 4y + 6y^2) \frac{\partial^2 E}{\partial y^2} + b \left( \frac{-5 + 20y - 18y^2}{1 - y} \right) \frac{\partial E}{\partial y} \quad (4.20)
\]

\[
= b R(y) \frac{\partial^2 E}{\partial y^2} + b Q(y) \frac{\partial E}{\partial y} \quad (4.20a)
\]

where \( R(y) = 1 - 4y + 6y^2 \)

\[
Q(y) = \frac{-5 + 20y - 18y^2}{1 - y}
\]

Now the above partial differential equation was replaced by a finite difference form of the implicit type. This form was suggested by Crank and Nicholson (14).

\[
\frac{E_{r,s+1} - E_{r,s}}{\Delta t} = \frac{bR_{r}}{2\Delta y^2} \left[ (E_{r+1,s+1} - 2E_{r,s+1} + E_{r-1,s+1}) + (E_{r+1,s} - 2E_{r,s} + E_{r-1,s}) \right] + \frac{bQ_{r}}{4\Delta y} \left[ (E_{r+1,s+1} - E_{r-1,s+1}) + (E_{r+1,s} - E_{r-1,s}) \right] \quad (4.21)
\]

where \( r \) and \( s \) represent "mesh points" for \( y \) and \( t \), respectively.

Rearranging:

\[
A_rE_{r+1,s+1} + B_rE_{r,s+1} + C_rE_{r-1,s+1} \quad 1 \leq r \leq m \quad (4.22)
\]
where:

\[
A_r = \frac{bR_r \Delta t}{2 \Delta y^2} + \frac{bQ_r \Delta t}{4 \Delta y} \quad (4.21a)
\]

\[
B_r = -1 - \frac{2bR_r \Delta t}{2 \Delta y^2} = -1 - \frac{bR_r \Delta t}{\Delta y^2} \quad (4.22b)
\]

\[
C_r = \frac{bR_r \Delta t}{2 \Delta y^2} - \frac{bQ_r \Delta t}{4 \Delta y} \quad (4.21c)
\]

\[
D_r = \left(- \frac{bR_r \Delta t}{2 \Delta y^2} - \frac{bQ_r \Delta t}{4 \Delta y}\right) E_{r+1, s} + \left(-1 + \frac{bR_r \Delta t}{\Delta y^2}\right) E_{r, s} \quad (4.21d)
\]

\[
+ \left(- \frac{bR_r \Delta t}{2 \Delta y^2} + \frac{bQ_r \Delta t}{4 \Delta t}\right) E_{r-1, s+1}
\]

The above equations only hold for \( M \) points (from \( r = 1, 2, \ldots M \)).

At \( r = 0 \), i.e. \( y = 1 \) corresponding to the center of the torus and \( r = M + 1 \) i.e. \( y = 0 \) at the surface, the boundary conditions (equation 4.17 and equation 4.18) were used.

When \( s = 0 \) i.e., \( t = 0 \) we have the initial condition

\[
E = 0 \quad 0 \leq y \leq 1 \quad t = 0 \quad (4.19)
\]

The above boundary condition was used for the starting value for the solution.

At \( r = 0 \) or \( y = 1 \), equation (4.20a) does not exist. But it can be shown that at \( y = 1 \) equation (4.20) takes the following form by application of L'Hopital's rule (appendix F).

\[
\left. \frac{\partial E}{\partial t} \right|_{y=1} = 6b \left. \frac{\partial^2 E}{\partial y^2} \right|_{y=1} \quad (4.22)
\]
The above equation was replaced by the following implicit form:

\[
\frac{E_{o,s+1} - E_{o,s}}{\Delta t} = \frac{6b}{\Delta y^2} \left[ (E_{1,s+1} - 2E_{o,s+1} + E_{-1,s+1}) + (E_{1,s} - 2E_{o,s} + E_{1,s}) \right]
\]  

(4.23)

This is at the center of the torus, and because of symmetry we can assume:

\[
E_{-1,s} + E_{-1,s+1} = E_{1,s} + E_{1,s+1}
\]  

(4.24)

Equation (4.24) can also be obtained using boundary condition (4.18) in the following manner:

\[
\frac{\partial E}{\partial y} = 0 \quad y = 1 \quad t = t
\]  

(4.18)

An approximate difference form for the above boundary condition is:

\[
\frac{1}{4\Delta y} \left[ E_{1,s+1} - E_{-1,s+1} + E_{1,s} - E_{-1,s} \right] = 0
\]

or

\[
E_{-1,s} + E_{-1,s+1} = E_{1,s} + E_{1,s+1}
\]  

(4.24)

which is the same as equation 4.24. Substituting equation (4.24) in (4.23) and rearranging we have
\[
\left( -\frac{6b\Delta t}{\Delta y^2} \right) E_{1, s+1} + \left( 1 + \frac{6b\Delta t}{\Delta y^2} \right) E_{0, s+1} \\
= \frac{6b\Delta t}{\Delta y^2} E_{1, s} + \left( 1 - \frac{6b\Delta t}{\Delta y^2} \right) E_{0, s}
\]

(4.25)

or

\[
A_0 = -\frac{6b\Delta t}{\Delta y^2} \quad (4.25a)
\]

\[
B_0 = 1 + \frac{6b\Delta t}{\Delta y^2} \quad (4.25b)
\]

\[
D_0 = \frac{6b\Delta t}{\Delta y^2} E_{1, s} + \left( 1 - \frac{6b\Delta t}{\Delta y^2} \right) E_{0, s} \quad (4.25d)
\]

Now at the surface \( y = 0 \), \( r = M + 1 \), and equation (4.20) is reduced to

\[
\left. \frac{\partial E}{\partial t} \right|_{y=0} = \frac{\partial^2 E}{\partial y^2} \left|_{y=0} \right. - 5 \left. \frac{\partial E}{\partial y} \right|_{y=0} \quad (4.26)
\]

According to boundary condition (4.17)

\[
\left. \frac{\partial E}{\partial y} \right|_{y=0} = h(E-1) \quad y = 0 \quad t > 0 \quad (4.17)
\]

Equation 4.17 is reduced to

\[
\left. \frac{\partial E}{\partial t} \right|_{y=0} = \left. \frac{\partial^2 E}{\partial y^2} \right|_{y=0} - 5 \left. bh(E-1) \right|_{y=0} \quad (4.28)
\]

The corresponding implicit form of equation 4.28 is:

\[
\frac{E_{m+1, s+1} - E_{m, s+1}}{\Delta t} = \frac{b}{2\Delta y^2} \left[ (E_{m+2, s+1} - 2E_{m+1, s+1} + E_{m, s+1}) \right. \\
+ (E_{m+2, s} - 2E_{m+1, s} + E_{m, s}) \left. \right] - 5bh(E_{m+1, s} - 1) \quad (4.29)
\]
Now from boundary condition 4.17
\[
\frac{1}{4\Delta y} [ (E_{m+2, s+1} - E_m, s+1) + (E_{m+2, s} - E_m, s) ] = h(E_{m+1, s} - 1) \quad (4.30)
\]
or
\[
4\Delta y h (E_{m+1, s} - 1) + (E_m, s+1 + E_m, s) = E_{m+2, s+1} + E_{m+2, s} \quad (4.30a)
\]
Substituting equation (4.30a) in (4.29), the resulting rearranged expression is
\[
(1 + \frac{b\Delta t}{\Delta y^2}) E_{m+1, s+1} + \left( -\frac{\Delta t b}{\Delta y^2} \right) E_m, s+1 = \left( 1 - \frac{2\Delta t bh}{\Delta y} \right)
\]
\[- \frac{\Delta t b}{\Delta y^2} - 5bh\Delta t \right) E_{m+1, s} + \left( \frac{\Delta t b}{\Delta y^2} \right) E_m, s + \left( -\frac{2\Delta t bh}{\Delta y} - 5bh\Delta t \right) \quad (4.31)
\]
or
\[
B_{m+1} = 1 + \frac{b\Delta t}{\Delta y^2} \quad (4.31b)
\]
\[
C_{m+1} = -\frac{\Delta t b}{\Delta y^2} \quad (4.31c)
\]
\[
D_{m+1} = \left( 1 + \frac{2\Delta t bh}{\Delta y} - \frac{\Delta t b}{\Delta y^2} - 5bh\Delta t \right) E_{m+1, s} + \frac{\Delta t b}{\Delta y^2} E_m, s
\]
\[+ \left( -\frac{2\Delta t bh}{\Delta y} + 5bh\Delta t \right) E_{m-1, s} \quad (4.31d)
\]
Combining the equations (4.21), (4.25), (4.31) we have
\[
B_0 E_{0, s+1} + A_0 E_1, s+1 = D_0
\]
\[
C_1 E_{0, s+1} + B_1 E_1, s+1 + A_1 E_2, s+1 = D_1
\]
\[
C_2 E_1, s+1 + B_2 E_2, s+1 + A_2 E_3, s+1 = D_2 \quad (4.32)
\]
(4.32) is a system of equations with \( M + 2 \) unknown and \( M + 2 \)
equations which can be represented in the following matrix form:

\[
\begin{pmatrix}
B_0 & A_0 & 0 & \cdots & \cdots & 0 \\
C_1 & B_1 & A_1 & & & \\
& C_2 & B_2 & A_2 & & \\
& & \ddots & \ddots & \ddots & \\
& & & C_m & B_m & A_m \\
0 & \cdots & \cdots & \cdots & C_{m+1} & B_{m+1}
\end{pmatrix}
\begin{pmatrix}
E_0, s+1 \\
E_1, s+1 \\
\vdots \\
E_m, s+1 \\
E_{m+1}, s+1
\end{pmatrix}
=
\begin{pmatrix}
D_0 \\
D_1 \\
\vdots \\
D_m \\
D_{m+1}
\end{pmatrix}
\]

The above matrix is a tridiagonal matrix which can be solved by
the method of Thomas (14).

Now starting with \( s = 0 \), we can solve for different values of
\( E_s \) according to the size of the step, and at different times the con-
centration distribution was found throughout the droplet. The
average fraction extracted at different times was found by numerical
integration (see appendix C). The results are presented in graphical
form (fig. 4) in the next chapter.
V. RESULTS AND DISCUSSION

Computation of Eigenvalues. As described in the preceding chapter, the eigenvalues, $\lambda_n$, and coefficients, $B_n$, were calculated as a function of the modified continuous phase mass transfer coefficient, $h$, for $n = 1, 2, 3$ and $4$. The results are plotted in Figure 5.1 (also see Table 1). These results were obtained using the Runge-Kutta method. It can be easily observed that for a constant value of $h$, as $n$ increases the values of $\lambda_n$ increase rapidly, e.g. for $h = 1.0$, $\lambda_1 = 1.276$, $\lambda_2 = 9.19$ and $\lambda_3 = 33.35$. As $\lambda_n$ increases very rapidly, it is obvious from equation (3.41) that the values of $\lambda_n$ where $n>5$ will not affect the computation of $E_m$, the fraction extracted. This is particularly true at large values of $t$.

$$E_m = 1 - 2 \sum_{n=1}^{\infty} B_n^2 \exp (-\lambda_n bt)$$  \hspace{1cm} (3.41)

The first eigenvalue, $\lambda_1$, varies rapidly as a function of $h$, until the value of $h$ reaches 10, and then $\lambda_1$ remains nearly constant. The variation with $h$ in the case of second eigenvalue, $\lambda_2$, is relatively less than the variation of the $\lambda_1$. For the values of $h$ less than 0.1, the value of $\lambda_2$ increases slowly; as $h$ becomes greater than 0.1, $\lambda_2$ again reaches an approximately constant value when the value of $h$ becomes greater than 20. This behavior is consistent with the physical situation; as the value of modified continuous phase mass transfer coefficient, $h$, increases, the resistance to transfer
in the continuous phase becomes less and does not appreciably affect the eigenvalues.

The eigenvalues, \( \lambda_n \), were also obtained using Hamming's method (Table 2) to check the eigenvalues obtained by Runge-Kutta method. The results obtained coincide with the results of the Runge-Kutta method to within 2\%. The coefficients \( B_n \) for \( n = 1 \), are positive for all values of \( h \). For \( n = 2 \), \( B_n \), for all values of \( h \), are negative. For \( n = 3 \), \( B_n \), for \( h \geq 10 \) are negative and for \( h < 10 \) are positive. The coefficients \( B_n \), for \( n = 4 \), are negative for all values of \( h \). This strange behavior of \( B_n \) was carefully considered. The values of the coefficients, \( B_n \), calculated by the two methods also agreed with each other to within 2\%.

The space in the memory of the IBM-1620 (model 2) was limited and could not be used to calculate all the eigenvalues using Hamming's method for \( h = 100 \), which was not the case with the Runge-Kutta method. Therefore, the eigenvalues obtained by the Runge-Kutta method are recommended.

\( E_m \) vs. \( b t \). The fraction extracted, \( E_m \), was computed using eigenvalues and coefficients obtained by the Runge-Kutta and Hamming's methods. The results obtained by both techniques are in close agreement with each other. It can be observed from Figure 5.2 and Figure 5.3 that for particular values of \( bt \) the fraction extracted increases with an increase in the value of \( h \).
which is consistent with physical expectation. As the values of h get larger, the fraction extracted approaches unity at a lower value of bt. This is consistent with expectations because as values of h get larger, $k_c$ gets larger, and, therefore, the resistance to transfer in the continuous phase decreases. For the low values of bt, the fraction extracted remains approximately constant with time. As the value of bt increases and after a certain value of bt, the fraction extracted approaches unity asymptotically, which is expected physically.

The same family of curves was also obtained using the finite difference method (see figure 5.4). The only notable difference between these two sets of curves is that, as bt approaches zero, $E_m$ approaches zero in the case of the finite difference method, while in the case of the other two methods this is not observed. Physically when bt approaches zero, $E_m$ should approach zero. This implies that the results of the finite difference method are consistent with the physical situation at low values of bt, whereas the other results obtained in this work do not satisfy this requirement.

Comparison of Results with Grober and Elzinga and Banchero

Modification. The families of curves ($E_m$ vs. time factor) for Grober (7), Elzinga and Banchero (4), Wellek and Skelland (26) and the results in this work have a similar pattern. With the exception of the families of curves obtained by using the finite difference method (continued on p. 59)
<table>
<thead>
<tr>
<th>h</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
<th>$B_1$</th>
<th>$B_2$</th>
<th>$B_3$</th>
<th>$B_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>0.002</td>
<td>6.87</td>
<td>31.06</td>
<td>365</td>
<td>0.5073</td>
<td>-0.873(10)$^{-4}$</td>
<td>0.152(10)$^{-4}$</td>
<td>-0.814(10)$^{-6}$</td>
</tr>
<tr>
<td>0.002</td>
<td>0.004</td>
<td>6.88</td>
<td>31.06</td>
<td>365</td>
<td>0.5071</td>
<td>-0.178(10)$^{-3}$</td>
<td>0.303(10)$^{-4}$</td>
<td>-0.163(10)$^{-5}$</td>
</tr>
<tr>
<td>0.010</td>
<td>0.020</td>
<td>6.89</td>
<td>31.06</td>
<td>365</td>
<td>0.5053</td>
<td>-0.889(10)$^{-3}$</td>
<td>0.152(10)$^{-3}$</td>
<td>-0.816(10)$^{-5}$</td>
</tr>
<tr>
<td>0.05</td>
<td>0.096</td>
<td>6.98</td>
<td>31.07</td>
<td>365</td>
<td>0.4964</td>
<td>-0.443(10)$^{-2}$</td>
<td>0.757(10)$^{-3}$</td>
<td>-0.408(10)$^{-4}$</td>
</tr>
<tr>
<td>0.1</td>
<td>0.188</td>
<td>7.10</td>
<td>31.08</td>
<td>365</td>
<td>0.4859</td>
<td>-0.881(10)$^{-2}$</td>
<td>0.151(10)$^{-2}$</td>
<td>-0.815(10)$^{-4}$</td>
</tr>
<tr>
<td>0.5</td>
<td>0.785</td>
<td>8.03</td>
<td>32.5</td>
<td>366</td>
<td>0.4207</td>
<td>-0.414(10)$^{-1}$</td>
<td>0.750(10)$^{-2}$</td>
<td>-0.407(10)$^{-3}$</td>
</tr>
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<td>0.147(10)$^{-1}$</td>
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<td>-0.123</td>
<td>0.332(10)$^{-1}$</td>
<td>-0.201(10)$^{-2}$</td>
</tr>
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<td>-0.531(10)$^{-2}$</td>
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<td>396</td>
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<td>-0.121</td>
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<td>-0.120(10)$^{-1}$</td>
</tr>
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<td>407</td>
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<td>-0.410(10)$^{-1}$</td>
<td>-0.138(10)$^{-1}$</td>
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<td>2.779</td>
<td>20.04</td>
<td>94.7</td>
<td>411</td>
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<td>-0.141(10)$^{-1}$</td>
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<td>96.7</td>
<td>419</td>
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<td>96.8</td>
<td>420</td>
<td>0.2353</td>
<td>-0.111</td>
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<td>96.9</td>
<td>420</td>
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<td>$\infty$</td>
<td>2.816</td>
<td>20.49</td>
<td>97.1</td>
<td>421</td>
<td>0.2350</td>
<td>-0.111</td>
<td>-0.399(10)$^{-1}$</td>
<td>-0.142(10)$^{-1}$</td>
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</tbody>
</table>
### TABLE 2

**EIGENVALUES FOR WELLEK-SKELLAND MODIFICATION (BY HAMMING'S METHOD)**

<table>
<thead>
<tr>
<th>h</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
<th>$B_1$</th>
<th>$B_2$</th>
<th>$B_3$</th>
<th>$B_4$</th>
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<tbody>
<tr>
<td>0.001</td>
<td>0.002</td>
<td>6.96</td>
<td>31.9</td>
<td>369</td>
<td>0.5150</td>
<td>-0.882(10)^{-4}</td>
<td>0.151(10)^{-4}</td>
<td>-0.827(10)^{-6}</td>
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<tr>
<td>0.002</td>
<td>0.004</td>
<td>6.96</td>
<td>31.9</td>
<td>369</td>
<td>0.5148</td>
<td>-0.177(10)^{-3}</td>
<td>0.303(10)^{-4}</td>
<td>-0.166(10)^{-5}</td>
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<tr>
<td>0.010</td>
<td>0.019</td>
<td>6.98</td>
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<td>369</td>
<td>0.5129</td>
<td>-0.886(10)^{-3}</td>
<td>0.152(10)^{-3}</td>
<td>-0.829(10)^{-5}</td>
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<tr>
<td>0.10</td>
<td>0.185</td>
<td>7.18</td>
<td>32.1</td>
<td>369</td>
<td>0.4938</td>
<td>-0.878(10)^{-2}</td>
<td>0.151(10)^{-2}</td>
<td>-0.829(10)^{-4}</td>
</tr>
<tr>
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<td>8.11</td>
<td>32.8</td>
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<td>0.4289</td>
<td>-0.413(10)^{-1}</td>
<td>0.750(10)^{-2}</td>
<td>-0.414(10)^{-3}</td>
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<tr>
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<td>0.597(10)^{-1}</td>
<td>-0.541(10)^{-2}</td>
</tr>
<tr>
<td>10.0</td>
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<td>17.56</td>
<td>84.5</td>
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<td>-0.359(10)^{-1}</td>
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<td>19.38</td>
<td>91.5</td>
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<td>0.2483</td>
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<td>-0.123(10)^{-1}</td>
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<td>92.5</td>
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<td>0.2469</td>
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<td>-0.422(10)^{-1}</td>
<td>-0.130(10)^{-1}</td>
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<td>50.0</td>
<td>2.778</td>
<td>20.02</td>
<td>94.6</td>
<td>411</td>
<td>0.2442</td>
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<td>-0.143(10)^{-1}</td>
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<td>0.2430</td>
<td>-0.116</td>
<td>-0.418(10)^{-1}</td>
<td>-0.146(10)^{-1}</td>
</tr>
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<td>100.0</td>
<td>2.804</td>
<td>20.34</td>
<td>96.3</td>
<td>418</td>
<td>0.2421</td>
<td>-0.115</td>
<td>-0.416(10)^{-1}</td>
<td>-0.148(10)</td>
</tr>
</tbody>
</table>
Figure 5.1 Eigenvalue vs Continuous Phase Mass Transfer Coefficient
Figure 5.2 Fraction Extracted Versus Dimensionless Time. Solution Using Runge-Kutta Method
Figure 5.3 Fraction Extracted Versus Dimensionless Time. Solution Using Hamming’s Method.
Figure 5.4 Fraction Extracted Versus Dimensionless Time.
Solution By Finite Difference Method.
Figure 5.5 Fraction Extracted Versus Dimensionless Time. Not to be used for low values of bt. Solution by Wellek-Skelland (26).
Figure 5.6  Fraction Extracted Versus Dimensionless Time.
Solution for Grober Modification (7), Internally Stagnant Droplets.
Figure 5.7  Fraction Extracted Versus Dimensionless Time.
Solution for Elzinga and Banchero (4), Hadamard Internal Circulation Patterns.
for the Wellek-Skelland modification and the curves of Wellek and 
Skelland (26), $E_m$ does not approach zero as $bt$ approaches zero 
for all other families of curves. This is not consistent with the 
physical situation. This would imply that at lower value of $bt$ results 
obtained by finite difference method should be used and at larger 
value of $bt$ results obtained by Runge-Kutta method can be used.

One unusual behavior in the case of the Elzinga and Banchero 
model, which is not observed in other cases, is the intersection of 
various curves in the same families (see figure 5.7). This variation 
may be due to the difference in the means used to obtain their mathe-
matical solution. They obtained a solution with the aid of an elec-
tronic differential analyzer, i.e., an analog computer, while all 
other solutions were obtained by analytic or numerical methods using 
a digital computer.

Comparison with Wellek-Skelland Eigenvalues. It may be observed 
that eigenvalues obtained by Wellek (26) for his modification of the 
Handlos and Baron model (Table 3 in appendix E) and the values 
obtained by the author using the Runge-Kutta and Hamming's methods 
do not necessarily coincide. The first eigenvalue is generally in 
agreement within 5%. Since only $\lambda_1$ is important at large contact 
times, the difference in results should be negligible at large contact 
times. The results obtained for the Wellek-Skelland modification 
using the behavior of the curve is consistent with the physical
situation, i.e., $E_m$ approaches zero as $bt$ approaches zero and $E_m$ approaches unity as $bt$ approaches infinity. As the Wellek-Skeland relation was obtained for large contact time, Wellek-Skeland results should not be used for small value of $bt$, although it does appear to agree with the physical situation.

Comparison of Solutions by Different Methods. Solutions obtained by Runge-Kutta and Hamming's methods are in agreement with each other. The solution by the finite difference method is presented in figure 5.1. At lower values of $bt$, solutions obtained by Runge-Kutta and Hamming's methods are not in agreement with the solutions obtained by the finite difference method. But at the higher values of $bt$, all the solutions for $E_m$ approach unity, as expected. Now for $bt = 1$ and $h = 0.5$ as an arbitrary example:

- $E_m = 0.8345$ (Runge-Kutta method)
- $E_m = 0.832$ (Hamming's method)
- $E_m = 0.663$ (Finite difference method)
- $E_m = 0.750$ (Wellek-Skeland)

From the above it is clear that for Hamming's and Runge-Kutta methods the results agree with each other. The value obtained by Wellek-Skeland is low, and the value obtained by the finite difference method is even lower than the results of the Runge-Kutta method. A further comparison is made for specific droplet systems later in this chapter and in appendix D.
For the larger values of \( h (> 100) \) all the curves coincide with each other. This behavior is observed in all cases. The curves obtained at higher values of \( h (> 100) \) are in fair agreement with the solution obtained for the Handlos and Baron model (i.e. \( k_c \to \infty \), or no resistance to transfer in continuous phase). The eigenvalues obtained for the Handlos and Baron model (\( h = \infty \)) using the Runge-Kutta method are:

\[
\begin{align*}
\lambda_1 &= 2.816 \\
\lambda_2 &= 20.49
\end{align*}
\]

These values agree with the eigenvalue obtained for \( h = 10^{10} \). Handlos and Baron (8) found \( \lambda_1 = 2.88 \).

The Handlos and Baron model was also solved by the finite difference method for \( h \to \infty \) and the solution obtained when plotted coincided with the solution for \( h = 100 \).

**Computational Errors.** To calculate eigenvalues, Runge-Kutta and Hamming's methods were used. The interval of integration selected was 0.005 to keep the truncation error low. When the interval of integration was changed from 0.005 to 0.0025 for \( h = 1 \), the following results were obtained.
The results obtained for $\lambda_n$ and $B_n$ using two different intervals (0.005 and 0.0025) are in agreement with each other to within 0.5% as shown in table 5.3. For Hamming's method the truncation error was less than $5(10)^{-4}$. A double precision routine was used for the Runge-Kutta method to keep the round-off error to a minimum.

To obtain a solution by the finite difference method the implicit form suggested by Crank and Nicholson was used to make the solution stable. The interval selected in the $y$ direction was 0.1, and in the $bt$ direction was 0.005 in most cases ($h$ ranging from 0.01 to 10).

For this case

$$\beta = \frac{bA_t}{\Delta y^2} = \frac{0.005}{(.1)^2} = 0.5$$

For this value of $\beta$, solution of a parabolic partial differential equation satisfies the stability and convergence criteria. For the implicit representation there is no restriction.
on the size of $\beta$. For all values of $\beta$, the implicit method is stable, but the explicit method is not stable for all values of $\beta$. When the first eight digits were used in the computation, the results obtained for $E_m$ were negative. Results obtained using the double precision and triple precision routine were the same and were not negative. To keep the round-off error low, a double precision routine was used which made a significant difference in the results. For the values of $h = 100$, the interval selected in the $bt$ direction was 0.0005 to keep computational errors low.

Application of the Results. To illustrate the application of solutions obtained by different methods, consider the following two single droplet systems. In the first, most of the resistance to mass transfer is in the droplet phase. In the second, the resistance is about half in the continuous phase and half in the dispersed phase.

Consider a drop of benzene saturated with acetic acid, 0.503 cm in diameter, rising in a large quantity of water with a velocity of 11.3 cm/sec as reported by Handlos and Baron (8). (Details of the calculations are in appendix D). For the above system, $N_{Re} = 595$. Using the Garner and Tayeban correlation (Equation 2.24) for the continuous phase mass transfer coefficient:

$$k_C = 0.0171 \text{ cm/sec}$$

$$h = 63$$

$$b = 0.108$$
The time of contact is 8.5 sec. Therefore

\[ bt = 0.92 \]

The following results are obtained:

\[ K_d = 0.0218 \text{ cm/sec} \] (using Figure 2, Runge-Kutta)

\[ K_d = 0.0278 \text{ cm/sec} \] (using Figure 4, Finite difference)

\[ K_d = 0.0218 \text{ cm/sec} \] (Wellek-Skelland, Rayleigh-Ritz)

\[ K_d = 0.0253 \text{ cm/sec} \] (Handlos and Baron, assuming \( h \to \infty \))

\[ K_d = 0.0213 \text{ cm/sec} \] (observed experimentally)

The above results show satisfactory agreement with each other. However, it appears that the results obtained by Runge-Kutta, Wellek-Skelland and Handlos and Baron compare very favorably with the experimental value of \( K_d \). In this case, as reported by Handlos and Baron, the resistance in the continuous phase was negligible.

Let us consider another case where resistance in both phases is nearly the same. In this case, a benzene drop 0.481 cm containing acetone rises with the velocity of 10.6 cm/sec through a continuous phase of water.

\[ N_{Re} = 531, \text{ and using the Garner and Tayeban correlation the continuous phase mass transfer coefficient is:} \]

\[ k_c = 0.013 \text{ cm/sec} \]

\[ h = 0.91 \]

\[ b = 0.1051 \]
The time of contact is equal to 9.41 sec. Therefore,

\[ bt = 0.99 \]

The following results are obtained:

\[
\begin{align*}
K_d &= 0.0084 \text{ cm/sec} \quad \text{(using Figure 2, Runge-Kutta)} \\
K_d &= 0.0064 \text{ cm/sec} \quad \text{(using Figure 4, Finite difference method)} \\
K_d &= 0.0089 \text{ cm/sec} \quad \text{(Wellek-Skelland, Rayleigh-Ritz method)} \\
K_d &= 0.0109 \text{ cm/sec} \quad \text{(Handlos and Baron, assuming h \to \infty)} \\
K_d &= 0.0094 \text{ cm/sec} \quad \text{(observed experimentally)}
\end{align*}
\]

The above results show that the results obtained by the Runge-Kutta and finite difference methods differ considerably from each other. In this case, the Runge-Kutta and Wellek-Skelland results are slightly lower than experimental value while the results obtained from the Handlos and Baron model are higher. In this case the finite difference method gives very low results.

Although there is no experimental observation for \( K_d \) at very short contact times, let us consider the case of an arbitrary contact time, i.e.

\[ bt = 0.099 \]

which is one tenth that used in the above case.

The following results are obtained:

\[
\begin{align*}
K_d &= 0.0129 \text{ cm/sec} \quad \text{(using Figure 2, Runge-Kutta method)} \\
K_d &= 0.0076 \text{ cm/sec} \quad \text{(using Figure 4, Finite difference method)}
\end{align*}
\]
It is clear from the above example that there is a significant difference between the results obtained by the Runge-Kutta and finite difference methods.

At the short contact time the difference between the Runge-Kutta method and the finite difference method is approximately 40%. Figure 4 (finite difference method) agrees with the physical situation; therefore, the results obtained from figure 4 (finite difference method) should be considered more accurate.

The value of $K_{dr}$ obtained using the Wellek-Skelland (26) relation will not change with changes in contact time as the relation is independent of contact period. This is because it was derived for large contact times using the first eigenvalue, even though the higher values were calculated. This implies that at a lower contact time ($bt < 0.5$) higher eigenvalues should be considered. Hence the application of the Wellek-Skelland relation is restricted to the higher values of $bt$. The values obtained for $K_{dr}$ for the higher values of $bt$ by Wellek-Skelland relation and by the author using Runge-Kutta method are in agreement with each other and with the observed value.

The restrictions apply to the relations obtained by the Runge-Kutta method because the results obtained for $bt < 0.5$ remain constant instead of asymptotically approaching zero. At short contact times, although there is no experimental evidence, the results obtained using finite difference method should be considered more accurate as the fraction extracted does approach zero.
**Recommendations:**

The following recommendations are suggested for further investigation in this field:

1. The Wellek-Skelland modification and the Handlos and Baron model should be solved in toroidal coordinates. (see appendix H.)

2. The results obtained here by the theoretical treatment should be compared with experimental data in more detail.
VI. CONCLUSION

The purpose of this study was to attempt to describe more accurately the modification of the Handlos and Baron model for mass transfer to droplets for turbulent internal circulation which considers the effect of a finite continuous phase resistance.

The investigation was divided into two projects (1) to use some method other than the Rayleigh-Ritz variational technique in order to check the accuracy of eigenvalues, $\lambda_n$, calculated by Wellek and Skelland and in addition to determine the constants $B_n$ in the series solution and (2) to obtain the solution for the Wellek-Skelland modification by a finite difference method. Ideally the results of these two methods for calculating the dispersed phase mass transfer coefficient should agree with each other.

The following conclusions are presented following the analysis of results:

1. The eigenvalues, $\lambda_n$, and the coefficients, $B_n$, obtained by the Runge-Kutta and Hamming's methods are in agreement with each other, within 2% and 2% to 4%, respectively.

2. The eigenvalues obtained by Wellek using the Rayleigh-Ritz technique and by the author using the Runge-Kutta method are in agreement for the first eigenvalues within 5%, but the higher eigenvalues differ considerably. It should be noted, however, that the Rayleigh-Ritz variational technique gives a good approximation for only lower eigenvalues.
3. At lower values of $bt$, solutions obtained by the Runge-Kutta and the Hamming's methods are not in agreement with the solutions obtained by finite difference method. In the case of the finite difference method $E_m$ approaches zero as $bt$ approaches zero while this is not observed in the case of the Runge-Kutta method. The results obtained by the finite difference method agree with the physical situation.

4. The results obtained for $h > 100$ for the Wellek-Skelland modification using the Runge-Kutta method and the finite difference method coincide with results obtained for the Handlos and Baron model using $h = \infty$ which implies that for $h = 100$ the solutions may be treated as $k_c \to \infty$ (i.e., $h = \infty$).

5. The families of curves of $E_m$ versus $bt$ with varying $h$ are similar in nature for the Grober (stagnant drop), the Elzinga and Banchero (laminar circulation) and the modification of the Handlos and Baron model as calculated in this work. That is as $bt$ approaches to zero, $E_m$, the fraction extracted, does not approach zero. This is not consistent with the physical expectation.

6. The families of curves obtained by the finite difference method and by the Wellek-Skelland relation are almost identical and are also in agreement with the physical situation. That is, as $bt$ approaches zero, $E_m$ approaches zero; and as $bt$ assumes higher values, $E_m$ approaches unity. Therefore, these results are more representative of the actual physical situation.
7. The values of $K_{dr}$, overall mass transfer coefficient, at higher values of $bt$ obtained using the results from the Runge-Kutta method and using the Wellek-Skelland relation agree with the observed value of $K_{dr}$ to within 1.5% and 2%, respectively. But results obtained by the finite difference method do not agree with observed values of $K_{dr}$ (per cent average deviation 20%). For the short contact times, the values of $K_{dr}$ obtained using results from the Runge-Kutta method and finite difference method differ considerably (approximately 40%) from each other. Therefore, at the higher values of $bt$ (> 0.5) the results from the Runge-Kutta method or the Wellek-Skelland relation should be used. For short contact times (or values of $bt$ < 0.5), the results obtained using the finite difference method should be considered more accurate; although it should be recognized that this recommendation should be compared with the experimental values of $K_{dr}$ which will have to be obtained from future experiments.
VII. APPENDICES
Appendix A

General solution of equation 3.19 will be outlined here. The equation 3.19 is:
\[
\frac{\partial \phi}{\partial t} = \frac{b}{1-y} \frac{\partial}{\partial y} \left[ (1 - 5y + 10y^2 - 6y^3) \frac{\partial \phi}{\partial y} \right] \quad (3.19)
\]

and relevant boundary conditions are:
\[
\begin{align*}
\frac{\partial \phi}{\partial y} &= h(C - C_i), \quad y = 0, \quad t > 0 \\
\frac{\partial \phi}{\partial y} &= 0, \quad y = 1, \quad t = t \\
C &= C_0, \quad 0 \leq y \leq 1, \quad t = 0
\end{align*}
\]

By the method of separation of variables, the solution is assumed to be:
\[
C(y, t) = T(t) \cdot Y(y) \quad (3.26)
\]

Therefore:
\[
\frac{\partial \phi}{\partial t} = T'(t) \cdot Y(y) \quad (A.2)
\]

and
\[
\frac{\partial \phi}{\partial y} = T(t) \cdot Y'(y) \quad (A.3)
\]

Substituting equations (A.2) and (A.3) in equation 3.19 and rearranging we have:
\[
\frac{T'(t)}{bT(t)} = \frac{1}{Y(y) \cdot (1-y)} \frac{d}{dy} \left[ (1 - 5y + 10y^2 - 6y^3) \frac{dY}{dy} \right] = -\lambda \quad (A.4)
\]

where \( \lambda = \text{constant} \).

The constant \( \lambda \) may be either positive, negative or zero.
Equation (A. 4) will give the following two ordinary differential equations:

\[ T'(t) + \lambda b T(t) = 0 \]  \hspace{1cm} (A. 5)

\[ \frac{d}{dy} \left( P(y) \frac{dY}{dy} \right) - Q(y) \frac{dY}{dy} = 0 \]  \hspace{1cm} (A. 6)

where

\[ P(y) = 1 - 5y + 10y^2 - 6y^3 \]

\[ Q(y) = 1 - y \]

The solution of equation (A. 5) is

for \( \lambda = \) positive value

\[ T(t) = A \exp(-b \lambda t) \]  \hspace{1cm} (A. 7)

for \( \lambda = \) negative value

\[ T(t) = B \exp(b \lambda t) \]  \hspace{1cm} (A. 8)

for \( \lambda = 0 \)

\[ T(t) = D \]  \hspace{1cm} (A. 9)

where \( A, B, \) and \( D \) are constants.

Also there will be 3 solutions for equation (A. 6)

for \( \lambda = \) positive value

\[ Y(y) = Y(y) \]  \hspace{1cm} (A. 10)

for \( \lambda = \) negative value

\[ Y(y) = Y^*(y) \]  \hspace{1cm} (A. 11)

for \( \lambda = 0 \)

\[ Y(y) = \int \frac{b'}{1 - 5y + 10y^2 - 6y^3} \, dy \]  \hspace{1cm} (A. 12)
Therefore, the total solution is

\[ C(y,t) = \sum_{n=1}^{\infty} b_n Y_n \exp(-b_\lambda_n t) + \Sigma' b'_n Y'_n \exp(b'_\lambda_n t) \]

\[ + \int \frac{b'}{1 - 5y + 10y^2 - 6y^3} \, dy \]

(A. 13)

It is clear from the above equation (A. 13) that for large values of \( t \) (i.e., \( t \to \infty \)), \( C(y, \infty) = \infty \) which is not true physically. \( C(y, \infty) \) should approach \( C_i \), the equilibrium concentration (where \( C_i = mC_c \)). Therefore, the second term in equation (A. 13) is omitted (or \( b'_n = 0 \)).

When \( t \to \infty \), the following is obtained

\[ C(y, \infty) = C_i \int \frac{b'}{1 - 5y + 10y^2 - 6y^3} \, dy \]

or

\[ C_i = b' Y''(y) + b'' \]

(A. 14)

where \( b' \) and \( b'' \) are constants of integration.

As \( C_i \) is constant, \( b' = 0 \) and \( b'' = C_i \)

Therefore, equation (A. 13) reduces to

\[ C(y,t) = \sum_{n=1}^{\infty} b_n Y_n \exp(-b_\lambda_n t) + C_i \]

(A. 15)

In this work it is assumed that the concentration of solute in the continuous phase is very dilute, i.e. \( C_c = 0 \) and therefore

\[ C_i = 0 \]

As a consequence the final solution is:

\[ C(y,t) = \sum_{n=1}^{\infty} b_n Y_n \exp(-b_\lambda_n t) \]

(A. 16)
As $C_i = 0$ the boundary condition (A. 1) will reduce to

$$\frac{\partial c}{\partial y} = hc \quad y = 0 \quad t > 0$$  

(3.24)

Equation (A. 6) is:

$$\frac{d}{dy} \left( P(y) \frac{dY}{dy} \right) - Q(y) \lambda Y(y) = 0$$  

(A. 6)

and relevant boundary conditions are

$$\frac{dY}{dy} = hY, \quad y = 0$$  

(A. 17)

$$\frac{dY}{dy} = 0, \quad y = 1$$  

(A. 18)

Equation (A. 6), (A. 17) and (A. 18) belong to the class of Sturm-Liouville problems (2). A Sturm-Liouville system has an infinite number of eigenvalues

$$\lambda_1 < \lambda_2 < \lambda_3 \ldots$$

and corresponding eigenfunctions $Y_n$

Now from boundary condition (3.22),

$$C(0, y) = C_0 = \sum_{n=1}^{\infty} b_n Y_n$$  

(A. 19)

From the orthogonal properties of Sturm-Liouville systems:

$$b_n = C_0 \int_0^1 (1-y) Y_n dy = B_n C_0$$  

(A. 20)

where

$$B_n = \int_0^1 (1-y) Y_n dy$$

$$C(y, t) = C_0 \sum_{n=1}^{\infty} B_n Y_n \exp(-b \lambda_n t)$$  

(A. 21)
Appendix B

Equation 4.4 will be developed here. Equation 3.28 is:

\[ \frac{d}{dy} \left( (1 - 5y + 10y^2 - 6y^3) \frac{dY}{dy} \right) + \lambda (1 - y) Y = 0 \tag{3.28} \]

rearranging we have:

\[ \frac{d^2Y}{dy^2} = -\frac{\lambda Y}{(6y^2 - 4y + 1)} - \frac{(18y^2 - 20y + 5)}{(y - 1)(6y^2 - 4y + 1)} \frac{dY}{dy} \tag{B.1} \]

and relevant boundary conditions are:

\[ Y'(0) = \lambda Y \tag{B.2} \]
\[ Y'(1) = 0 \tag{B.3} \]
\[ Y(1) = 2 \tag{B.4} \]

Equation B.1 has a regular singular point at \( y = 1 \). \( Y(y) \) can also be represented by the following generalized series (9) where \( y_0 = 1 \).

\[ Y = \sum_{n=1}^{\infty} a_n(y - y_0)^n \tag{B.5} \]
\[ Y' = \sum_{n=1}^{\infty} a_n(n-1)(y - y_0)^{n-1} \tag{B.6} \]
\[ Y'' = \sum_{n=2}^{\infty} a_n(n-1)(y - y_0)^{n-2} \tag{B.7} \]

Applying boundary condition B.3 to equation B.6 we have:

\[ Y'(1) = 0 = a_1 \tag{B.8} \]

and at \( y = 1 \)

\[ Y'' = 2a_2 \tag{B.9} \]
and using boundary condition B.4

\[ Y(1) = a_0 = 1 \quad (B.10) \]

Rearranging equation B.6 we have

\[ \frac{Y'}{(y-y_0)} = \sum_{n=1}^{\infty} n a_n (y-y_0)^{n-2} \quad (B.11) \]

or

\[ \left( \frac{Y}{(y-y_0)} \right)_{y=1} = 2a_2 \quad (B.12) \]

Substituting equations B.10 and B.12 in equation B.1, we have:

\[ \frac{d^2Y}{dy^2} (1) = -\frac{\lambda}{3} - 2a_2 \quad (B.13) \]

And combining equation B.13 and B.9 we get

\[ a_2 = -\frac{\lambda}{12} \quad (B.14) \]

substituting equation B.14 in B.9 we get:

\[ \frac{d^2Y}{dy^2} (1) = -\frac{\lambda}{6} \quad (B.15) \]
Appendix C

The finite difference method described in chapter IV gives $E'_m$, fraction extracted, as the function of $y$, which also is a function of time. To get average $E'_m$ as a function of time the following procedure was adopted.

$$E'_m = \frac{C_o - C}{C_o} \quad (C. 1)$$

Now if $\bar{C}$ represents average concentration in drop, then

$$\bar{C} = \frac{\int_0^V C dV}{\int_0^V dV} \quad (C. 2)$$

Now

$$E_m = \frac{C_o - \bar{C}}{C_o} = 1 - \frac{\bar{C}}{C_o} \quad (C. 3)$$

From equation C. 1

$$C = C_o(1 - E'_m) \quad (C. 1a)$$

Substituting in equation C. 3, we get

$$E_m = 1 - \frac{\int_0^V (1 - E'_m) dV}{\int_0^V dV} \quad (C. 4)$$

or in terms of $y$

$$E_m = 1 - 2 \int_0^1 (1 - E'_m)(1 - y) dy \quad (C. 5)$$
Appendix D

In this section the use of figures 2, 4 to calculate the overall mass transfer coefficient, $K_d$, will be shown for two different droplet systems.

1. System: Acetic acid, water, benzene
2. System: Acetone, water, benzene

Temperature of systems = 25°C ± 0.1

1. Consider a drop of benzene saturated with acetic acid, 0.503 in diameter, rising in large quantity of water with velocity of 11.3 cm/sec as reported by Handlos and Baron.

\[
\mu_c = 0.95 \text{ c. p.} (19)
\]

\[
\mu_d = 0.60 \text{ c. p.} (19)
\]

\[
\rho_c = 0.998 \text{ gm/cu. cm.} (19)
\]

\[
D_{ab} = 1.58 \times 10^{-5} \text{ sq. cm/sec (calculated using Wilke and Chang relation)}
\]

\[
m = 0.023 \text{ distribution coefficient}
\]

Evaluation of $k_c$:

The $N_{Re}$ for this droplet is 595, which suggests that the Garner and Tayeban correlation is applicable, (equation 2.24).

\[
k_c = \frac{D_{ab}}{d_e} \left[ 50 + 0.0085 (N_{Re})^{1.0} (N_{Sc})^{0.7} \right]
\]

\[
= \frac{1.58 \times 10^{-5}}{0.503} \left[ 50 + 0.0085 (595) (602)^{0.7} \right]
\]

\[
= 0.0171 \text{ cm/sec}
\]
Evaluation of $h$:

\[ h = \frac{512 k_c (1 + \mu_d / \mu_c)}{\mu u} \]

\[ = \frac{512 (0.0171) (1 + 0.6/0.95)}{(0.023) (11.3)} \]

\[ = 63 \]

\[ b = \frac{u}{128 (1 + \mu_d / \mu_c) d_e} \]

\[ = \frac{11.3}{128 (1 + 0.6/0.95) (0.503)} \]

\[ = 0.108 \]

For an assumed distance of 100 cms, the contact time

\[ t = \frac{100}{11.3} = 8.5 \text{ sec} \]

\[ b.t = (0.108) (8.5) = 0.92 \]

From figure 2

\[ E_m = 0.895 \]

\[ k_d = -d_e / 6t \ln (1 - E_m) \]

\[ = - \frac{0.503}{(6) (8.5)} \ln (0.105) \]

\[ = 0.0224 \text{ cm/sec} \]

$k_d$ (using the Wellek and Skelland modification):

\[ k_d = \frac{u \lambda_1}{768 (1 + \mu_d / \mu_c)} \]

\[ \lambda_1 = 2.848 \text{ (see appendix F, table 3)} \]

\[ k_d = \frac{(2.848) (11.3)}{768 (1 + 0.6/0.95)} \]
The document contains a mathematical derivation and explanation of certain physical phenomena. It starts by calculating a constant $k_c$ using figure 4:

From figure 4, $E_m = 0.94$

$$k_d = \frac{-d_e}{6t} \ln(1 - E_m)$$
$$= \frac{-0.503}{(6)(8.5)} \ln(0.06)$$
$$= -(0.00985)(-2.81)$$
$$= 0.0277$$

Now

$$\frac{1}{K_d} = \frac{1}{k_d} \pm \frac{1}{k_c}$$

$K_d = 0.0218 \text{ cm/sec}$ (using Figure 2, Runge-Kutta)

$K_d = 0.0278 \text{ cm/sec}$ (using Figure 4, Finite difference)

$K_d = 0.0218 \text{ cm/sec}$ (Wellek-Skelland, Rayleigh-Ritz)

$K_d = 0.0253 \text{ cm/sec}$ (Handlos and Baron, assuming $h \to \infty$)

$K_d = 0.0213 \text{ cm/sec}$ (observed experimentally)

2. Let us consider another case where a benzene drop, containing acetone rises with velocity of 10.6 cm/sec, 0.481 cm in diameter

$$D_{aw} = 1.121 \times 10^{-5} \text{ sq cm/sec}$$

$$k_c = \frac{D_{aw}}{d_e} \left\{ \frac{50 + 0.0085 \left( \frac{(0.481)(10.6)(0.998)}{(0.0095)} \right)}{(0.998)(1.121 \times 10^{-5})} \right\}^{0.7}$$
\[ 2.33 \times 10^{-5} \times 50 + 0.0085(535)(85)^{0.7} \]
\[ = 2.33 \times 10^{-5}(50 + 510) \]
\[ = 0.013 \text{ cm/sec} \]

Evaluation of \( h \):
\[ h = \frac{512 k_c (1 + \mu_d/\mu_c)}{mu} \]
\[ = \frac{(512)(0.013)(1 + 0.006/0.0095)}{(0.899)(10.6)} \]
\[ = 0.91 \]

\[ b = \frac{u}{128(1 + \mu_d/\mu_c) d_e} \]
\[ = \frac{10.6}{128(1 + 0.006/0.0095) 0.481} \]
\[ = 0.1051 \]

For a distance of 100 cms the contact time is:
\[ t = \frac{100}{10.6} \]
\[ t = 9.41 \text{ sec} \]
\[ (b) (t) = (9.41)(0.1051) = 0.99 \]

From figure 2 for \( h = 0.91 \)
\[ E_m = 0.945 \]
\[ k_d = -\frac{d}{6t} \ln (1 - E_m) \]
\[ = -\frac{0.481}{6(9.41)} \ln (1 - 0.945) \]
\[ = 0.02 \text{ cm/sec} \]

\( k_d \) by Wellek and Skelland:
\[ k_d = \frac{u \lambda_1}{768 \left( 1 + u_d/u_c \right)} \]

\[ \frac{(2.2) (10.3)}{768 \left( 1 + 0.006/0.0095 \right)} = 0.0228 \text{ cm/sec} \]

\( k_d \) by finite difference method:

\[ E_m = 0.775 \]

\[ k_d = -\frac{d}{6t} \ln (1 - E_m) \]

\[ = -\frac{0.481}{6 (9.41)} \ln (1 - 0.74) \]

\[ = 0.0125 \text{ cm/sec} \]

Now

\[ \frac{1}{K_d} = \frac{1}{k_d} + \frac{1}{k_c} \]

\[ K_d = 0.0084 \text{ cm/sec} \quad \text{(using Figure 2, Runge-Kutta)} \]

\[ K_d = 0.0064 \text{ cm/sec} \quad \text{(using Figure 4, Finite difference)} \]

\[ K_d = 0.0089 \text{ cm/sec} \quad \text{(Wellek-Skelland, Rayleigh-Ritz)} \]

\[ K_d = 0.0109 \text{ cm/sec} \quad \text{(Handlos and Baron, assuming } h \to \infty) \]

\[ K_d = 0.0094 \text{ cm/sec} \quad \text{(observed experimentally)} \]

Although there is no experimental observation for very short contact time, let us consider an assumed length of 10 cm for the second case.

\[ bt = 0.099 \]


\[ E_m = 0.75 \quad \text{(from figure 2, Runge-Kutta)} \]
\[ k_d = -\frac{d}{6t} \ln\left(1 - E_m\right) \]
\[ = -\frac{0.481}{6(0.941)} \ln(0.25) \]
\[ = 0.118 \text{ cm/sec} \]

From figure 4

\[ E_m = 0.15 \]
\[ k_d = \frac{0.481}{6(0.941)} \ln\left(1 - 0.15\right) \]
\[ = 0.0138 \]

\[ K_d = 0.0129 \text{ cm/sec} \quad \text{(using figure 2, Runge-Kutta)} \]
\[ K_d = 0.0076 \text{ cm/sec} \quad \text{(using figure 4, Finite difference)} \]

The above example shows that there is a significant difference for shorter contact time between the two solutions.
Appendix E

TABLE E. 1 EIGENVALUES AND COEFFICIENTS FOR STAGNANT DROPS DUE TO CROVER (7)

<table>
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<tr>
<th>$\frac{h_0d}{k}$</th>
<th>$\psi_1$</th>
<th>$\psi_2$</th>
<th>$\psi_3$</th>
<th>$\psi_4$</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$A_4$</th>
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<td>8.069</td>
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### TABLE E.3

EIGENVALUES FOR HANDLOS AND BARON MODEL CALCULATED BY WELLEK AND SKELLAND (26)

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<td>41.6</td>
<td>302</td>
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<tr>
<td>1.</td>
<td>1.980</td>
<td>14.27</td>
<td>45.4</td>
<td>304</td>
</tr>
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<td>2.5</td>
<td>2.445</td>
<td>19.54</td>
<td>55.9</td>
<td>311</td>
</tr>
<tr>
<td>5.</td>
<td>2.674</td>
<td>23.42</td>
<td>77.2</td>
<td>322</td>
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<tr>
<td>7.</td>
<td>2.708</td>
<td>23.76</td>
<td>80.0</td>
<td>327</td>
</tr>
<tr>
<td>10</td>
<td>2.731</td>
<td>23.72</td>
<td>78.6</td>
<td>332</td>
</tr>
<tr>
<td>25</td>
<td>2.821</td>
<td>25.26</td>
<td>97.4</td>
<td>355</td>
</tr>
<tr>
<td>50</td>
<td>2.847</td>
<td>25.54</td>
<td>99.5</td>
<td>366</td>
</tr>
<tr>
<td>70</td>
<td>2.850</td>
<td>25.24</td>
<td>91.2</td>
<td>365</td>
</tr>
<tr>
<td>100</td>
<td>2.852</td>
<td>24.88</td>
<td>83.5</td>
<td>364</td>
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<td>250</td>
<td>2.861</td>
<td>24.85</td>
<td>80.9</td>
<td>367</td>
</tr>
<tr>
<td>500</td>
<td>2.864</td>
<td>24.76</td>
<td>78.8</td>
<td>367</td>
</tr>
<tr>
<td>700</td>
<td>2.864</td>
<td>24.64</td>
<td>77.0</td>
<td>366</td>
</tr>
<tr>
<td>1000</td>
<td>2.865</td>
<td>24.56</td>
<td>75.8</td>
<td>366</td>
</tr>
<tr>
<td>$\infty$</td>
<td>2.866</td>
<td>24.58</td>
<td>75.6</td>
<td>367</td>
</tr>
</tbody>
</table>
Appendix F

Equation 4.22 will be developed in this section. Equation 4.20 is:

\[
\frac{\partial E}{\partial t} = b(1 - 4y + 6y^2) \frac{\partial^2 E}{\partial y^2} + b \left( \frac{-5 + 20y - 18y^2}{1 - y} \right) \frac{\partial E}{\partial y}
\]

\[= b \frac{\partial^2 E}{\partial y^2} + b \frac{\partial E}{\partial y}
\]

where \( R(y) = 1 - 4y + 6y^2 \)

\[Q(y) = \frac{-5 + 20y - 18y^2}{1 - y}
\]

Now at \( y = 1 \) we have

\[Q(1) \frac{\partial E}{\partial y} = 0 \]

which is indeterminant. So using L'Hopital's rule

\[Q(y) \frac{\partial E}{\partial y} = \frac{(20 - 36y) \frac{\partial E}{\partial y} + (-5 + 20y - 18y^2) \frac{\partial^2 E}{\partial y^2}}{-1}
\]

Now at \( y = 1 \)

\[Q(1) \frac{\partial E}{\partial y} = 3 \frac{\partial^2 E}{\partial y^2}
\]

Substituting equation F. 2 in equation 4.20 at \( y = 1 \), we have:

\[\frac{\partial E}{\partial t} \bigg|_{y=1} = 6 \frac{\partial^2 E}{\partial y^2} \bigg|_{y=1}
\]

which is not indeterminant.
Appendix G

Solution by Finite Difference Method (flow chart)

*DIMENSION H(25), R(25), W(25)

*DIMENSION A(20), C(21), E(20), D(21), F(22), E(21), Y(21)

***READ 100, DY, DT, R, FH, N

***PRINT 101, FH, DT, DY

I

M = ABSF(1. / DY) + 1.0

M = M - 1

MB = M + 1

I

+---------------------+

DO

+---------------------+

2

E(I) = 0.0

Y(I) = 1.0

I

+---------------------+

DO

+---------------------+

3

Y(I+1) = Y(I) + DY

I

T = 0.0

I

+---------------------+

DO

+---------------------+

1

I

K = 1, N

+---------------------+

A(I) = -6. * R * DT / (DY**2)

G(I) = 1. + 6. * R * DT / (DY**2)

D(I) = 6. * R * DT * E(2) / (DY**2) + 1.

E(I) = -6. * R * DT / (DY**2) * E(1)
DO 11  I=1,MA  
  
I K = K - 1  
I F(K) = H(K) - R(K) * F(K+1)  
  
11 CONTINUE  
  
IT = T + DT  
IBT = B * T  
  
DO 5  I=1,M  
  
I E(I) = F(I)  
  
5 CONTINUE  
  
I S1 = 0.0  
I S2 = 0.0  
I S3 = 0.0  
I S1 = S1 + (1. - E(I)) * (1. - Y(I)) + (1. - E(M)) * (1. - Y(M))  
  
7 CONTINUE  
  
I S2 = S2 + (1. - E(I)) * (1. - Y(I))  
I MN = MA - 1
I
-----------
+ DO +
+++++++  I = 3, HN, 2 +
+ I +
I

R  ++++++++ I S3 = S3 + (1. - E(I)) * (1. - Y(I))  I
+  I HA = ABSF(DY)  I
+  I SIM = HA * (S1 + 4. * S2 + 2. * S3) / 3.  I
+  I EV = 1. - 2. * SIM  I

I

***PRINT 103, BT, EV
+
1 ++++++++CONTINUE

CALL EXIT

100  FORMAT(4F10.5, I10)
103  FORMAT(F12.3, F18.6)
101  FORMAT(4F18.8)

END
C SOLUTION OF HANDLOS AND BARON MODEL BY FINITE-DIFFERENCE

DIMENSION H(25),R(25),W(25)
DIMENSION A(20),B(21),C(20),D(21),F(22),E(21),Y(21)
READ 100,DY,DT,B,FH,N
PRINT 101,FH,DT,DY
M=ABS(1./DY)+1.0
MA=M-1
MB=M+1
DO 2 I=1,M
2 E(I)=0.0
Y(I)=1.0
DO 3 I=1,MA
3 Y(I+1)=Y(I)+DY
T=0.0
DO 1 IK=1,N
A(I)=-6.*B*DT/(DY**2)
G(I)=1.+6.*B*DT/(DY**2)
C(I)=6.*B*DT*E(2)/(DY**2)+(1.-6.*B*DT/(DY**2))**E(1)
DO 4 I=2,MA
P=6.*Y(I)**2-4.*Y(I)+1.0
Q=1.-5.+20.*Y(I)-18.*Y(I)**2)/(1.-Y(I))
A(I)=DT*B*P/(2.*DY**2)+DT*B*Q/(4.*DY)
C(I)=DT*P*B/(2.*DY**2)-DT*B*Q/(4.*DY)
G(I)=DT*B*P/(DY**2)-1.0
D(I)=E(I+1)*(-A(I))+E(I)*((DT*P*B/(DY**2)-1.0)+E(I-1)*(-C(I))
4 CONTINUE
C(I)=DT*B/(DY**2)
C(I)=1.+DT*B/(DY**2)
D(M)=(1.+2.*FH*DT*B/DY-5.*B*DT*FH)*E(M)
D(N)=D(M)+1.*DT*B*E(MA)/(DY**2)-5.*B*DT*FH/DY+5.*B*DT*FH
W(1)=G(1)
H(1)=D(1)/W(1)
DO 10 I=2,M
R(I-1)=A(I-1)/W(I-1)
W(I)=G(I)-C(I)*R(I-1)
H(I)=(D(I)-C(I)*H(I-1))/W(I)
10 CONTINUE
F,N)=H(M)
K=M
DO 11 I=1,MA
K=K-1
F(I)=H(K)-R(K)*F(K+1)
11 CONTINUE
T=T+DT
6T=B*T
DO 5 I=1,M
E(I)=F(I)
5 CONTINUE
S1=0.0
S2=0.0
S3=0.0
S1=S1+(1.-E(1))*(1.-Y(1))+(1.-E(M))*(1.-Y(M))
S2=S2+(1.-E(I))*(1.-Y(I))
MN=MA-1

DO 8 I=3,MN,2
  S3=S3+(1.-E(I))*(1.-Y(I))
  HA=ABSF(DY)
  SIM=HA*(S1+4.*S2+2.*S3)/3.
  EV=1.-2.*SIM
  PRINT 103,BT,EV
  1 CONTINUE
CALL EXIT

100 FORMAT(4F10.5,I10)
103 FORMAT(F12.3,F18.6)
101 FORMAT(4F18.8)
END

Finite Difference Method

DY = step size in y direction

DT = step size in t direction

B = \frac{U}{128 \left(1 + \frac{\mu_d}{\mu_c}\right)d_e}

= 1, used in this program

FH = modified continuous phase mass transfer coefficient

N = number of increments in time

BT = (B)(N)(DT) = bt

EV = average fraction extracted of the drop
Hamming's method (flow chart)

\[
\text{DIMENSION } G(10), EF(10), ED(10), BN(10)
\]

\[
\text{DIMENSION } Y(300), VP(300), PV(300), PY(300), YM(300), VM(300)
\]

\[
\text{DIMENSION } YD(300), VD(300), CY(300), CV(300)
\]

\[
\text{DIMENSION } V(300), YP(300), A(10), B(10), C(10), FH(10)
\]

\[
\text{I} +------------+ \\
\text{IO} + \\
\text{JMP=1,16} + \\
\text{I} + \\
\text{+++**READ 300,K} + \\
\text{+++**READ 101,(A(M),B(M),C(M),FH(M),M=1,K} + \\
\text{I} + \\
\text{+++DO} + \\
\text{50} + \\
\text{M=1,K} + \\
\text{I} + \\
\text{I} \\
\text{I E =A(M) I} \\
\text{I E1 =B(M) I} \\
\text{I H =C(M) I} \\
\text{I J =1 I} \\
\text{I} \\
\text{I W =1.0 I} \\
\text{I D =1./H I} \\
\text{I N =ABSF(D)-2.0 I} \\
\text{I Y(1) =1.0 I} \\
\text{I YP(1)=0.0 I} \\
\text{I KJ =1 I} \\
\text{I KM =4 I} \\
\text{I} + \\
\text{+++DO} + \\
\text{10} + \\
\text{I=KJ,KM} + \\
\text{I} + \\
\text{I} \\
\text{I X =W I} \\
\text{I W1 =E*H/6.0 I} \\
\text{CONTINUED
\[ Y_{I+1} = Y(I-3) + (4.9 * H/3) * (2.1 * Y(I_-1)) \]
\[ PV_{I+1} = V(I-3) + (4.9 * H/3) * (2.1 * VP(I_-1)) \]
\[ YM_{I+1} = Y_{I+1} - 112.0 * (PY(I) - CY(I)) \]
\[ VM_{I+1} = VP_{I+1} - 112.0 * (PV(I) - CV(I)) \]
\[ YD_{I+1} = VM(I+1) \]
\[ P = 5.0 - (20.0 * X) + (18.0 * X * X) \]
\[ Q = 1.0 - (5.0 * X) + (10.0 * X * X) - (6.0 * X * X * X) \]
\[ S = 1.0 - X \]
\[ CY_{I+1} = (9.0 * Y(I) - Y(I-2) + 3.9 * H * (YD(I) + 1) + 2.1 * YP(I) - YP(I-1)) / 8.0 \]
\[ CV_{I+1} = (9.0 * V(I) - V(I-2) + 3.9 * H * (VD(I) + 1) + 2.1 * VP(I) - VP(I-1)) / 8.0 \]
\[ Y(I+1) = CY_{I+1} + 9.0 * (PY(I+1) - CY(I) + 1) / 121.0 \]
\[ I\ V(I+1) = CV(I+1) + 9 \cdot (PV(I+1) - CV(I+1)) \]
\[ I\ YP(I+1) = V(I+1) \]
\[ I\ VP(I+1) = (P \cdot V(I+1) - (E \cdot S \cdot Y(I+1))) \]
\[ I\ \frac{YP(I+1)}{Q} \]

**CONTINUED**
I * * * IF *(ABSF(F2)-5.E-05) * I * * * * I I 

- I 0 I + I I 22 I I 22 I I 30 I

I

I

I

I 31 I

22 + ***PRINT 102,E

***PRINT 104,Y(N)

***PRINT 103,YP(N)

***PRINT 105,H

***PRINT 106,FH(M)

I G(M) =E I

I ED(M)=YP(N) I

I EF(M)=Y(N) I

I BN(M)=ED(M)/G(M) I

50 +++++++CONTINUE

***PRINT 205

***PRINT 200

:CONTINUED
***PRINT 211
***PRINT 210
***PRINT 201, (G(M), M=1, K)
***PRINT 210
***PRINT 202, (EF(M), M=1, K)
***PRINT 210
***PRINT 203, (ED(M), M=1, K)
***PRINT 210
***PRINT 204, (BN(M), M=1, K)
***PRINT 210
***PRINT 106, FH(1)
***PRINT 210
***PRINT 105, H
***PRINT 205

500 +++++++CONTINUE

CALL EXIT

205 FORMAT(I1)
102 FORMAT(22H E1GEN VALUE =E18.8)
104 FORMAT(22H E1GEN FUNCTION Y(0) =E18.8)
103 FORMAT(22H YP(0) =E18.8)
105 FORMAT(22H DELTA X =E18.8)
106 FORMAT(22H FILM COEFFICIENT =E18.8)
101 FORMAT(4E18.8),
300 FORMAT(I5)
211 FORMAT(31X3H(1),14X3H(2),14X3H(3),14X3H(4))
200 FORMAT(/)
210 FORMAT(/)
201 FORMAT(22H E1GEN VALUE =4E18.8) CONTINUED
202  FORMAT(22H EIGEN FUNCTION Y(O) =4E18.8)
203  FORMAT(22H YP(O) =4E18.8)
204  FORMAT(22H B(N)) =4E18.8)

END
C C**09817CMX021 PATEL J H 01/13/66 FORTRAN 2 0450 021
C SOLUTION OF HANDLOS AND BARGIN MODEL BY RUNGA-KUTTA AND HAMINGS
DIMENSION G(10),EF(10),ED(10),BN(10)
DIMENSION Y(300),VP(300),PV(300),PY(300),YM(300),VM(300)
DIMENSION YD(300),VD(300),CY(300),CV(300)
DIMENSION V(300),VP(300),A(10),B(10),C(10),FH(10)
DO 50 M=1,16
READ 300,K
READ 101,(A(M),B(M),C(M),FH(M),M=1,K)
DO 50 M=1,K
E=A(M)
F=B(M)
H=C(M)
I=1
51 ...=1.0
D=1./H
F=ABS(D)-2.0
Y(I)=1.0
YP(I)=0.0
K=1
53 DO 10 I=KJ,KM
10 X=H
W1=-(20.*X)+(18.*X*X)
7 P=5.0-(20.*X)+(18.*X*X)
Q=1.0-(5.*X)+(10.*X*X)-(6.*X*X*X)
S=1.0-X
51 I=H:*((P*YP(I)-(E*S*YP(I)))/Q
6 X=X+H/2.0
U=Y(I)+(H*YP(I)/2.0)
UP=YP(I)+(H/2.0)
P=5.0-(20.*X)+(18.*X*X)
Q=1.0-(5.*X)+(10.*X*X)-(6.*X*X*X)
S=1.0-X
51 W2=H*((P*UP)-(E*S*U))/Q
U=U+(H*W2/4.0)
U=YP(I)+(H*W2/4.0)
P=5.0-(20.*X)+(18.*X*X)
Q=1.0-(5.*X)+(10.*X*X)-(6.*X*X*X)
S=1.0-X
51 W3=H*((P*UP)-(E*S*U))/Q
X=X+H/2.0
U=Y(I)+(H*YP(I)+(H*W2/2.0)
UP=YP(I)+W3
P=5.0-(20.*X)+(18.*X*X)
Y(I+1) = Y(I) + (H * YP(I)) + ((W1 + W2 + W3) * H / 6.0)
YP(I+1) = YP(I) + ((W1 + W2 + 2.0) + (2.0 * W3) + W4) / 6.0)

10 N = N + 1
N = 1.0
DO 11 I = XN, KM
X = H
YP(I) = YP(I)
VP(I) = -E / 6.0
IF(I - 1) = 11, 11, 5
5 P = 5.0 - (20.0 * X) + (18.0 * X * X)
Q = 0.0 - (5.0 * X) + (10.0 * X * X) - (6.0 * X * X * X)
S = 1.0 - X
VP(I) = P * V(I) - E * S * Y(I)
11 N = N + 1
N = N + 1
DO 40 I = 4, N
42 X = X
YP(I+1) = Y(I - 3) + (4.0 * H / 3.0) * (2.0 * YP(I) - YP(I - 1) + 2.0 * YP(I - 2))
VP(I+1) = V(I - 3) + (4.0 * H / 3.0) * (2.0 * VP(I) - VP(I - 1) + 2.0 * VP(I - 2))
IF(I - 4) = 16, 16, 17

16 YH(I+1) = PY(I+1)
WH(I+1) = PV(I+1)
GO TO 18

17 YH(I+1) = PY(I+1) - 112.0 * (PY(I) - CY(I)) / 121.0
WH(I+1) = PV(I+1) - 112.0 * (PV(I) - CV(I)) / 121.0

18 YD(I+1) = VH(I+1)
P = 5.0 - (20.0 * X) + (18.0 * X * X)
Q = 0.0 - (5.0 * X) + (10.0 * X * X) - (6.0 * X * X * X)
S = 1.0 - X
VH(I+1) = (P * VH(I+1) - (E * S * VH(I+1))) / Q
CY(I+1) = (9.0 * Y(I) - Y(I - 2) + 3.0 * H * (YD(I+1) + 2.0 * YP(I) - YP(I - 1))) / 8.0
CV(I+1) = (9.0 * V(I) - V(I - 2) + 3.0 * H * (VD(I+1) + 2.0 * VP(I) - VP(I - 1))) / 8.0

61 YP(I+1) = Y(I+1)
VP(I+1) = (P * V(I+1) - (E * S * Y(I+1))) / Q

40 N = N + 1
PRINT 101, E, Y(N), YP(N), H
IF(J = 2) = 1, 3, 3
1 F(I) = YP(N) - Y(N) * FH(M)
R = E1 - E
E = E1
J = J + 1
GO TO 31
3. F2=YP(N)-Y(N)*FH(N)
   IF(ABS(F2)-5.E-05)22,22,30
30 J=J+1
   P=(F2-F1)/R
   E1=E-(F2/P)
   F1=F2
   R=E1-E
   E=E1
   GO TO 31
22 PRINT 102,E
   PRINT 104,Y(N)
   PRINT 103,YP(N)
   PRINT 105,H
   PRINT 106,FH(M)
   G(M)=E
   ED(M)=YP(N)
   EF(M)=Y(N)
   BN(M)=ED(M)/G(M)
50 CONTINUE
   PRINT 205
   PRINT 200
   PRINT 211
   PRINT 210
   PRINT 201,(G(M),M=1,K)
   PRINT 210
   PRINT 202,(EF(M),M=1,K)
   PRINT 210
   PRINT 203,(ED(M),M=1,K)
   PRINT 210
   PRINT 204,(BN(M),M=1,K)
   PRINT 210
   PRINT 106,FH(1)
   PRINT 210
   PRINT 105,H
   PRINT 205
500 CONTINUE
   CALL EXIT
205 FORMAT(1H1)
102 FORMAT(22H E1GEN VALUE =E18.8)
104 FORMAT(22H E1GEN_FUNCTION Y(0) =E18.8)
103 FORMAT(22H YP(0) =E18.8)
105 FORMAT(22H DELTA X =E18.8)
106 FORMAT(22H FILM COEFFICIENT =E18.8)
101 FORMAT(4E18.8)
300 FORMAT(15)
A = first approximation of eigenvalues, 0.5% less than Wellek-Skelland eigenvalue.

B = second approximation of eigenvalues, 0.5% more than Wellek-Skelland eigenvalue.

C = interval of integration

FH = modified continuous phase mass transfer coefficient

K = number of eigenvalues to be computed

G = eigenvalue computed

EF = derivative of eigenfunction

ED = eigenfunction

BN = constant for series solution, Bn
Runge-Kutta method (flow chart)

DIMENSION G(10), EF(10), ED(10), BN(10)
DIMENSION Y(500), YP(500), A(10), B(10), C(10), FH(10)

***READ 300, K

***READ 101, (A(M), B(M), C(M), FH(M), M=1, K)

I

+------------+
+      DO     +
+       50     +
+       M=1, K  +
+               +
+               I
+               +
+               +
I E = A(M)    I
I E1 = B(M)   I
I H = C(M)    I
I J = 1       I

I

31 +

I V = 1.0  I
I D = 1.0/H I
I D = ABSF(D) I
I N = D    I
I Y(1) = 1.0 I
I YP(1) = 0.0 I

+-------+
+       I
+-------+
+       I
+       +
+       +
+       +
+       +
+       +
+       +
+       +
+       +
+       +
+       +
+       +
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+       +
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+       +
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+       +
+       +
+       +
+       +
+       +
+       +
+       +
+       +
+       +

CONTINUED
**continued**

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```

```
1 IJ = J+1
   IF (F2-F1)/R.
      (J-2)
      IF
         (J-2)
      ELSE
         EXIT
      IF
         (J-2)
   I

1 22
   I
1 30
   I
```

```
1 31
   I
1
```
\[ \begin{align*}
I E_1 &= E - \left( \frac{F_2}{P} \right) \\
I F_1 &= F_2 \\
I R &= E_1 - E \\
I E &= E_1 \\
\end{align*} \]

---

```
22 + ***PRINT 102, E
    ***PRINT 104, Y(N)
    ***PRINT 103, YP(N)
    ***PRINT 105, H
    ***PRINT 106, FH(M)
```

```
I G(M) = E
I ED(M) = YP(N)
I EF(M) = Y(N)
I BN(M) = ED(M) / G(M)
```

```
50 +++++++CONTINUE
    ***PRINT 200
    ***PRINT 211
    ***PRINT 210
    ***PRINT 201, (G(M), M=1, K)
    ***PRINT 210
    ***PRINT 202, (EF(M), M=1, K)
    ***PRINT 210
    ***PRINT 203, (ED(M), M=1, K)
    ***PRINT 210
    ***PRINT 204, (BN, M), M=1, K)
```

(Continued)
***PRINT 210
***PRINT 106,FH(1)
***PRINT 210
***PRINT 105,H

CALL EXIT

102 FORMAT(18H EIGEN VALUE =E18.8)
104 FORMAT(18H EIGEN FUNCTION =E18.8)
103 FORMAT(18H YP(0) =E18.8)
105 FORMAT(18H DELTA X =E18.8)
106 FORMAT(18H FILM COFF. =E18.8)
101 FORMAT(4E18.8)
300 FORMAT(I5)
211 FORMAT(25X4HE(1),14X4HE(2),14X4HE(3),14X4HE(4))
200 FORMAT(/)
210 FORMAT(/)
201 FORMAT(18H EIGEN VALUE =4E18.8)
202 FORMAT(18H EIGEN FUNCTION =4E18.8)
203 FORMAT(18H YP(0) =4E18.8)
204 FORMAT(18H B(N) 4E18.8)

END
SOLUTION OF HANDLOS AND BARON MODEL BY RUNGA-KUTTA METHOD

DIMENSION G(10), EF(10), ED(10), BN(10)
DIMENSION Y(500), YP(500), A(10), B(10), C(10), FH(10)

READ 300, K
READ 101, (A(M), B(M), C(M), FH(M), M=1, K)
DO 50, K=1, K
E=A(M)
E1=B(M)
H=C(M)

J=1
V=1.0
D=1.0/H
D=M*SF(D)
N=D
Y(1)=1.0
YP(1)=0.0
DO 10 I=1, N
X=V
W1=-E*H/6.0
IF(I=1)16, 6, 7
P=5.0-(20.*X)+(18.*X*X)
Q=1.0-(5.*X)+(10.*X*X)-(6.*X*X*X)
S=1.0-X
H1=H*((P*YP(I))-(E*S*Y(I)))/Q

X=X+(H/2.0)
U=Y(I)+(H*YP(I)/2.0)
P=5.0-(20.*X)+18.*X*X)
Q=1.0-(5.*X)+(10.*X*X)-(6.*X*X*X)
S=1.0-X
W2=H*((P*UP)-(E*S*U))/Q
U=U+((H*W1)/4.0)
UP=YP(I)+(H*W2/2.0)
P=5.0-(20.*X)+(18.*X*X)
Q=1.0-(5.*X)+(10.*X*X)-(6.*X*X*X)
S=1.0-X
W3=H*((P*UP)-(E*S*U))/Q
X=X+(H/2.0)
U=Y(I)+(H*YP(I))+(H*W2/2.0)
UP=YP(I)+W3
P=5.0-(20.*X)+(18.*X*X)
Q=1.0-(5.*X)+(10.*X*X)-(6.*X*X*X)
S=1.0-X
W4=H*((P*UP)-(E*S*U))/Q

110

\[ Y(I+1) = Y(I) + (H \times YP(I)) + ((W1+W2+W3) \times H/6.0) \]
\[ YP(I+1) = YP(I) + ((W1+(W2*2.0)+(2.0*W3)+W4) \times H/6.0) \]

10 \( v = v + H \)
PRINT 101, E, Y(N), YP(N), H
PRINT 101, V
IF(J-2)<1,3,3
F1 = YP(N) - Y(N) \times FH(M)
R = E1 - E
J = J + 1
GO TO 31
3 F2 = YP(N) - Y(N) \times FH(M)
IF(ABS(F2) = 5.0E-05) 22, 22, 30
J = J + 1
P = (F2 - F1)/R
E1 = E - (F2/P)
F1 = F2
R = E1 - E
E = E1
GO TO 31
22 PRINT 102, E
PRINT 104, Y(N)
PRINT 103, YP(N)
PRINT 105, H
PRINT 106, FH(M)
G(M) = E
ED(M) = YP(N)
EF(M) = Y(N)
BN(M) = ED(M)/G(M)
50 CONTINUE
PRINT 200
PRINT 211
PRINT 210
PRINT 201, (G(M), M=1,K)
PRINT 210
PRINT 202, (EF(M), M=1,K)
PRINT 210
PRINT 203, (ED(M), M=1,K)
PRINT 210
PRINT 204, (BN(M), M=1,K)
PRINT 210
PRINT 106, FH(1)
PRINT 210
PRINT 105, H
CALL EXIT
102 FORMAT(18H EIGEN VALUE = E18.8)
Same nomenclature as Hamming's method.
Appendix H

If one rotates bipolar coordinates about the perpendicular bisector of the line between the two poles, toroidal coordinates are obtained. Using the following transformation, Fick's second law can be transformed to the toroidal coordinates (17a, 17b).

See figure H. 1.

\[
x = \frac{a \sinh \mu \cos \phi}{\cosh \mu - \cos \eta} \quad (H. 1)
\]
\[
y = \frac{a \sinh \mu \sin \phi}{\cosh \mu - \cos \eta} \quad (H. 2)
\]
\[
z = \frac{\sin \eta}{\cosh \mu - \cos \eta} \quad (H. 3)
\]
\[
h_{\nu} = h_{\eta} = \frac{a}{\cosh \mu - \cos \eta} \quad (H. 4)
\]
\[
h_{\phi} = \frac{a \sinh \mu}{\cosh \mu - \cos \eta} \quad (H. 5)
\]

Where \( h_{\mu} \), \( h_{\phi} \) and \( h_{\eta} \) are unit vectors, \( \mu \) ranges from 0 to \( \infty \), \( \eta \) ranges from 0 to 2\( \pi \) and \( \phi \) ranges from 0 to 2\( \pi \).

Fick's second law is

\[
\frac{\partial C}{\partial t} = D \nabla^2 C \quad (H. 6)
\]

\[
\frac{\partial C}{\partial t} = \frac{D}{h_{\mu}^3} \left\{ \frac{1}{\sinh \mu} \left( \frac{\partial}{\partial \mu} \left( h_{\mu} \sinh \mu \frac{\partial C}{\partial \mu} \right) \right) + \frac{\partial}{\partial \eta} \left( h_{\eta} \frac{\partial C}{\partial \eta} \right) + \frac{h_{\mu}}{\sinh 2\mu} \frac{\partial^2 C}{\partial \phi^2} \right\} \quad (H. 7)
\]
Equation (H. 7) represents Fick's second law in toroidal coordinates (figure H. 1), but due to symmetry equation (H. 1) reduces to

\[
\frac{\partial C}{\partial t} = \frac{D}{h^{3}_{\mu}} \left\{ \frac{1}{\sinh \mu} \frac{\partial}{\partial \mu} \left( h_{\mu} \sinh \mu \frac{\partial C}{\partial \mu} \right) \right\} + \frac{\partial}{\partial \eta} \left( h_{\eta} \frac{\partial C}{\partial \eta} \right) 
\]

The following boundary conditions (29) can be applied to solve equation (H. 8)

\begin{align*}
C &= C_{0} \quad \mu = \mu_{0} \quad \eta = \eta \quad t = 0 \quad (H. 9) \\
\frac{\partial C}{\partial \eta} &= 0 \quad \mu = \mu \quad \eta = \pi \quad t = t \quad (H. 10) \\
\frac{\partial C}{\partial \eta} &= 0 \quad \mu = \mu \quad \eta = 0 \quad t = t \quad (H. 11) \\
\frac{\partial C}{\partial \mu} &= 0 \quad \mu = \infty \quad \eta = \eta \quad t = t \quad (H. 12) \\
C &= 0 \quad \mu = \mu_{0} \quad \eta = \eta \quad t = t \quad (H. 13)
\end{align*}

The boundary condition (H. 13) assumes that there is no resistance in continuous phase (i.e. \( k_{c} \to \infty \)). To consider the effect of continuous phase resistance boundary condition (H. 13) should be replaced by the following boundary condition.

\[
\frac{\partial C}{\partial \mu} = h \mu \quad \mu = \mu_{0} \quad \eta = \eta \quad t = t 
\]

where \( h \) includes the effect of continuous phase resistance:

Equation (H. 8) using boundary condition (H. 9), (H. 10), (H. 11), (H. 12),
Figure H. 1 Toroidal Coordinates
(H. 13) and/or (H. 14) could be solved and the results compared with the results obtained by the author. Time did not permit obtaining this solution.

Figure (H. 1) represents the cross sectional view of toroidal coordinates. It is clear from the above figure that for different value of \( \mu \), a system of tori is obtained which is not concentric as is the case for the Handlos and Baron model.

Handlos and Baron derived their model in cylindrical coordinates assuming infinite cylinder for the system of tori. The solution of equation (H. 8) will avoid the assumption made by Handlos and Baron for the system of tori.
VIII. Bibliography


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