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To My Beloved Parents

"My Lord, grant me more knowledge"

(Quran)

STUDY OF MIXING
IN NATURAL STREAMS AND AIR AGITATED TANKS

A Dissertation
Submitted to the Faculty of Graduate Studies through the
Department of Chemical Engineering in Partial Fulfilment
of the Requirements for the Degree of
Doctor of Philosophy at the
University of Windsor

by

Waseem Akhtar

Windsor, Ontario

1978

ABSTRACT

This investigation was concerned with an indepth examination of mixing characteristics encountered in natural streams and in air agitated mixing devices.

In the investigation on natural streams, mathematical models for describing dispersion of soluble wastes in the St. Clair River have been developed. Waste outfalls originating from two Sarnia industries situated along the St. Clair shore were considered in the development of these models. The models equations were comprised of two or three dimensional steady state conservation equations. For both two and three dimensional models, the longitudinal dispersion term was considered negligible in comparison to the corresponding convective term. The two dimensional model incorporated lateral dispersion, while both lateral and vertical dispersion were considered in the three dimensional model. The necessary dispersion coefficients were estimated from correlations proposed in literature. The model equations were solved numerically by using Forward Marching and Crank Nicholson procedures. The results from the two procedures were found to be similar but for the latter procedure the computation time was five to six times higher than for

the former case. Some stability criteria for these procedures were also developed.

Theoretical predictions from the two dimensional model have been compared to the experimental work on the St. Clair river performed by the Ontario Ministry of the Environment. It was found that the results from the two dimensional model using a value of lateral diffusion coefficient significantly higher than that proposed in literature for open channel flow gave a better agreement with the experimental results.

The investigation into mixing by air agitation consisted of two phases. In the first phase of the work, a model that describes the mixing process in a batch air agitated tank was developed. The model is based on the data obtained in a rectangular batch air agitated tank equipped with a line diffuser placed at the bottom of one end of the tank. The experimental work was conducted for different conditions of airflow rates, depths and lengths of the tank. Detailed velocity measurements were made for one base case in order to establish the velocity profile for the air agitated tank. It was found that the velocity profile resembled a forced vortex and could be correlated in terms of the liquid circulation rate and the tank geometry. Using the information revealed from the velocity profile, a mathematical formulation of the mixing

process based on a two-dimensional unsteady state conservation statement was put forward. This led to the model equation, which was a partial differential equation containing a convective term superimposed by longitudinal and vertical diffusion terms. This equation was solved numerically using an alternating-direction implicit finite difference method proposed by Peaceman and Rachford. Model parameters such as the longitudinal and the vertical turbulent diffusion coefficients were deduced from correlations proposed in literature. The adjustable model parameter was the multiplier for the longitudinal diffusion coefficient. Good agreement was obtained with the experimental results for the seventeen mixing time runs. The diffusion multiplier was found to correlate to the length/depth ratio for the tank.

The second phase of the work was concerned with the development of design procedures for the batch air agitated tanks using the mixing model developed in the first phase. Based on the existing practices, two distinct design situations were identified. One used mixing time as the design criterion, whereas the other used the bulk velocity as a measure of the induced degree of agitation. For the first situation the mixing model was shown to be directly usable in a design procedure. Stepwise procedures proposed for both cases require information regarding the kind of treatment

and the volume of the tank as an input. The design equations relate surface, bottom and bulk velocities to stipulated tank geometry and air flow rate. The velocity correlations were checked against limited large scale measurements reported in a previous investigation. The design decisions were shown to involve a trade-off between power requirement and mixing time.

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I. INTRODUCTION

Mixing is a phenomenon of great importance. It occurs naturally on a global scale and is deliberately induced in many engineering operations.

Mixing plays a significant role in many aspects of air and water pollution control. For example, the dispersion of gaseous or finely divided material released into the atmosphere near or above the ground level depends on the natural mixing processes which are a direct consequence of turbulent and convective motions within the atmosphere. Similarly, when a mass of domestic or industrial soluble wastes is discharged into a river, ocean or a lake, it undergoes mixing with the water resulting in the dilution of the wastes.

In processes used for waste water treatment, mixing is an integral unit operation in many phases of the treatment. Some of these treatment processes are as follows.

1. In the coagulation process, chemical coagulants are mixed into the wastewater. This is a rapid process and requires intense mixing in order to insure uniform chemical distribution and exposure of the suspended particles in the water to the coagulating agent within a short time.

2. In the flocculation process which follows the coagulation process, mixing is again required, though not with as high a degree of agitation as in the previous process. The purpose of the flocculation is to aggregate the coagulated particles into floc particles which are readily removeable in the subsequent processes of sedimentation or filtration (1).
3. In the sludge treatment, chemicals are mixed with sludge to improve its dewatering characteristics before vacuum filtration.
4. In biological treatment, mixing is employed to assure intimate contact between micro-organisms and their nutrients (2).

There are a number of mixing devices which are used to accomplish the mixing operation in the wastewater treatment units. These may be classified into three broad groups, namely, gravitational, mechanical and pneumatic. The baffled channel and hydraulic-jump mixers are examples of gravitational mixers. Impellers such as paddles, turbines and propellers are generally employed for mechanical mixing. In pneumatic mixing compressed air is diffused into the liquid content, which generates mass circulation of liquid and turbulence (3). Out of these three types of mixing

pneumatic mixing is the one which has been the least investigated.

A. Scope of Present Work:

The present work reports the results of an effort to study the mixing process in a natural stream and in an air agitated tank.

The city of Sarnia has a number of chemical industries situated along the Canadian bank of the St. Clair river. This river has long been used as a means for disposal of the industries' wastes. It is important to know the mixing characteristics for the river in order to determine its capacity for assimilation of the wastes. This kind of information is essential for establishing satisfactory control on the water quality of the river, as well as in determining the criterion for such control. In this investigation, two mixing models were developed for the St. Clair river in the neighbourhood of two industries, based on discharge data obtained from these industries.

In the second phase of this research work, the nature of mixing in an air agitated tank was studied. Despite the widespread use of air agitated tanks, especially in wastewater treatment operations, the nature of mixing in these devices has not yet been that fully explored. In this investigation, a mixing model has been developed for the air agitated batch tanks of a rectangular geometry with a line diffuser placed at the bottom of one side of the tank.

a

4

B. Dissertation Outline :

Chapter II describes briefly the theoretical background on mixing and presents the basic equations which have been used to describe the mixing process in turbulent systems.

In Chapter III, two mathematical models are developed to describe the mixing of soluble waste outfalls originating from two Sarnia industries situated along the river.

In Chapter IV, experimental results obtained using a laboratory scale air agitated tank are presented. The experiments conducted covered a wide range of air flow rates. In addition, the geometry of the tank was varied to a limited degree. Mixing times were determined using tracer technique. Detailed velocity profile determination was made to provide the necessary data for developing the mixing model.

Chapter V presents the development of the mixing model for the air agitated tank on the basis of the experimental results presented in Chapter IV.

In Chapter VI, some procedures for designing the air agitated tanks are presented. These design procedures are based on the correlations obtained on the basis of all available data on air agitated batch tanks, and include some information from previous researchers that has not previously been published.

Chapter VII summarizes the findings and presents some conclusions.

II. THEORETICAL BACKGROUND OF MIXING AND LITERATURE REVIEW

Mixing is defined as the intermingling of two or more dissimilar portions of materials, resulting in the attainment of a desired level of uniformity either physical or chemical in the final product. In fluid mixing the intermingling of one substance with another is accomplished by diffusion and fluid motion. Thus, the basic equation of the mixing process, which relates the variables affecting uniformity of composition of the system, is that of mass conservation describing the diffusion and convection of the material in the system. For laminar fluid motion involving molecular diffusion, the mathematical formulation of the mixing processes can be done easily by using Fick's law of diffusion. But difficulties arise in the formulation of turbulent mixing processes because of the dynamic and complex nature of the turbulent motion itself.

Based on the work of earlier investigators such as Reynolds (5) and Taylor (6,7), a reasonably rigorous mathematical representation of the turbulent mixing has been attempted by a number of investigators (8,9,10). In the following section, basic mathematical representations used to describe mixing phenomena are briefly outlined.

A. General Equation for Turbulent Mixing

Based on Fick's law of diffusion, the mass conservation equation describing the mixing process in a laminar flow system can be formulated as

$$\frac{\partial c}{\partial t} = E_m \left[\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right] - \frac{\partial uc}{\partial x} + \frac{\partial vc}{\partial y} + \frac{\partial wc}{\partial z} \quad \dots 2.1$$

where

c = point concentrations of material, lbm/ft³

t = time, sec

x,y,z = cartesian coordinates (longitudinal, lateral and vertical) respectively.

u,v,w = point velocity components in x,y,z direction, respectively, ft/sec

E_m = molecular diffusion coefficient, ft²/sec

It should be noted that equation 2.1 involves only two transport mechanisms, the velocity transport and molecular diffusion according to Fick's law. Equation 2.1 is not suitable for analysis of mixing in turbulent flows which involve velocity and concentration fluctuations. However, this equation can be modified by adding terms which account

for turbulence. The nature of the additional terms was first investigated by Reynolds (5). He suggested that the point velocities in the laminar flow equations may be replaced by instantaneous point velocities in turbulent motion. The same reasoning can be applied to concentration fluctuations. These considerations suggest that the concentration and the velocity vector be replaced by a time-averaged value plus a term to represent the fluctuations. Thus,

$$c = \bar{c} + c'$$

$$u = \bar{u} + u'$$

$$v = \bar{v} + v'$$

$$w = \bar{w} + w'$$

.... 2.2

where

\bar{c} = time-averaged value of concentration, lbm/ft³

c' = concentration fluctuation, lbm/ft³

$\bar{u}, \bar{v}, \bar{w}$ = time-averaged velocities in x, y, z directions respectively, ft/sec

u', v', w' = velocities fluctuations in x, y, z directions, respectively, ft/sec

Substitutions of these relations in equation 2.1 and time averaging the resulting equation lead to

$$\frac{\partial \bar{c}}{\partial t} = E_m \left[\frac{\partial^2 \bar{c}}{\partial x^2} + \frac{\partial^2 \bar{c}}{\partial y^2} + \frac{\partial^2 \bar{c}}{\partial z^2} - \frac{\partial \bar{u}\bar{c}}{\partial x} + \frac{\partial \bar{v}\bar{c}}{\partial y} + \frac{\partial \bar{w}\bar{c}}{\partial z} \right. \\ \left. - \frac{\partial \overline{u'c'}}{\partial x} + \frac{\partial \overline{v'c'}}{\partial y} + \frac{\partial \overline{w'c'}}{\partial z} \right] \quad \dots 2.3$$

In the above equation, the time averaged concentrations and velocities have replaced the concentrations and velocities in equation 2.1, but three new terms accounting for the fluctuations in velocity and concentrations also appear. These terms, analogous to Reynolds stresses in momentum transport, have been referred to as turbulent mass fluxes (11). The turbulent mass fluxes are often assumed to be proportional to the gradient of averaged concentrations, a suggestion made first by Boussinesq (12) for momentum transport and applied to mass transport according to Reynolds analogy (5). Thus, the new terms in equation 2.3 are defined as

$$\overline{u'c'} = -E_x \frac{\partial \bar{c}}{\partial x} \\ \overline{v'c'} = -E_y \frac{\partial \bar{c}}{\partial y} \\ \overline{w'c'} = -E_z \frac{\partial \bar{c}}{\partial z} \quad \dots 2.4$$

where E_x, E_y, E_z = turbulent diffusion coefficients in x,y,z

directions, respectively, ft^2/sec

Substituting equation 2.4 in equation 2.3 gives

$$\begin{aligned} \frac{\partial \bar{c}}{\partial t} = & E_m \left(\frac{\partial^2 \bar{c}}{\partial x^2} + \frac{\partial^2 \bar{c}}{\partial y^2} + \frac{\partial^2 \bar{c}}{\partial z^2} \right) + \frac{\partial}{\partial x} E_x \frac{\partial \bar{c}}{\partial x} + \frac{\partial}{\partial y} E_y \frac{\partial \bar{c}}{\partial y} + \frac{\partial}{\partial z} E_z \frac{\partial \bar{c}}{\partial z} \\ & - \frac{\partial \bar{u}\bar{c}}{\partial x} - \frac{\partial \bar{v}\bar{c}}{\partial y} - \frac{\partial \bar{w}\bar{c}}{\partial z} \end{aligned} \quad \dots 2.5$$

Since the molecular and turbulent diffusivities are additive, equation 2.5 becomes

$$\begin{aligned} \frac{\partial \bar{c}}{\partial t} = & \frac{\partial}{\partial x} (E_m + E_x) \frac{\partial \bar{c}}{\partial x} + \frac{\partial}{\partial y} (E_m + E_y) \frac{\partial \bar{c}}{\partial y} \\ & + \frac{\partial}{\partial z} (E_m + E_z) \frac{\partial \bar{c}}{\partial z} - \left(\frac{\partial \bar{u}\bar{c}}{\partial x} + \frac{\partial \bar{v}\bar{c}}{\partial y} + \frac{\partial \bar{w}\bar{c}}{\partial z} \right) \end{aligned} \quad \dots 2.6$$

Equation 2.6 may be further simplified if flow is incompressible.

In addition, the contribution of molecular diffusion for most turbulent systems may be considered to be negligible. Thus equation 2.6 reduces to

$$\begin{aligned} \frac{\partial \bar{c}}{\partial t} = & \frac{\partial}{\partial x} \left(E_x \frac{\partial \bar{c}}{\partial x} + \frac{\partial}{\partial y} E_y \frac{\partial \bar{c}}{\partial y} + \frac{\partial}{\partial z} E_z \frac{\partial \bar{c}}{\partial z} \right) \\ & - \bar{u} \frac{\partial \bar{c}}{\partial x} + \bar{v} \frac{\partial \bar{c}}{\partial y} + \bar{w} \frac{\partial \bar{c}}{\partial z} - \bar{c} \left(\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} \right) \end{aligned} \quad \dots 2.7$$

Applying the equation of continuity, $\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = 0$

and transferring convective terms to left side of the equation 2.7, one obtains

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z} = \frac{\partial}{\partial x} E_x \frac{\partial c}{\partial x} + \frac{\partial}{\partial y} E_y \frac{\partial c}{\partial y} + \frac{\partial}{\partial z} E_z \frac{\partial c}{\partial z} \dots 2.8$$

Note that in equation 2.8, the bars above c,u,v and w have been dropped for convenience.

Equation 2.8 is the basic equation that describes the mixing of the material in the turbulent flow. In the following section, a summary of literature is presented which illustrates the application of this equation in studying different mixing processes.

B. Literature Review

1. Mixing in Natural Streams

A complete mathematical model for the mixing process in natural streams is represented by equation 2.8. The solution of this equation with appropriate boundary conditions would predict the concentration of a material at any point of the stream. However,

the formidability of obtaining solutions to equation 2.8 is apparent. This has led most researchers to use of simplified versions. The most common version has been a one dimensional model along the line proposed by G.I. Taylor (7). In Taylor's treatment, no variation in stream properties with any direction other than longitudinal is taken into account. In addition, the longitudinal turbulent diffusion coefficient is considered to be constant. Thus, the one dimensional model is expressed as

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = E_x \frac{\partial^2 c}{\partial x^2} \quad \dots 2.9$$

Equation 2.9 can be solved analytically for various boundary conditions. For an initial material distribution concentrated in the plane $x = 0$ at time t , the solution is

$$c = \frac{M}{A'' \sqrt{2 \pi E_x t}} e^{-\frac{(x-ut)^2}{4E_x t}} \quad \dots 2.10$$

where M = the total mass of material, lbm and A'' = the cross sectional area of flow normal to x , ft^2 .

Equation 2.10 has been applied to describe the mixing of material in laboratory flumes and in natural streams (13-16).

In many circumstances, however, it would be apparent that the one dimensional description can not adequately describe the mixing process. Fisher (17) reports a detailed study of dispersion of pollutants in natural streams. He found that after a slug of pollutant has been discharged into the stream, the mixing that takes place may be divided into two separate periods (a) an initial period in which the convective transport produces a markedly skewed distribution of the pollutant, and (b) a later period, after turbulent cross sectional mixing has reduced cross sectional concentration gradients to very small values, during which Taylor's one dimensional approach is valid. Using experimental results on natural streams, Fisher found a criterion for estimating the downstream distance from the pollutant source after which Taylor's one dimensional model equation 2.9 may be applied. The criterion is

$$X > 1.8 \frac{x'^2}{H} \frac{\bar{u}}{u^*} \quad \dots 2.11$$

where X = the distance from the source of pollutant, ft

x' = characteristic length, defined as the distance from the point of maximum surface velocity to the most distance bank, ft.

H = depth of the flow, ft.

\bar{u} = cross-sectional averaged velocity, ft/sec

u^* = shear velocity, ft/sec

Yotsukura and Fiering (18) used a two dimensional model for an open channel flow. They made two assumptions: (a) $v, w,$ and $\partial c / \partial y$ are zero and (b) the longitudinal diffusion term is negligible in relation to the longitudinal convective term. On the basis of these two assumptions, equation 2.8 reduced to a two dimensional equation as follows

$$-\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = \frac{\partial}{\partial z} E_z \frac{\partial c}{\partial z} \quad \dots 2.12$$

Yotsukura and Fiering solved equation 2.12 on a computer using numerical techniques.

In applying the general equation 2.8 or its modified versions to describe the mixing process in pipes, open channels and natural streams, one requires a knowledge of parameters such as longitudinal, lateral and vertical turbulent diffusions coefficients. Table 2.1 summarizes the results of previous studies of estimating these coefficients. From the Table, it would appear that the turbulent diffusion coefficients may be expressed as a product of the shear velocity u^* and the depth of flow H .

$$E_x, E_y \text{ or } E_z = \lambda H u^* \quad \dots 2.13$$

TABLE 2.1
Equations For Estimating Turbulent Diffusion Coefficients
Recommended by Various Investigators.

Investigator	Flow Channel	Equations For Turbulent Diffusion Coefficient
Longitudinal Turbulent Diffusion		
Taylor (7)	Pipe Flow	$E_x = 10.11 u^* r$
Elder (19)	Open Channel	$E_x = 5.93 u^* H$
Yotsukura & Fiering (18)	Open Channel	
	Rough Boundary	$E_x = 9.0 u^* H$
Glover (20)	Smooth Boundary	$E_x = 13.0 u^* H$
	Open Channel	
	Triangular Flume	$E_x = 18.0 u^* H$
"	Natural Stream (south Platte River)	$E_x = 500 u^* H$
Godfrey & Frederick(21)	Natural Stream (Church River)	$E_x = 50.5 u^* H$
	Power River	$E_x = 654 u^* H$
Lateral Turbulent Diffusion		
Elder (19)	Open Channel	$E_y = 0.23 u^* H$
Fischer (22)	Open Channel (canal)	$E_y = 0.24 u^* H$
Glover (20)	Natural Stream (Columbia River)	$E_y = 0.72 u^* H$
Yotsukura, Fischer & Sayre (23)	Natural Stream (Missouri River)	$E_y = 0.62 u^* H$
Kinkead & Handy(24)	Natural Stream †	$E_y = 0.97 u^* H$
Vertical Turbulent Diffusion		
Vanoni (25)	Open Channel	$E_z = k(1 - \frac{z}{H}) zu^*$ or $E_z = 0.067^* H u^*$

† (St. Clair River)

where λ = a constant termed as a dimensionless diffusion coefficient

The shear velocity u^* is defined by the following equation

$$u^* = \sqrt{\frac{\tau_0}{\rho}} \quad \dots 2.14$$

where τ_0 = wall stress, $\text{lbm}/(\text{sec.}^2 \text{ft})$, and ρ = fluid density, lbm/ft^3 .

As shown in Table 2.1, the numerical values of the dimensionless diffusion coefficient for longitudinal and lateral directions are reported to be different by various investigators. For longitudinal turbulent diffusion, Taylor (7) obtained a value of 10.11 for a pipe flow. He carried out his analysis for an empirical velocity distribution in a circular straight pipe and assumed that the turbulent eddy diffusivities were isotropic and could be defined by the Reynolds analogy, which states that the mass transport is analogous to momentum transport. In his results, the depth of flow H was replaced by the radius of the pipe.

Elder (19) extended Taylor's work to a two dimensional flow in a very wide open channel of depth 1.5 cm. He estimated a value of λ equal to 5.93. Yotsukura and Fiering (18) reported value of λ ranging from 9 to 13 for open channels of smooth and rough boundaries. For natural streams Glover (20) and Godfrey and

Frederick (21) found a higher value of λ which was reported to be in the range of 50 to 654.

The numerical values of dimensionless coefficient of lateral turbulent coefficient are found to be much less than that of longitudinal. Elder (19) obtained a value of λ for lateral diffusion equal to 0.23 for a wide channel. Fisher (22) used a canal and estimated a value of λ equal to 0.24. Some studies on natural streams have shown that the value of dimensionless lateral diffusion coefficient is higher than that for open channel flows. For examples, Glover (20) and Yotsukura, Fisher and Sayre (23) have obtained for Columbia and Missouri rivers, values of λ equal to 0.72 and 0.62 respectively. Recently Kinkead and Hamdy (21) have done a study of the St. Clair river near Sarnia region and obtained a rather high value of λ equal to 0.97.

A correlation for vertical turbulent diffusion has been obtained by Vanoni (25). He studied the distribution of concentration of small sediment particles with respect to depth in a laboratory flume and obtained theoretically the following expression for the vertical turbulent diffusion coefficient ' E_z '

$$E_z = k \left(1 - \frac{z}{H}\right) z u^* \quad \dots 2.15$$

where $k = 0.4$, von Karman constant

z = vertical downward distance from the surface of channel

Equation 2.15 may be averaged over entire depth to obtain the following expression,

$$E_z = 0.067 u^* H \quad \dots 2.16$$

Expressions 2.15 and 2.16 have been used as a basis for predicting the distribution of sediment in streams and have been confirmed by laboratory and field measurement (26,27)

2. Mixing in Agitated Tanks:

a. Mechanically Agitated

Mixing in mechanically agitated tanks has been studied extensively. There is abundant literature available on this subject. Uhl and Gray (4), Sterbacek and Tausk (28) and Nagata (29) have presented an exhaustive survey of the literature on the theoretical and practical aspects of mechanical agitation. Recently a series of articles (30) written by researchers of Chemineer, Inc., Dayton, Ohio have been published. These

describe in detail design methods for mechanically agitated tanks. In the following paragraphs, some of the works which are general in nature would be reviewed.

In mechanical agitation, the turbulence and fluid motion which results in the mixing of material in the tank is caused by the momentum transfer from the rotating impeller to the liquid content. Thus the basic relationships among the variables affecting the performance of the tank are governed by the basic equations for mass balances and momentum balances. Due to complex nature of boundary conditions caused by the complex shapes of mixing vessels, impellers and the flow patterns of contained fluids induced by impellers, the formidability of solving the basic equations is apparent. This has led investigators to use simple methods such as dimensional analysis in order to get performance correlations for agitated tanks. For example, a rather simple dimensional analysis of Navier Stokes momentum balance equation yields the following result (4,31).

$$\frac{P_g}{\rho N^3 D^5} = f(N_{Re}) \quad \dots 2.17$$

where P = Power consumptions, ft-lbf/sec

N = impeller speed, revolutions/sec

D_I = impeller diameter, ft

ρ = fluid density, lbm/ft³

N_{Re} = Reynolds number for impeller expressed as $ND_I^2\rho/\mu$

$g_c = 32.2$ lbm.ft/lbf.sec²

The group on left hand side of equation 2.17 is termed the power number. A number of plots having the power number as ordinate against the impeller Reynolds number have been obtained for different kinds of impellers (4,31,32). These plots are used in designing the equipment.

Since the action of a mechanical impeller resembles to a certain degree that of a centrifugal pump, the basic principles which relate the head developed, fluid velocities, flow rates, power consumption and equipment geometry are applicable also to rotating impeller in agitated tanks. Like the pumps, there are two important factors characterizing the action of mixer. One is the hydrodynamic head ' H_m ' and other is the volumetric discharge rate of liquid termed as pumping capacity, Q_m . The hydrodynamic head and pumping capacity of the mixer is related to power

consumption by the following equation (28).

$$P = Q_m \rho H_m \quad \dots 2.18$$

where P = power consumption, ft-lbf/sec

Q_m = pumping capacity, ft³/sec

ρ = density, lbm/ft³

H_m = hydrodynamic head, ft.

- The calculations of the pumping capacity for mixers has been set out from the analogy with pumps (33). There are different relations obtained for different kinds of impellers. For curved and pitch blade turbines and propellers, the following relations are reported (4).

Curved-bladed Turbines

$$Q_m = \pi^2 b N D_I^2 (1-k') \quad \dots 2.19$$

Pitch-blade Turbines

$$Q_m = \pi^2 N D_I^3 (1-k') \left[(1/6) \sin \alpha \cos \alpha + (b/D_I) \sin^2 \alpha \right] \quad \dots 2.20$$

Propeller

$$Q_m = \pi/4 N D_I^2 p' \quad \dots 2.21$$

where b' = axial impeller blade width, ft

k' = ratio of tangential fluid velocity at the periphery of an impeller to peripheral impeller velocity

N = impeller speed, revolutions/sec

α' = angle of pitch of the blade face

p' = propeller pitch, ft.

The pumping capacity of the mixer when divided by the cross-sectional area of the tank yields the bulk velocity, which is considered to be a characteristic quantity that measures the dynamic response of agitated tanks (34). In order to establish impeller performance criteria, a scale of agitation, numbered from 1 to 10, has been obtained in terms of the bulk velocities ranging from 6 to 60 ft/min (34). These scales indicate capabilities of the various agitation intensities to obtain a number of different process results.

Van de Vusse (33) developed correlations that relate batch mixing time of agitated tank to various operating and equipment variables. Using dimensional analysis, he obtained the following relation

$$t_m Q_m / V = K'' N_{Re}^a F_{rm}^b \quad \dots 2.23$$

where t_m = mixing time, sec

V = volume of tank, ft^3

N_{Re} = Reynolds number defined as $\frac{D_I^2 N_p}{\mu}$

F_{rm} = a modified Froude number defined as $\frac{D_I^2 N_p^2}{gH\Delta\rho}$ in

which $\Delta\rho$ is the difference of density of the individual component and H is liquid depth in the tank.

K, a, b = correlation constants

The exponents a & b have been determined from experimental data (33).

The values of a are found to be -3 and zero for laminar and turbulent flows respectively. The values of b are found to be in the range of -0.25 to -0.3 depending upon the kind of impeller.

b. Air-Agitated

In wastewater treatment as well as in other mixing operations, two types of air agitated tanks are in use: continuous and batch operated. Despite the widespread use of these units, there is very little literature available on either the theoretical or the practical aspects of designing these tanks.

Most of the reported work is on continuous air agitated tanks in which air agitation is used to achieve oxygen transfer from

diffused air to the liquid content of the tank. Morgan and Bewtra (35) and Bewtra (36) have studied extensively the effects of several factors involved in the process of oxygen transfer in continuous air agitated tanks. Some fundamental research work on mixing characteristics of continuous air agitated tank has been reported by Thomas and McKee (37), Murphy and Timpany (38) and Murphy and Boyko (39). Murphy and co-workers (38,39) used one dimensional model equation 2.9 to predict the tracer response curves from a pulse input to the continuous air agitated tanks. The solution to the one dimensional equation 2.9, which defines the effluent response curve to a pulse input of an inert tracer for a tank, has been given by Thomas and McKee (37) and Miyauchi (40) and is of the form

$$\frac{c_e}{c_o} = 2 \sum_{n=1}^{\infty} \frac{\alpha_n (T \sin \alpha_n + \alpha_n \cos \alpha_n)}{(\alpha_n^2 + 2T + \alpha_n^2)} \exp \left[T - \frac{T^2 + \alpha_n^2}{2T} s \right] \quad \dots 2.23$$

where

c_e = exit concentration of tracer at time t , lbm/ft³

c_o = mass of tracer added divided by tank volume, lbm/ft³

$T = 1/2 \left[\frac{uL}{E_x} \right]$

u = horizontal velocity of liquid calculated as volumetric flow rate of liquid divided by cross sectional area of tank perpendicular

to the flow, ft/sec

L = tank length, ft

ϵ = t/t_d

t_d = detention time calculated as volume of the tank divided by volumetric flow rate of liquid, sec

$$\alpha_n = \text{Cot}^{-1} \left[1/2 \left(\frac{\alpha_n}{T} - \frac{T}{\alpha_n} \right) \right]$$

This expression was used to generate theoretical response curves which were compared to the experimental response curves obtained by Murphy and Timpany (38) and Murphy and Boyko (39) from both a laboratory scale tank (5.0' x 3.0' x 2.5') and a full scale tank (270' x 27' x 15'). They concluded from their results that the one dimensional dispersion model appeared to be an adequate model to describe mixing in continuous air agitated tanks.

For batch air agitated tanks, the nature of mixing has not been studied extensively. Kaufman (41) has suggested practical amounts of air for various intensities of agitation, referring specifically to the petroleum industry. According to him the following quantities of air per square foot of tank cross sectional area may be used to obtain a certain degree of agitation in a liquid depth of 9 feet.

	Free air per min.
Moderate agitation	0.65 cu.ft.
Complete agitation	1.30 cu.ft.
Violent agitation	3.1 cu.ft.

Kaufman presents no foundation for his statements and does not define "degree of agitation". His figures may be based on the appearance of the surface of the fluid.

Lamont (42) has reported results concerned mostly with actual practices in pachuca tanks. A pachuca tank, employed in the metallurgical industry for ore leaching operations, is a circular tank with a 60° cone at the bottom and a central column for almost the full tank depth. Air is introduced at the bottom of the column causing ore pulp to rise in the column thereby developing circulation in the tank..

Szabo (43), in 1971, studied the mixing characteristics of a small scale circular batch mixing tank. In this study a tank of 5 feet in diameter and 4 feet depth was used. Air was diffused through a pipe located either at the centre or the periphery of the tank. Based on the experimental results, Szabo developed the following correlations relating the performance of the mixing time with the tank geometry and the air flow rate.

$$\log t_m = 0.57 + 0.34 \frac{D_c}{H} + 0.35 \frac{Q'_a}{V} \quad \dots 2.24$$

$$u_s = \frac{Q'_a}{e + f Q'_a} \quad \dots 2.25$$

where

t_m = mixing time, sec

D_c = diameter of the tank, ft

H = liquid depth, ft

Q'_a = air flow rate, ft³/min

V = volume of the tank, ft³

u_s = surface velocity, ft/sec

e & f = correlations constants

From the experimental procedure, it appears that the values of air flow rates reported by Szabo are in error because she did not measure the air pressure. Nevertheless, her results seem to indicate some general trends for the batch air agitated tanks of circular geometry.

III. MIXING MODELS FOR NATURAL STREAMS:

A Case Study of St. Clair River

St. Clair river, with an average discharge of 117,000 cubic feet per second, drains an area of 220,000 sq.miles (44). It starts from Lake Huron and ends at Lake St. Clair. The Canadian shore of the St. Clair river has long been used as a means for disposal of wastes from industries, mainly chemical industries, situated along the shore. In this study a region of the river of approximately ~~one mile~~ covering two chemical industries, namely Polysar Corporation Ltd and Dow Chemical Ltd, was taken into consideration for the development of the mathematical models. This region includes a dozen waste outfalls originating from the said two companies. The details of their locations and waste discharge rates are given in Figure 3.1

A. Development of Mixing Models:

As discussed in Chapter II, mixing of soluble wastes in a natural stream may be described by equation 2.8, which is an unsteady state conservation statement for mass in a three dimensional form. The formidability of obtaining a solution to

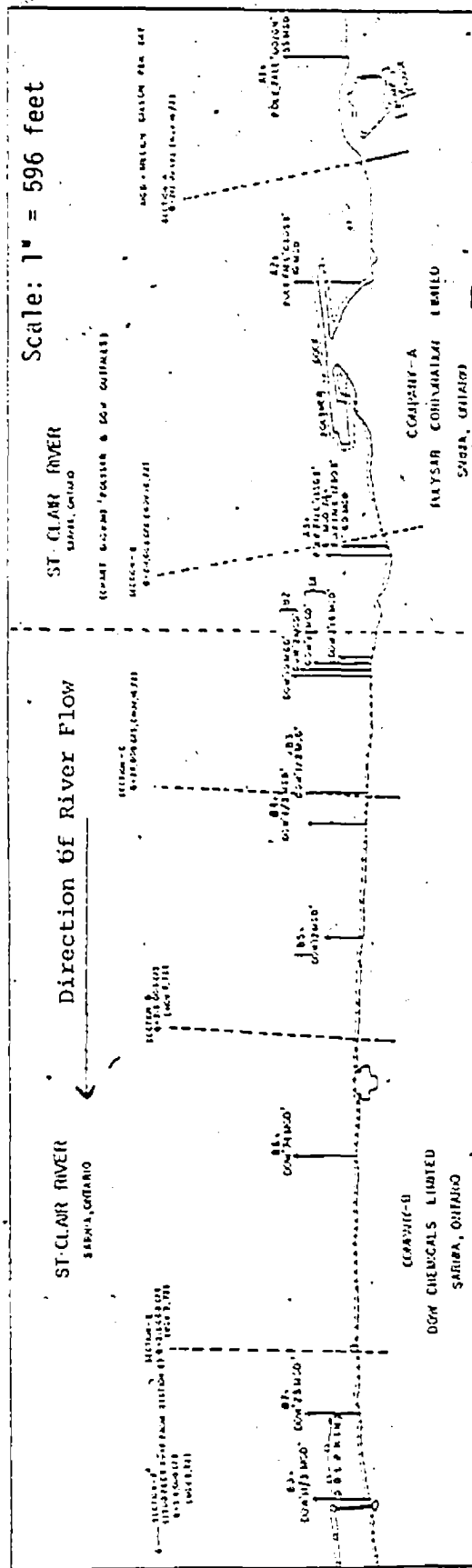


FIGURE 3-1— LOCATIONS, AND FLOW RATES OF OUTFALLS
& RIVER DISCHARGE RATE

equation 2.8 is apparent. Therefore, assumptions are usually made to modify equation 2.8 to simpler forms more amenable to solution by contemporary techniques. The following models are therefore simplified versions of the general description that seem appropriate for the particular case under consideration.

1. Two Dimensional Model

The following assumptions were made to simplify the general equation 2.8 to a two dimensional form:

- i) lateral and vertical velocity components i.e. v and w are zero
- ii) $\frac{\partial C}{\partial t} = 0$ (The waste streams are being released at the shore continuously.)
- iii) The longitudinal diffusion term $\frac{\partial}{\partial x} (E_x \frac{\partial C}{\partial x})$ is negligible as compared to longitudinal convective term $u \frac{\partial C}{\partial x}$ (18).
- iv) Concentration gradient along vertical direction is negligible, i.e., the waste mixes instantaneously in the vertical direction. Therefore $\frac{\partial C}{\partial z} = 0$.

Based on these assumptions, equation 2.8 reduces to a steady state two dimensional form

$$\bar{u} \frac{\partial \bar{C}}{\partial x} = \frac{\partial}{\partial y} (E_y \frac{\partial \bar{C}}{\partial y}) \quad \dots 3.1$$

where $\bar{C}(x,y)$ is the concentration of waste, averaged along the vertical direction and \bar{u} is the velocity in downstream direction at any point on lateral direction, averaged from velocities measured at fraction 0.2 and 0.8 of the river depth.

The boundary conditions for equation 3.1 are:

$$\frac{\partial \bar{C}}{\partial y} = 0 \quad \text{at } y = 0 \text{ (Canadian shore)} \quad \dots 3.2$$

$$\frac{\partial \bar{C}}{\partial y} = 0 \quad \text{at } y \rightarrow \infty \text{ (Set at } y = 500 \text{ feet)}$$

Since wastes are being added continuously from several outfalls located at various points downstream, a new initial concentration distribution has to be defined at the region of each outfall. To define the initial waste concentration, the following assumptions are made.

- i) velocities at outfalls are much lower than the river velocity.
- ii) wastes are uniformly diluted in a mixing zone extending to a certain distance from the shore.

Defining the location of the outfall 'i' by $x = x_i$, the initial

and subsequent distribution of waste concentration at different outfalls is given by:

At $x = x_1$ (First Outfall)

$$\bar{c}(x_1, y_1) = \frac{q_1}{Q_1 + q_1/\rho_1} F_{p1}$$

At $x = x_i$ (ith Outfall)

$$\bar{c}(x_i, y_i) = \frac{Q_i \bar{c}(y_i) \text{ prior to Fall } i}{Q_i + q_i/\rho_i} + \frac{q_i}{Q_i + q_i/\rho_i} F_{pi}$$

where

..... 3.3

$\bar{c}(x_i, y_i)$ = concentration of pollutant averaged over entire depth, at any point of downstream and lateral direction, lb/ft³

$\bar{c}(y_i)$ = average concentrations of pollutant of interest in the mixing zone, lb/ft³

q_i = total waste discharge rate for outfall 'i', lb/sec

ρ_i = density of waste discharge, lb/ft³

Q_i = local discharge rate of the river in mixing zone of width y_i feet, ft³/sec

F_{pi} = lb mass of pollutant of interest per lb of waste discharge

The weight fractions F_{pi} were all set at 1.0 for results presented in this work. The values of y_i were all set arbitrarily at 50 feet (unless otherwise stated). The density of waste discharge ρ_i was assumed to be equal to the water density i.e., 62.4 lb/ft³.

2. Three Dimensional Model

If the dispersion of waste in the vertical direction is also considered, then assumption iv made for the two dimensional model is no longer valid and a three dimensional model becomes necessary. In such a case, the model equation is

$$u \frac{\partial c}{\partial x} = \frac{\partial}{\partial y} (E_y \frac{\partial c}{\partial y}) + \frac{\partial}{\partial z} (E_z \frac{\partial c}{\partial z}) \quad \dots 3.4$$

where

$c(x,y,z)$ = concentration of pollutant at any point of downstream, lateral and vertical direction, lb/ft³

The boundary conditions for the model equation 3.4 are

$$\begin{aligned} \frac{\partial c}{\partial y} &= 0 && \text{at } y = 0 \\ & && \text{at } y = 500 \text{ feet} \\ \frac{\partial c}{\partial z} &= 0 && \text{at } z = 0 \text{ (surface of the river)} \\ & && \text{at } z = H \text{ (bottom of the river)} \\ & && \text{where } H \text{ is local depth of the river} \quad \dots 3.5 \end{aligned}$$

The initial and subsequent waste concentration distribution at each outfall has also to be defined in three dimensional form:

At $x = x_i$ (ith outfall)

$$c(x_i, y_i, z_i) = \frac{Q_i \bar{c}(y_i) \text{ prior to Fall } i}{Q_i + q_i/\rho_i} + \frac{q_i}{Q_i + q_i/\rho_i} F_{pi}$$

..... 3.6

B. Estimation of the Velocity Term and River Geometry

The velocity and depth data, to be used in the mathematical model, were provided by the companies. These data were collected by a consulting firm (James F. MacLaren Limited) during November 1972. A region of the river of approximately one mile downstream from the first wastefall of Polysar Ltd. and five hundred feet laterally from the Canadian shore was considered for flow and depth measurements. Six sections were arbitrarily chosen within the one mile downstream distance and velocity measurements, using a Price current meter, were made 50, 100, 250 and 500 feet offshore at each section. The method involved lowering the current meter to depths of 5 feet and 0.2 and 0.8 of the river depth. Readings were taken at each of the four points on the sections. River depths were measured by using a Ferrograph portable inshore echo sounder. The details of

the procedure are cited elsewhere (44). The velocity and depth data are tabulated in Appendix A.

C. Estimation of Parameters E_y and E_z :

The parameters of the model equations, i.e., the lateral and vertical turbulent diffusion coefficients, were estimated from correlations that have been recommended in published literature. As was observed in Chapter II, the values of lateral and vertical turbulent diffusion coefficients may be estimated from the following correlations

$$E_y = \epsilon H u^* \quad \dots 3.7$$

$$E_z = k \left(1 - \frac{z}{H}\right) z u^* \quad \dots 3.8$$

where

E_y and E_z = lateral and vertical turbulent diffusion coefficients, respectively, ft^2/sec

H = depth of flow, ft

u^* = shear velocity, ft/sec

ϵ = non-dimensional turbulent diffusion coefficient, defined as E_y/Hu^*

k = 0.4, von Karman constant

z = vertical downward distance from the surface of the river.

As shown in Table 2.1, values of ϵ ranging from 0.23 to 0.97 have been obtained by various investigators. In the present work, results were obtained using values of ϵ equal to 0.23 and 0.97.

The shear velocity term u^* in correlations 3.7 and 3.8 is defined by

$$u^* = \frac{\tau_o}{\rho} = \sqrt{g s r} \quad \dots 3.9$$

where

τ_o = shearing stress at the river surface

ρ = fluid density, lbm/ft³

g = 32, acceleration due to gravity, ft/sec²

s = slope of the river

r = hydraulic radius, ft = depth of flow, ft

The shear velocity u^* can be written in term of the river velocity using Manning's equation which may be expressed as:

$$u^* = \frac{1.486}{n} r^{2/3} s^{1/2} \quad \dots 3.10$$

where

n = Manning's roughness coefficient

u = velocity of river, ft/sec

Substituting equation 3.9 into equation 3.10 and replacing the hydraulic radius r by the depth of the river H, one gets

$$u^* = u \frac{n g^{1/2}}{1.486 H^{1/6}} \dots 3.11$$

A value of n = 0.0235 has been obtained for the St. Clair river by Corps of Engineers (45). Equation 3.11 was substituted in correlations 3.7 and 3.8 to estimate the lateral and vertical turbulent diffusion coefficients.

D. Solution of Model Equations:

The two and three dimensional model equations 3.1 and 3.4 with their boundary conditions were solved on an IBM 360/65 computer using finite difference techniques. For the two dimensional model Forward Marching and Crank Nicholson finite difference schemes were used. For the three dimensional model, only the forward marching scheme was applied. The details of the numerical procedures are given in Appendix B.

For a proper choice of grid size, both two and three dimensional models yield stable results. In the two dimensional model, the size of the grid in the longitudinal and lateral direction was 10 feet. In the step wise procedure for the two dimensional model, the

concentrations of wastes computed on each step were averaged over the entire depth before going to the next forward step. In other words, the correction due to the existent variable depth along the lateral and downstream were applied. For the solution of two dimensional model equation, the values of lateral turbulent diffusion coefficient were estimated from correlation 3.7.

For the three dimensional model, a variable grid size technique which accounted for the irregular boundaries at the bottom of the river was first used. But this resulted in unstable results. Consequently, this technique was abandoned and instead a fixed size three dimensional grid (10 x 10 x 4) was used ignoring the irregular boundaries. During the step wise solution of the three dimensional model, the values of lateral turbulent diffusion coefficient were estimated from correlation 3.7 by substituting the entire depth and the same values were used for all the grid points in the vertical direction. The values of the vertical turbulent diffusion coefficients were computed from correlation 3.8 for each grid point in the vertical direction.

Models Results

1. Sensitivity of Models to Diffusion Coefficients:

In the present work, parameters such as lateral and vertical turbulent diffusion coefficients were not experimentally determined for the actual system; instead, conventional values proposed in the literature have been used. Therefore, it was of considerable practical importance to study the sensitivity of models to the magnitudes of these diffusion coefficients. In order to study this, several computer runs were made using different values of lateral and vertical diffusion coefficients. The results are tabulated in Table 3.1. In this table, the terms E_y (Base) and E_z (Base) refer to the lateral and vertical turbulent diffusion coefficients estimated from equation 3.7 with $\alpha = 0.23$ and equation 3.8 respectively. The results indicate that the sensitivity to vertical variations in diffusion coefficient values is not significant. But the results are more sensitive to variations in the lateral coefficient. It is, therefore, quite important to obtain the lateral coefficient experimentally for the actual system. As indicated in Chapter II, the lateral diffusion coefficient for St. Clair river has recently been obtained by the Ontario Ministry of Environment. This value has been employed in the two dimensional model and the results thus obtained are discussed in

TABLE 3.1

Parametric Sensitivity of Mixing Models

Downstream Distance Mile	$E_y/E_{y(\text{base})}$	$E_z/E_{z(\text{base})}$	% Difference in Shore Concentration from base case
1	0.5	1	+17
	2	1	-29
	1	0.5	-5
	1	2	0
2	0.5	1	+60
	2	1	-47
	1	0.5	-2
	1	2	+5

Section 3. In sections 2 and 4, the results are obtained using the lateral turbulent diffusion coefficient values estimated from correlation 3.7 with $\alpha = 0.23$.

2. The Concentration Profiles:

Typical concentration profiles obtained from the two and three dimensional models are shown in Figures 3.2 and 3.3 for a downstream distance of one mile and greater. The figures presented are representative of the general nature of model results. It appears from the results that a rather large distance from the location of the outfalls is required to disperse the waste uniformly in the river.

In Figures 3.2 and 3.3, the comparison is made between the results obtained from two dimensional and three dimensional model. It appears that the results from the three dimensional model are a little more informative than those obtained from two dimensional model in that the former gives information of waste concentrations from the surface to bottom, whereas the later gives concentration of wastes averaged over the entire depth of the river. But these results obtained from the three dimensional model are achieved at the cost of long computation time. For example, to obtain concentration profiles for approximately two miles downstream of the

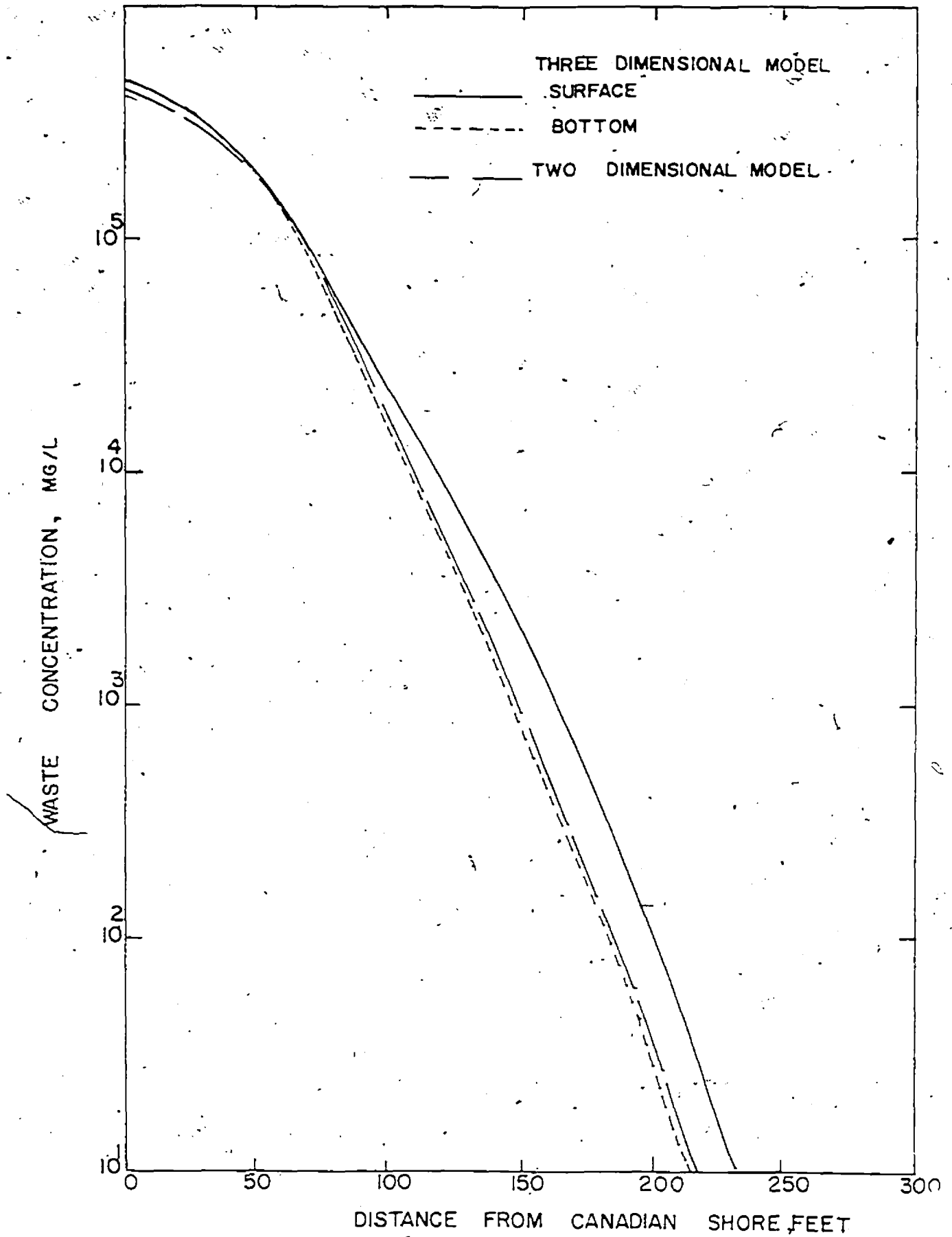


FIGURE 3.2 — LATERAL CONCENTRATION PROFILES
 DOWNSTREAM DISTANCE FROM OUTFALL A1=5300 FT.

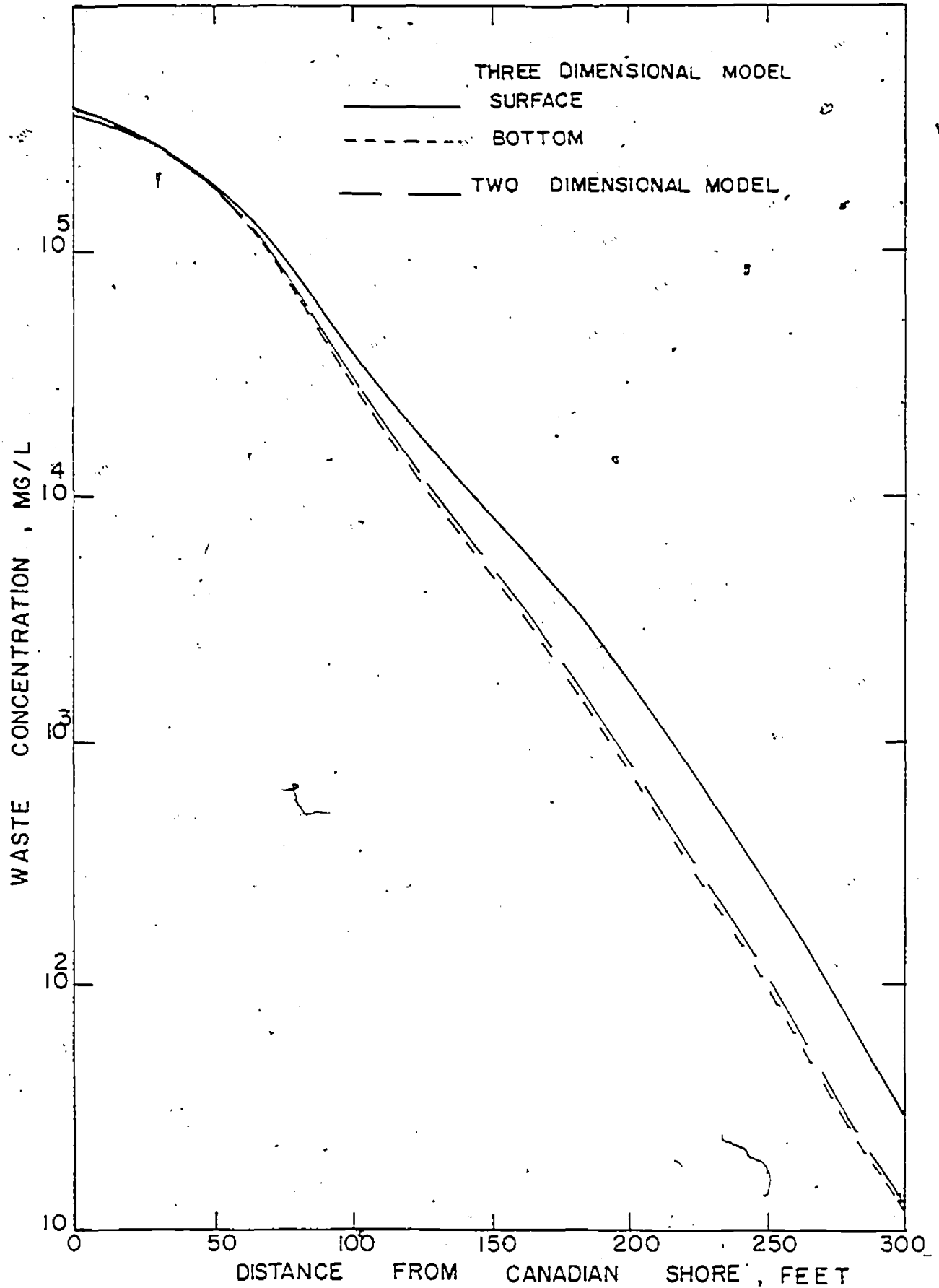


FIGURE 3.3 — LATERAL COCENTRATION PROFILES
 DOWNSTREAM DISTANCE FROM OUTFALL A1 = 9400 FT.

river, the three dimensional model requires one hour computer time as compared to 5 minutes required from two dimensional model. This makes the two dimensional model more advantageous over the three dimensional model.

3. Comparison of Model Results to Experimental Concentration Profiles.

The chloride concentrations just downstream of outfall B7 at points 25, 50 and 100 feet from Canadian shore were provided by the Ontario Ministry of Environment (46). Starting with these values the lateral concentration profiles at downstream distances of 1000 feet and 4224 feet from outfall B7 were obtained using two dimensional model. The results are plotted in Figures 3.4 and 3.5. The model was tested using two different values for lateral diffusion coefficients. These values estimated from correlation 3.7 with $\alpha = 0.23$ and $\alpha = 0.97$ represent lower and upper range of the coefficient as reported in literature. In Figures 3.4 and 3.5, the model results are compared with the experimental profiles for chloride concentrations obtained by the Ontario Ministry of Environment (46) at downstream distances of 1000 feet and 4224 feet from outfall B7. It appears that a better agreement with experimental values is obtained using a higher coefficient than those reported in the literature.

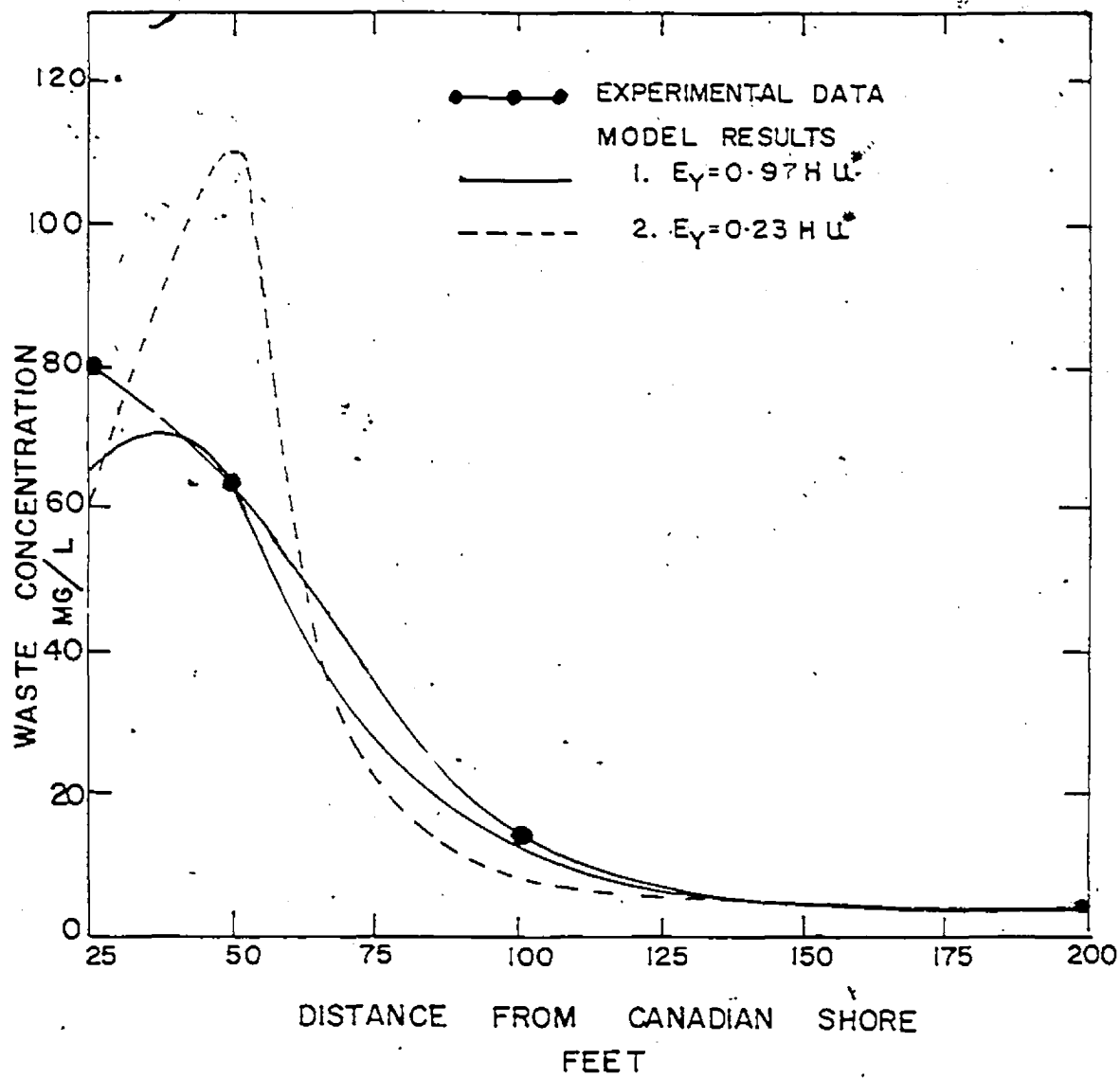


FIGURE 3-4 — LATERAL CONCENTRATION PROFILE AT A DISTANCE 1000 FEET FROM FALL B7

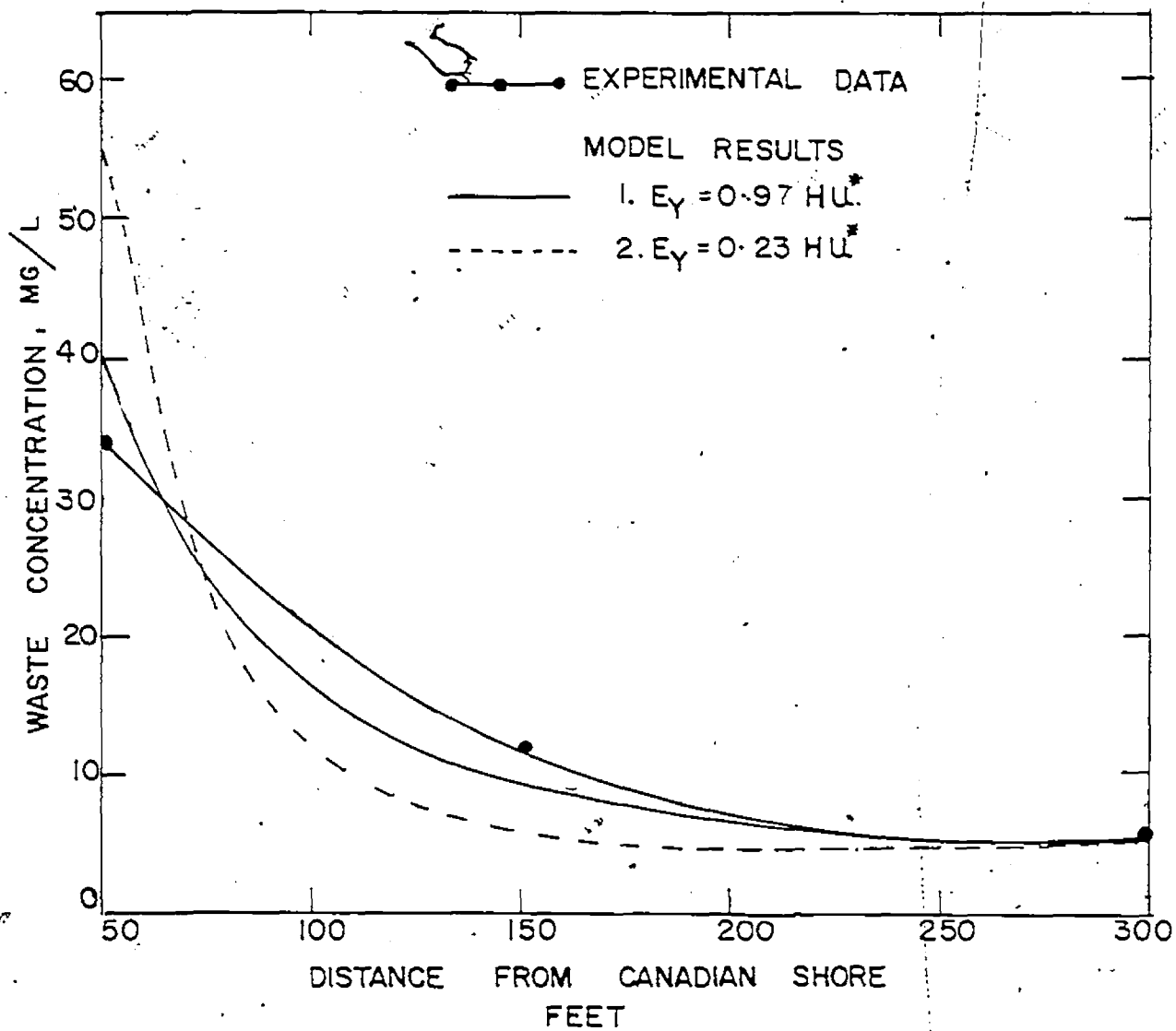


FIGURE 3.5 — LATERAL CONCENTRATION PROFILE
AT A DISTANCE 4224 FEET
FROM FALL B7

4. Model Applications

In the present work a preliminary attempt was made to illustrate the applications of the proposed two dimensional model in studying the effect of changing the location of outfalls and the width of initial mixing zones on the resultant concentration profiles. The results are presented in the following sections

a. Effects of Outfall Location on Overall Waste Dispersion:

Generally, wastes are released at the shore of the receiving stream from open end pipes or ditches. In such cases, the wastes disperse but slowly, thereby localizing the pollution to a zone near the shore. It may seem more advantageous to have outfalls a distance away from the shore so that the waste directly mixes with the receiving stream of considerable high velocity zone, resulting in a rapid dispersion. But the costs involved in moving outfalls away from the shore may offset this advantage. Therefore, to determine the optimum location of outfalls, both factors, location and cost, have to be considered simultaneously.

Figures 3.6 and 3.7 illustrates the effect of moving outfall A1 20 fifty feet offshore. It appears from the results that the localized pollution at the shore is reduced significantly by moving the outfall away from the shore. This reduction may be

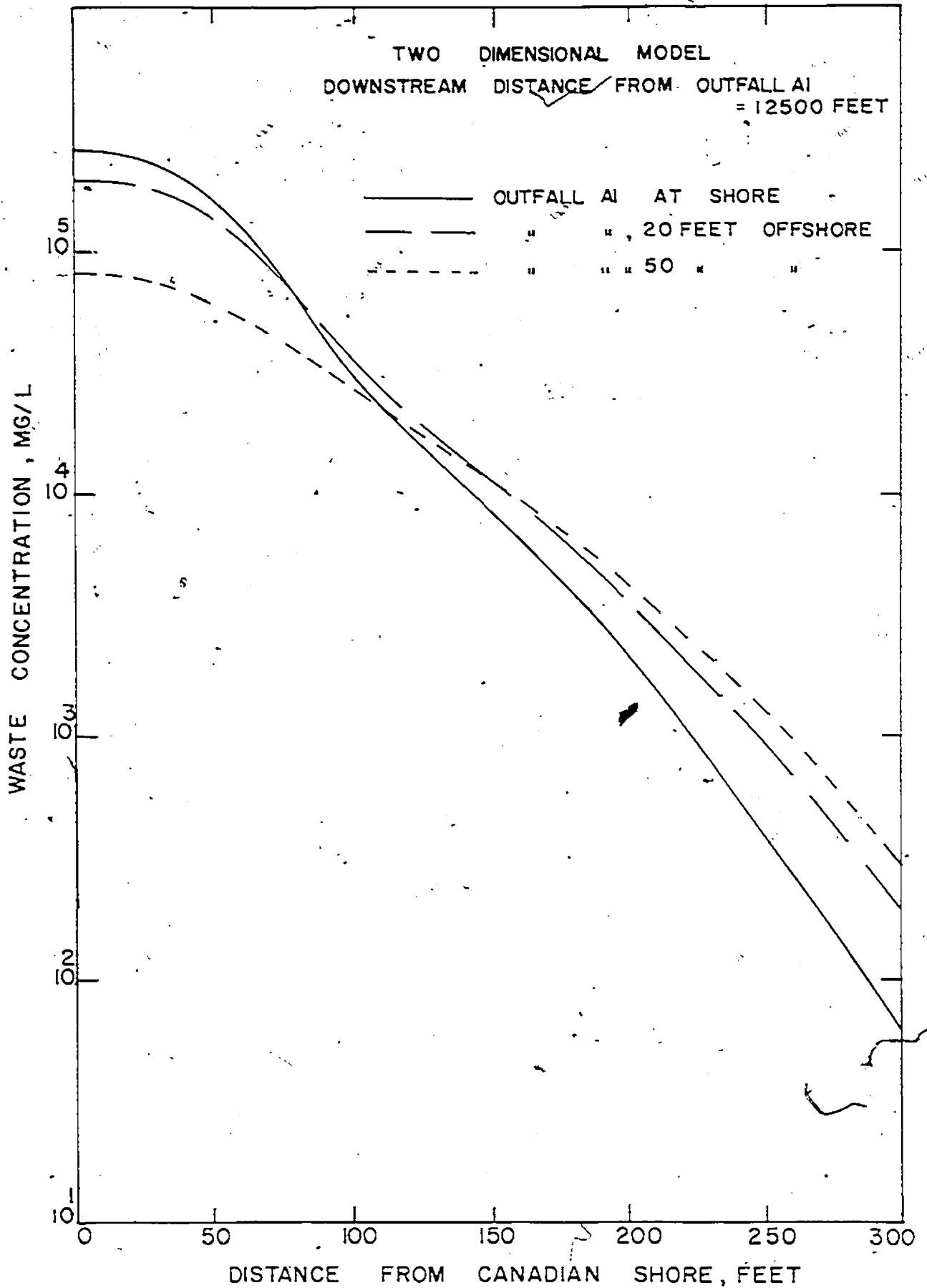


FIGURE 3-6—LATERAL CONCENTRATION PROFILES,
 VARIOUS LOCATIONS OF OUTFALL A1

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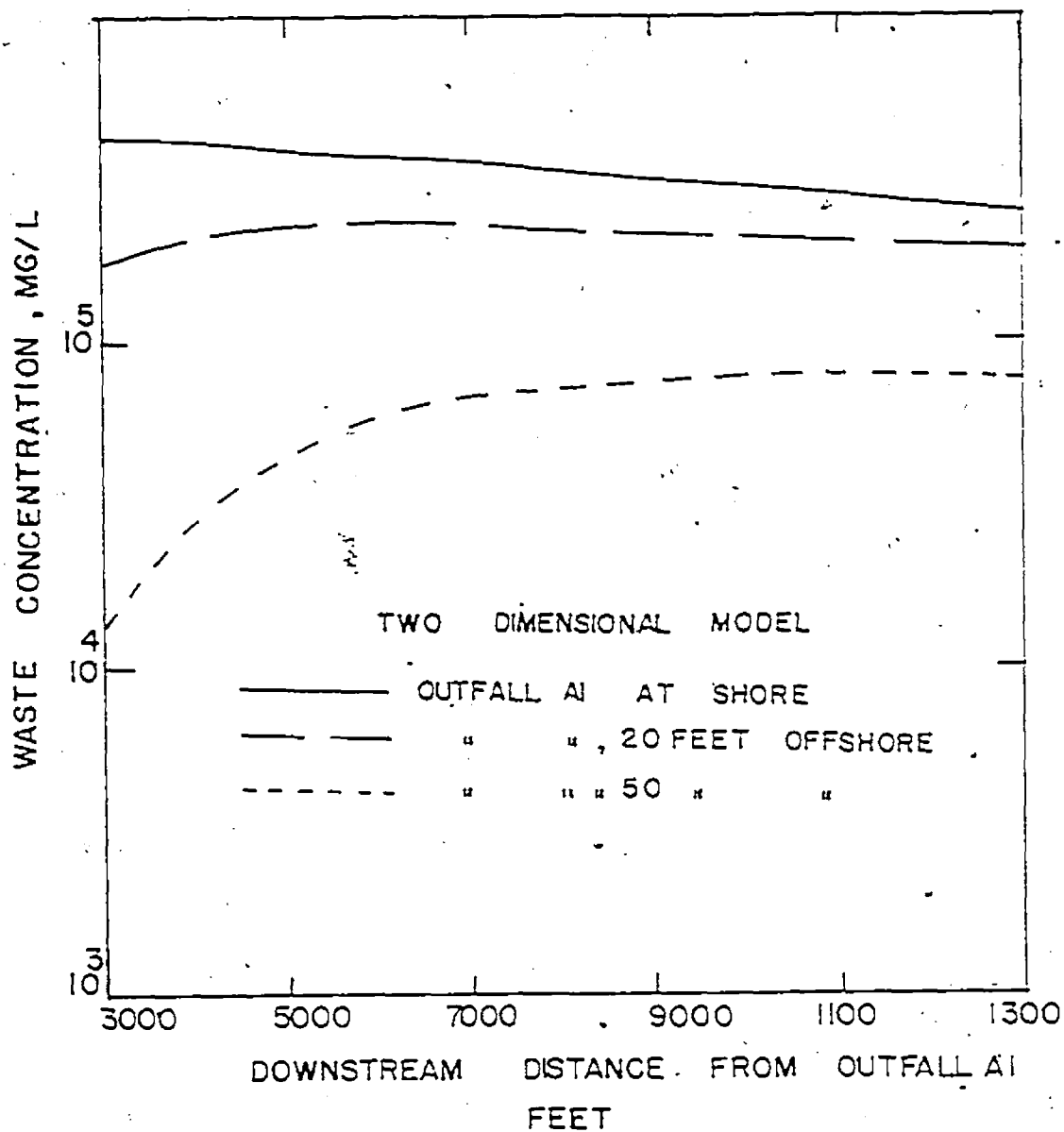


FIGURE 3-7 — LONGITUDINAL PROFILES OF SHORE CONCENTRATION, VARIOUS LOCATIONS OF OUTFALL A1

attributed not only to the availability of deeper stream but also to the existence of high velocities away from shore lines.

b. Effects of Initial Mixing Zones on Overall Waste Dispersion

In the present work, the velocity of waste discharge at each outfall has been assumed much less than the local velocity of the river and thus the effect of jet mixing in initial dilution of waste is ignored. This condition is true when outfalls are plane open channels or ditches. However, in cases where discharges are made from diffusers, the effect of jet mixing may be significant and the initial dilution of the waste will be governed by jet entrainment. Therefore, diffusion equations as proposed here, do not apply until a certain distance downstream where the jet effect becomes negligible.

An attempt was made in this work to examine the effect of mixing zone width on the overall dispersion of wastes. Runs were made assuming initial mixing zones of three different widths, as measured laterally from the Canadian shore. The results are shown in Figures 3.8 and 3.9. As expected, the larger the width of initial mixing zone, the greater is the dispersion of waste in lateral direction, bringing down the shore concentration considerably. For example, doubling the mixing zone

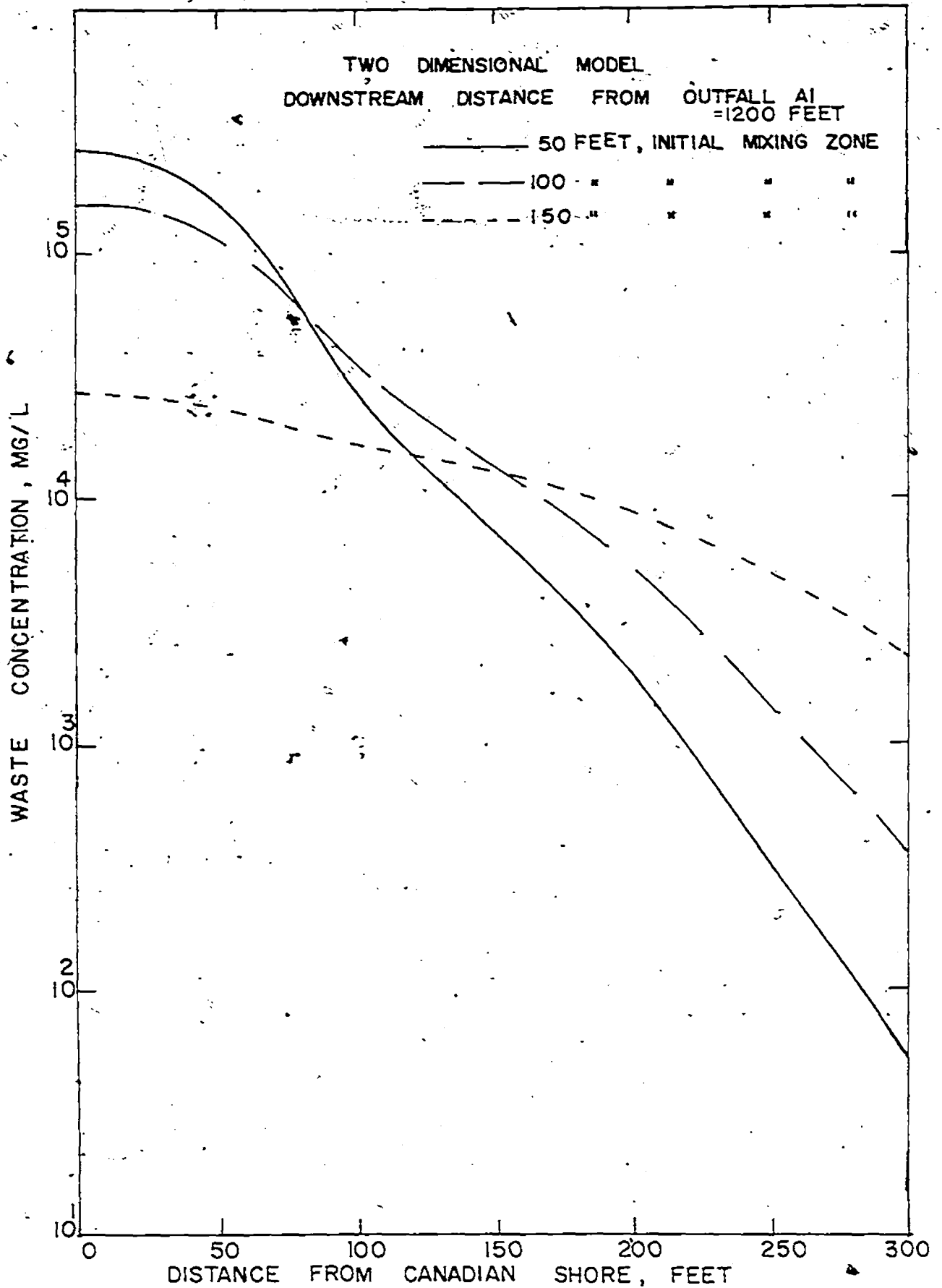


FIGURE 3.8.—LATERAL CONCENTRATION PROFILES
VARIOUS INITIAL MIXING ZONES

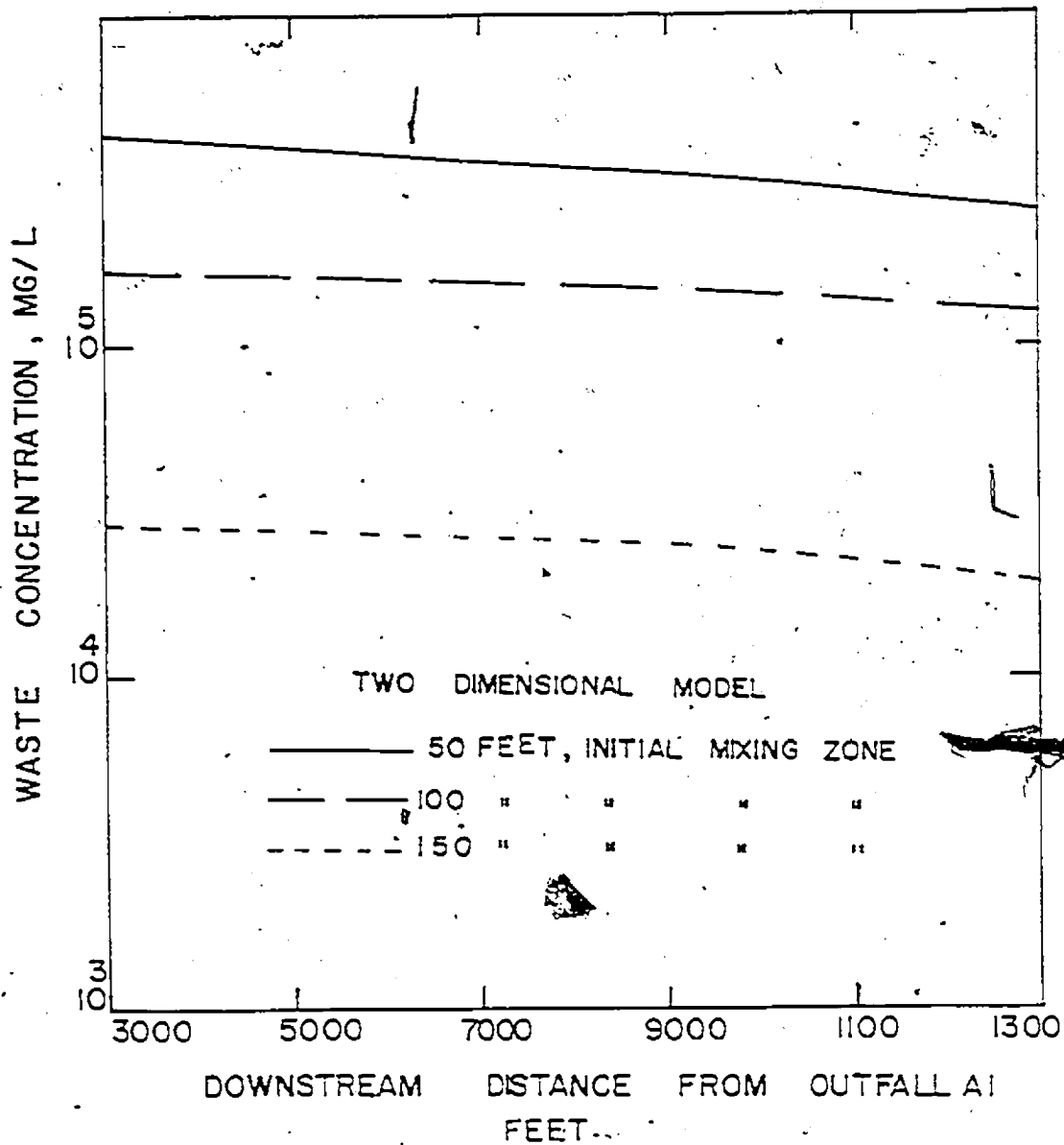


FIGURE 3-9— LONGITUDINAL PROFILES OF SHORE CONCENTRATION, VARIOUS INITIAL MIXING ZONES

from 100 feet to 200 feet, the waste concentration in the vicinity of the shore is 80% reduced. This considerable reduction in the waste concentration may be attributed to the initial availability of larger volume of the receiving stream to mix with discharge.

IV. MIXING IN AIR AGITATED TANKS: THE EXPERIMENTS

Mixing in fluids through air agitation is considered to be an economical and efficient technique for various processing industries. In particular, its application to wastewater treatment were discussed in Chapter II. An attempt was made in this investigation to obtain insights into the nature of mixing in air agitated batch tanks. This work may be considered in three parts. The experimental part where a laboratory scale tank was used to obtain mixing information under various conditions of air agitation. The model development part which utilized the information obtained in the experiments to get a mathematical description of the mixing process. Finally, a third part that examined the practical utility of the mixing model for design of large scale units. In this chapter, the first part of this work will be discussed. The second and third parts will be discussed in the following chapters.

A. The Experimental Set Up

The experimental work was carried out on a rectangular tank with a line diffuser placed at the bottom of the tank as shown in the schematic diagram (Figure 4.1). Photographs of top and side

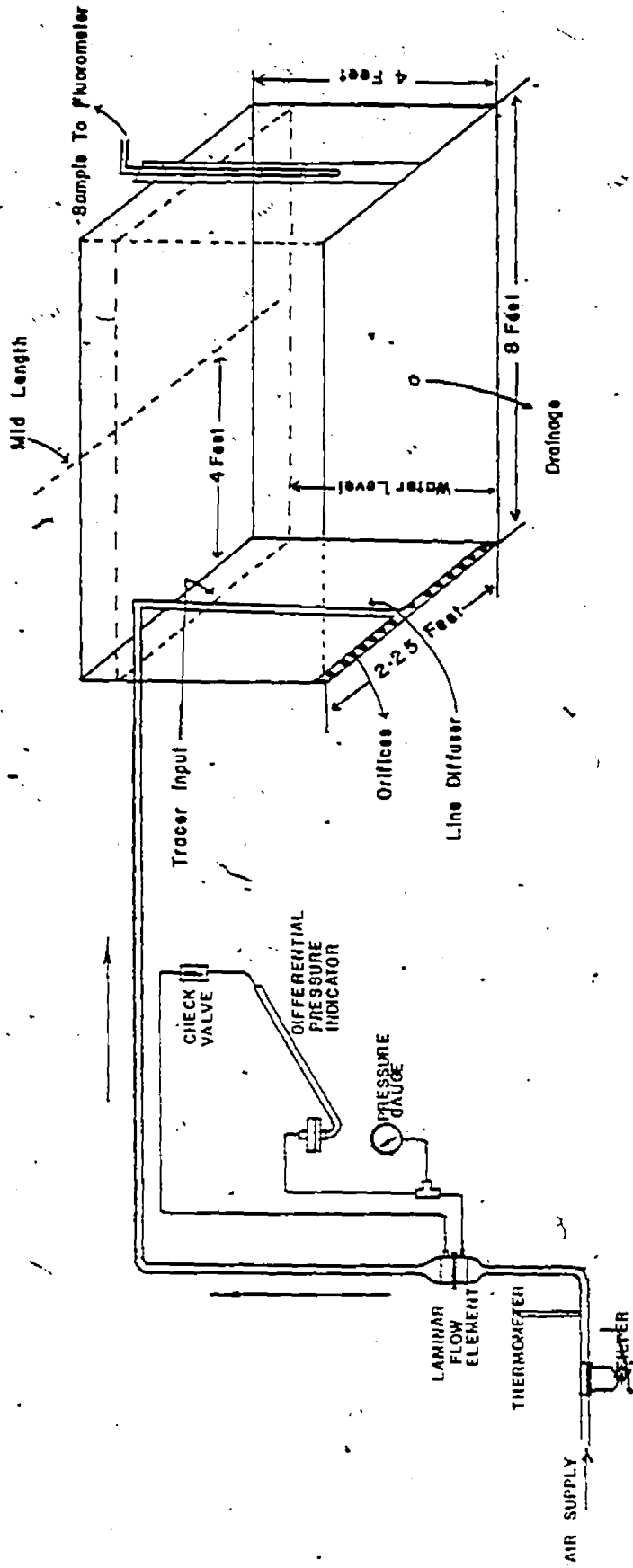


FIGURE 4-1 SCHEMATIC DIAGRAM OF THE MIXING TANK

views of the tank are given in Figure 4.2. The tank was 8 feet long, 2.25 feet wide and 4 feet high. The length of the tank could be altered by placing a partition made of iron plate. The tank itself was constructed of half an inch thick Plexiglass segments reinforced with iron frame. The line diffuser consisted of a one inch diameter copper pipe 2.25 feet long, with fourteen 1/8 inch diameter orifices two inches apart and facing towards the surface of the tank. The diffuser covered the entire width of the tank. Air flow was monitored through a Meriam Laminar Flow meter and a pressure gauge placed just upstream of the flow meter as shown in Figure 4.1. The flow meter calibration was supplied by the manufacturer. The flow measurements are estimated to be accurate to $\pm 0.5\%$ according to the instrument manual. Since errors can also arise from pressure measurement, overall air flow rates may be considered reliable to only $\pm 2\%$.

B. The Experimental Procedure

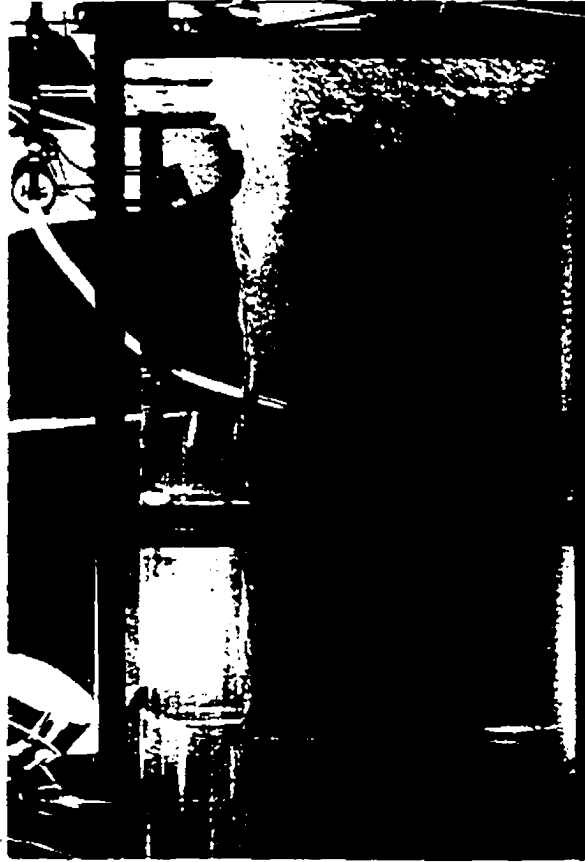
Two kinds of experiments were performed. One set of experiments was to determine mixing times at various experimental conditions. The second kind of experiment was to measure velocities in the tank in order to establish a characteristic velocity profile. A brief description of the experimental procedure is given below.

1. Mixing Time Determinations

Mixing times were determined by using Rhodamine B dye as a tracer. A concentrated solution of the tracer (10 gm/l) was injected on the



(b)



(a)

FIGURE 4.2 - Photographs of Air Agitated Tank

(a) Side View (b) Top View

diffuser side of the tank, as shown in Figure 4.1. On the other side of the tank, a sample was drawn continuously and its concentration was measured using a Turner Fluorometer (Model 111). The concentration-time curves were plotted using a chart recorder connected to the Fluorometer. A typical concentration-time curve is shown in Figure 4.3. Through replicate runs, the reproducibility of the mixing times reported in this work has been estimated to be ± 5 seconds.

2. Velocity Measurements

Velocity Measurements were made by a small current meter manufactured by A. OTZ KEMTEN (Type C1). The propeller used with the current meter was of 1.2 inch diameter. With this propeller the velocity measurements are effectively averages over an area of approximately one square inch. The equations that were used to calculate the water velocity are as follows.

$$u = 0.1289 n + 0.249 \text{ for } n < 1.68$$

$$u = 0.1797 n + 0.164 \text{ for } n > 1.68$$

where

u = horizontal velocity, ft/sec

n = number of revolutions of propeller per second

The current meter was investigated with respect to the nature of its observations from flows at different inclination to the propeller (yaw angle). By use of a flume, measurements were made at yaw angle of 0° , 20° , 45° and 90° . The actual velocities as measured are compared to expected values according to the formula $u_{\max} \cos \alpha$, as shown in Table 4.1. It can be seen that velocity estimates are quite close to the actual observation. The possible errors resulting from the current meter being at an angle

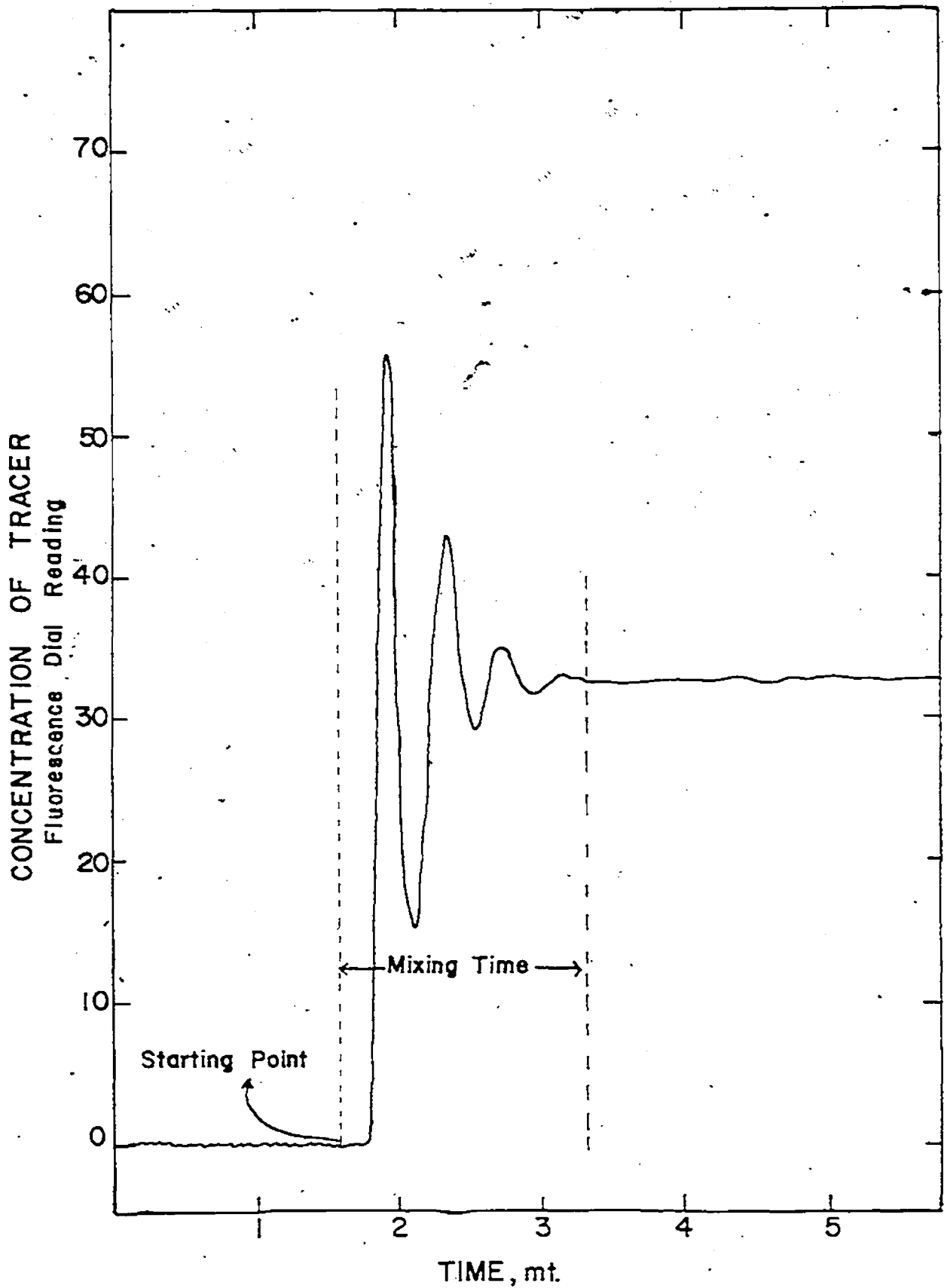


FIGURE 4.3- CONCENTRATION VS TIME CURVE
FOR RUN 5 (EXPERIMENT)

TABLE 4.1
Effect of Yaw Angle on Measured Velocity

Run	Yaw Angle α degrees	Measured Velocity ft/sec	Velocity Estimated from $u_{\max} \cos \alpha$ ft/sec*	% Error **
1	0	0.810	0.810	---
2	20	0.762	0.761	0.13
3	45	0.601	0.573	4.70
4	90	0	0	0

* u_{\max} = velocity at zero degree Yaw angle, ft/sec

** % error = $\frac{\text{measured velocity} - \text{estimated velocity}}{\text{measured velocity}} \times 100$

different than zero degrees may thus be estimated using the following expression

$$\% \text{ error} = \frac{u_{\max} - u_{\max} \cos \alpha}{u_{\max}} \times 100 = (1 - \cos \alpha) \times 100 \quad 4.1$$

where u_{\max} = velocity measured at zero degree of yaw angle, ft/sec
 α = yaw angle in degrees

Thus a 10° alignment of the current meter would produce an error of 1.5%. The current meter with yaw angle of zero degrees was further calibrated against a calibrated MINIFLO current meter (Type 265). It was found that the accuracy of the velocity measurements was $\pm 3\%$. During the measurements of the surface velocity, the propeller of the current meter was kept 2 inches below the water surface to keep it covered with water at all times. The bottom velocity was also measured 2 inches above the bottom of the tank.

The results from mixing time determinations and velocity measurements are presented in the next section.

C. The Experimental Results

1. The Mixing Time and Velocity Data

In all, seventeen experimental runs were made. The results are tabulated in Table 4.2. The depth of liquid content could be varied from 1.5 feet to 3.5 feet and the length of the tank, which was 8 feet for the first eleven runs, was altered to 6 feet and 4 feet for the next six runs. In order to make use of the entire capacity of the flow meter,

TABLE 4.2

Mixing Time and Velocity Data

Run	Depth H Feet	Length L Feet	Air Flow Rate Scfm	Surface Velocity Ft/sec	Bottom Velocity Ft/sec	Mixing Time From Experiments
1	3.5	8	17.82	2.15	1.29	121
2	3.5	8	9.45	1.54	1.00	141
3	3.5	8	3.85	1.19	0.81	197
4	3.0	8	15.28	2.07	1.25	98
5	3.0	8	8.10	1.28	0.94	110
6	3.0	8	3.30	1.00	0.71	187
7	2.0	8	15.28	1.34	0.85	65
8	2.0	8	10.18	1.03	0.69	79
9	2.0	8	5.40	0.98	0.58	83
10	2.0	8	2.20	0.70	0.44	111
11	1.5	8	15.28	1.11	0.58	63
12	3.5	6	13.37	2.11	1.33	100
13	2.0	6	11.46	1.75	1.25	91
14	2.0	6	7.64	1.40	0.84	74
15	3.5	4	8.91	2.26	1.45	91
16	3.0	4	7.64	2.11	1.40	85
17	2.0	4	5.09	1.53	0.90	76

the experiments were carried out at air flow rates ranging from 2.2 scfm to 17.82 scfm.

In one particular run (run 4) velocity measurements were made at regularly spaced locations in order to establish a characteristic velocity profile. For the other sixteen runs, only surface and bottom velocities at mid length of the tank were measured. The results from run 4 for the detailed velocity measurements are presented in the next section.

2. The Characteristics Velocity Profile Determination

In order to characterize the mixing process in the air agitated tank, it is first necessary to establish the nature of the velocity profile within the tank. Correlations for velocity profile were obtained in this work by carrying out one detailed run for which actual velocity measurements were made at closely spaced points in a three dimensional grid. For this run, the water depth and the length of the tank were 3.0 feet and 8.0 feet respectively and the air was introduced at the rate of 15.28 scfm. The magnitude and the direction of horizontal velocity were obtained at points on the grid by means of the current meter. The size of the grid near the diffuser was 6 inch x 6 inch x 6 inch (length x width x height), whereas after two feet distance from the diffuser the grid size was increased to 1 foot x 6 inch x 6 inch. The velocity data for a distance 4 feet from the diffuser are given in Table 4.3. The rest of the data are given in Appendix C.

TABLE 4.3
Velocity Data for Run 4

(+ ° Flow away from Diffuser, - ° Flow towards Diffuser).

Distance from one side of the tank ft. Liquid Depth from Bottom ft.	Velocity - 'u' ft/sec - 4.0 ft from diffuser					Average Velocity ft/sec	Direction of flow
	0.125	0.625	1.125	1.625	2.125		
3.0	2.04	2.10	2.10	2.07	2.02	2.07	+
2.5	0.94	1.13	1.40	1.20	0.96	1.13	+
2.0	-	-	-	-	-	-	random
1.5	-	-	-	-	-	-	random
1.0	0.70	0.68	0.79	0.75	0.71	0.73	-
0.5	0.93	0.97	1.14	0.98	0.95	1.00	-
0.0	1.29	1.22	1.28	1.24	1.23	1.25	-

A typical velocity profile for the tank is shown in Figure 4.4. The velocity data have been averaged over the width and are plotted against the depth. Positive and negative signs indicate the direction of the horizontal velocity. Positive sign is taken to be the direction away from the diffuser. During the experiments, it was observed that the propeller changed direction randomly for depths of 1.5 and 2.0 feet. A smooth velocity profile can only be drawn if the velocities for these points are obtained by interpolation from either end. In drawing the velocity profile the requirements to be met is that the areas under the positive and negative velocity zones be equal. From the velocity profiles, the next step is the calculation of integrated velocities. This is conveniently accomplished by starting the calculation from the point of zero velocity. The details of the calculation are given in Appendix C. The integrated velocities for four longitudinal distances are shown in Figure 4.5. From this figure, it is possible to obtain directly the streamlines of flow within the tank, as shown in Figure 4.6.

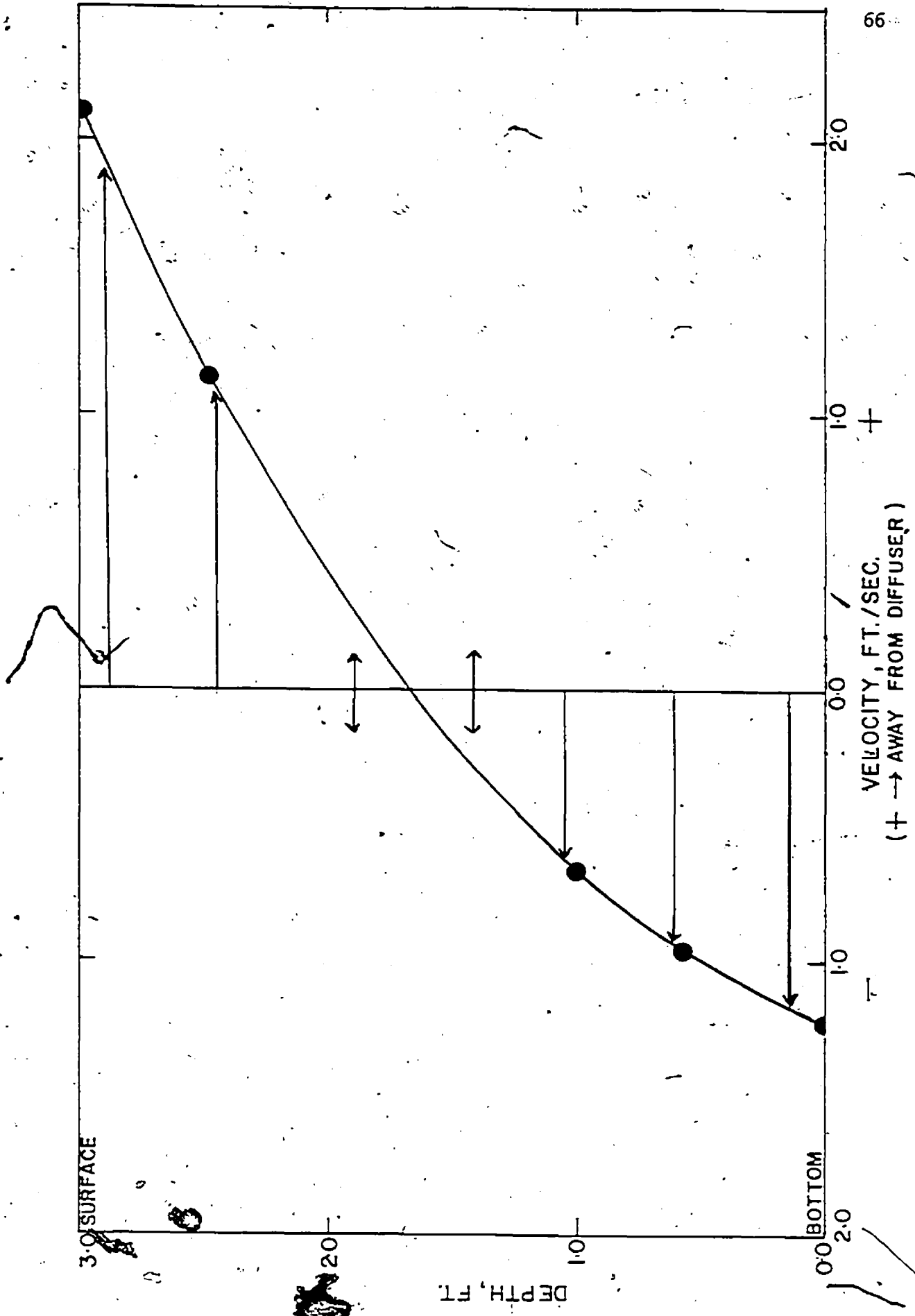


FIGURE 4.4— VELOCITY PROFILE, 4.0 FEET FROM DIFFUSER (RUN 4)

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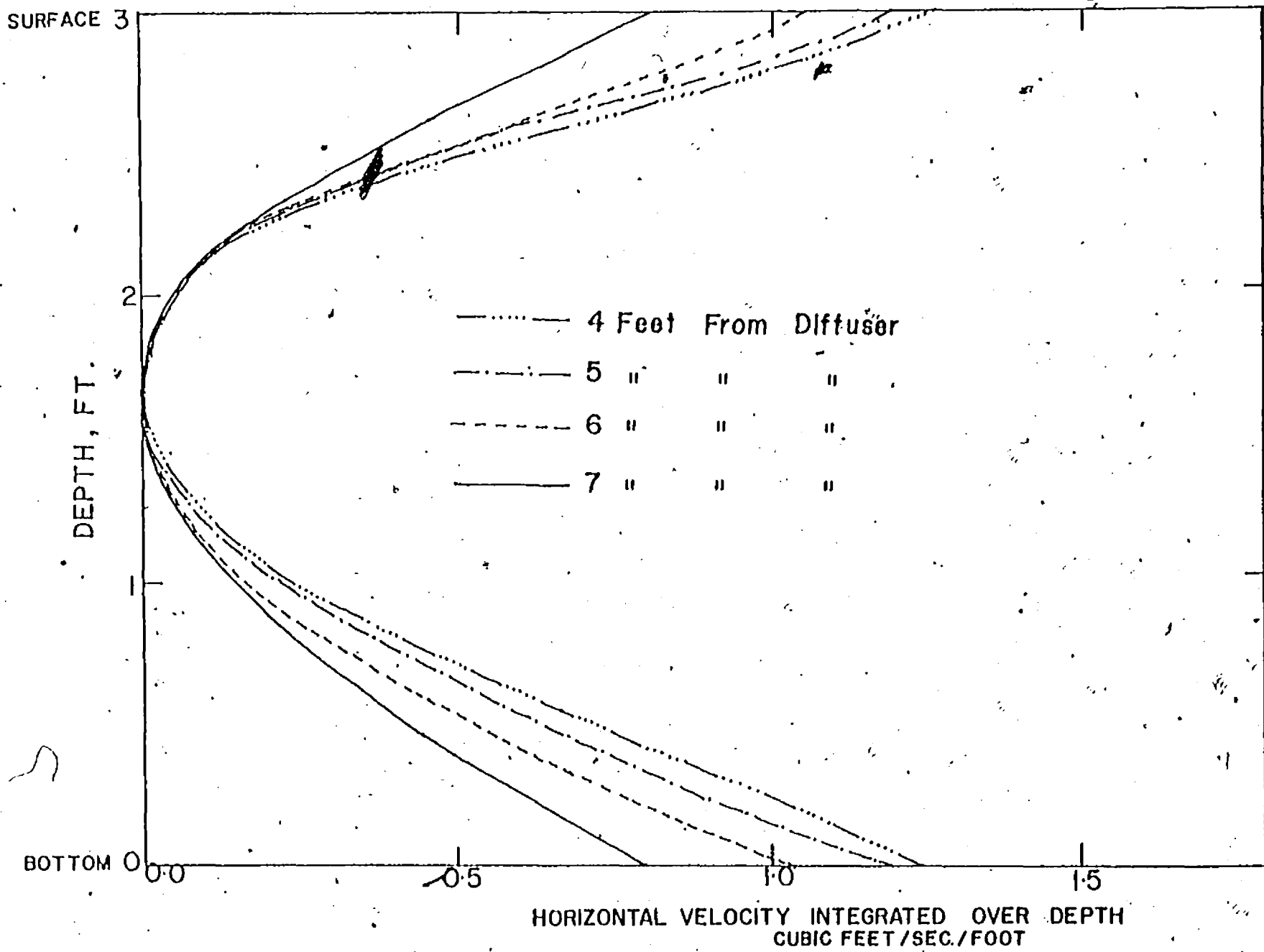
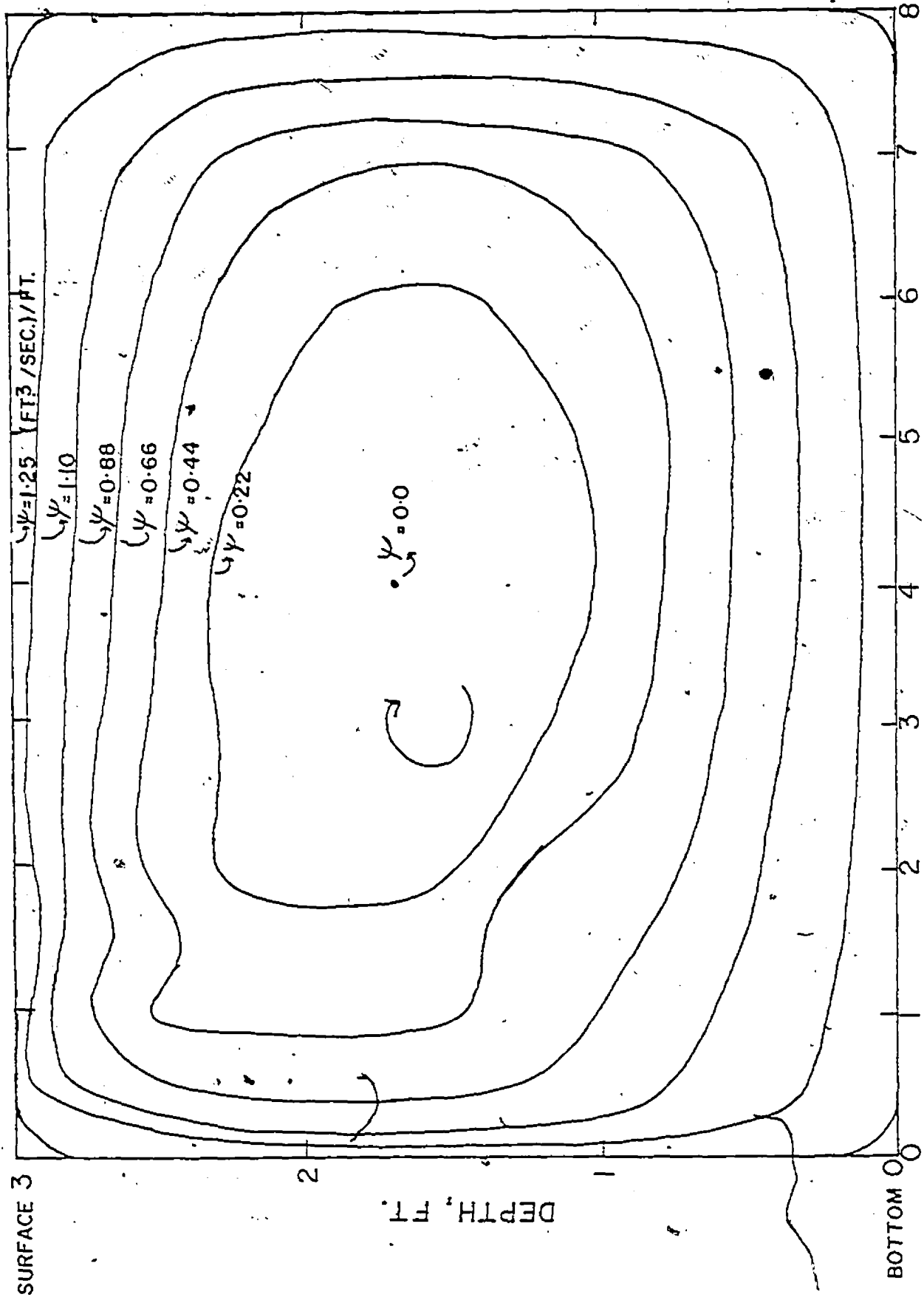


FIGURE 4.5— INTEGRATED HORIZONTAL VELOCITY VS. DEPTH



LONGITUDINAL DISTANCE FROM DIFFUSER, FT.
 FIGURE 4-6—STREAMLINES OF FLOW PATTERN IN THE TANK

V. MIXING IN AIR AGITATED TANK: THE MODEL

The general mathematical description of the phenomena of mixing under turbulent conditions was shown in Chapter II to pose a formidable challenge even with the fast computers. It was pointed out that simplified descriptions which ignore certain terms based on order of magnitude considerations have been investigated by various researchers for various mixing situations. The experimental results reported in Chapter IV indicate that none of the existing mixing models would be adequate in describing batch mixing in an air agitated tank. Therefore, a new model has been developed for this situation in the present work.

A. The Mixing Model Equations

The velocity profile established by the detailed run described in Chapter IV allows one to develop an appreciation of the nature of flow in air agitated tank. The forced vortex shape of the velocity profile indicates that the rising air bubbles generate a circulation pattern that is responsible for the mixing phenomena. A possible mathematical description of the mixing process may be obtained by keeping only the longitudinal and

vertical terms in the general equation 2.8. The proposed model, therefore, utilizes an unsteady mass balance equation containing convective flow terms superimposed by turbulent diffusion, as follows:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + w \frac{\partial c}{\partial z} = \frac{\partial}{\partial x} \left(E_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial z} \left(E_z \frac{\partial c}{\partial z} \right) \quad \dots 5.1$$

where

c = concentration of tracer at any point, lbm/ft³

u, w = velocity components in x (longitudinal) and z (vertical) directions respectively, ft/sec

E_x, E_z = turbulent diffusion coefficients in the x , and z directions respectively, ft²/sec

The model equation 5.1 is solved with the following initial and boundary conditions.

Initial Condition:

$$\text{for } t = 0 \quad c(0,0,0) = c_0$$

Boundary Conditions:

$$\text{at } x = L, \quad \frac{\partial c}{\partial x} = 0 \quad \text{for all } t \quad (\text{due to solid boundary})$$

$$\text{at } x = 0, \quad \frac{\partial c}{\partial x} = 0 \quad \text{for all } t \quad (\text{due to solid boundary})$$

$$\text{At } z = H, \quad \frac{\partial C}{\partial z} = 0 \quad \text{for all } t \quad (\text{due to liquid surface})$$

$$\text{At } z = 0, \quad \frac{\partial C}{\partial z} = 0 \quad \text{for all } t \quad (\text{due to solid boundary})$$

where

L = length of the tank, ft

H = depth of the liquid content, ft

The velocity terms in the model equation 5.1 can be determined from the stream function correlations. However, major difficulties arise in estimating the turbulent diffusion coefficients. These items are now discussed in turn.

B. Estimation Of The Velocity Terms

The velocity profile in the tank was established in terms of stream functions in Chapter IV. According to the definition of a stream function, the horizontal and vertical components of velocity can be obtained by differentiations:

$$u = \frac{\partial \psi}{\partial z} \quad \dots 5.2$$

$$w = - \frac{\partial \psi}{\partial x} \quad \dots 5.3$$

It is therefore desirable to obtain stream function correlations which can then be used to compute the velocity components. The following equations of elliptical form were tested for fit to the normalized profile.

$$\psi = k - C' \cdot [(x^2 - a^2)(z^2 - b^2)] \quad \dots 5.4$$

$$\psi = k - C' \cdot [((x^2 - Ae^{-k((x-A)^2 + (z-B)^2)})^2 - a^2)(z^2 - Be^{-k((x-A)^2 + (z-B)^2)})^2 - b^2] \quad \dots 5.5$$

$$\psi = k - C \cdot [((x^2 - Ae^{-k((x-A)^2 + (z-B)^2)})^2 - A^2)((z^2 - Be^{-k((x-A)^2 + (z-B)^2)})^2 - B^2)] \quad \dots 5.6$$

$$\psi = k - C \cdot [(x^2 - A^2)(z^2 - B^2)] \quad \dots 5.7$$

where

$$k = \psi_{\max} \text{ ft}^3/\text{sec ft}$$

$$\psi_{\max} = \text{maximum stream function (rate of liquid circulation per foot), ft}^3/\text{sec ft.}$$

$$C' = \psi_{\max}/a^2 b^2$$

$$C = \psi_{\max}/A^2 B^2$$

a = half of the length of the tank, ft

b = half of the liquid depth, ft

A = longitudinal distance from the point of zero velocity to either end of the tank, ft

B = vertical distance from the point of zero velocity to either the liquid surface or the bottom of the tank, as appropriate, ft

Equations 5.4 and 5.5 did not fit the ψ -data too well while 5.6 and 5.7 gave satisfactory fits. In subsequent model building equation 5.7 has been used.

Equation 5.7 is differentiated to estimate the velocity components u and w.

$$u = -2zC (x^2 - A^2) \quad \dots 5.8$$

$$w = 2xC (z^2 - B^2) \quad \dots 5.9$$

In order to use equations 5.8 and 5.9, only two parameters, namely ψ_{\max} and B, need to be determined, since $A = L/2$ and $C = \frac{\psi_{\max}}{A^2 B^2}$. In the detailed run, as described previously, the parameters of equations 5.8 and 5.9 were estimated from the actual profile. However, this would be an unwieldy requirement for a practical mixing model. The following procedure that minimize the data requirements was developed and used for all runs other than run 4. It is possible to estimate ψ_{\max} and B from just two velocity points, one at the surface and other at the bottom. Both of these

measurements have to be performed at mid length of the tank. The location of the zero stream function is then found by drawing two triangles of equal areas on the velocity vs depth plot, as shown in Figure 5.1. The value of B is the depth from the top or bottom of the tank, as appropriate, whereas ψ_{\max} is the area of either triangle.

C. Estimation of Parameters E_x and E_z

In open channel flow where irrotational flow patterns exist the values of E_x and E_z correspond directly to E_t and E_n (tangential and normal diffusion coefficients) respectively. But for rotational flow, such as encountered here, E_x and E_z have to be estimated from corresponding values of E_t and E_n , as follows

$$E_x = E_t \cos \theta - E_n \sin \theta \quad \dots 5.10$$

$$E_z = E_t \sin \theta + E_n \cos \theta \quad \dots 5.11$$

where

$$\theta = \tan^{-1} \frac{w}{u} \quad \dots 5.12$$

The methods for estimating values of E_t and E_n are now presented.

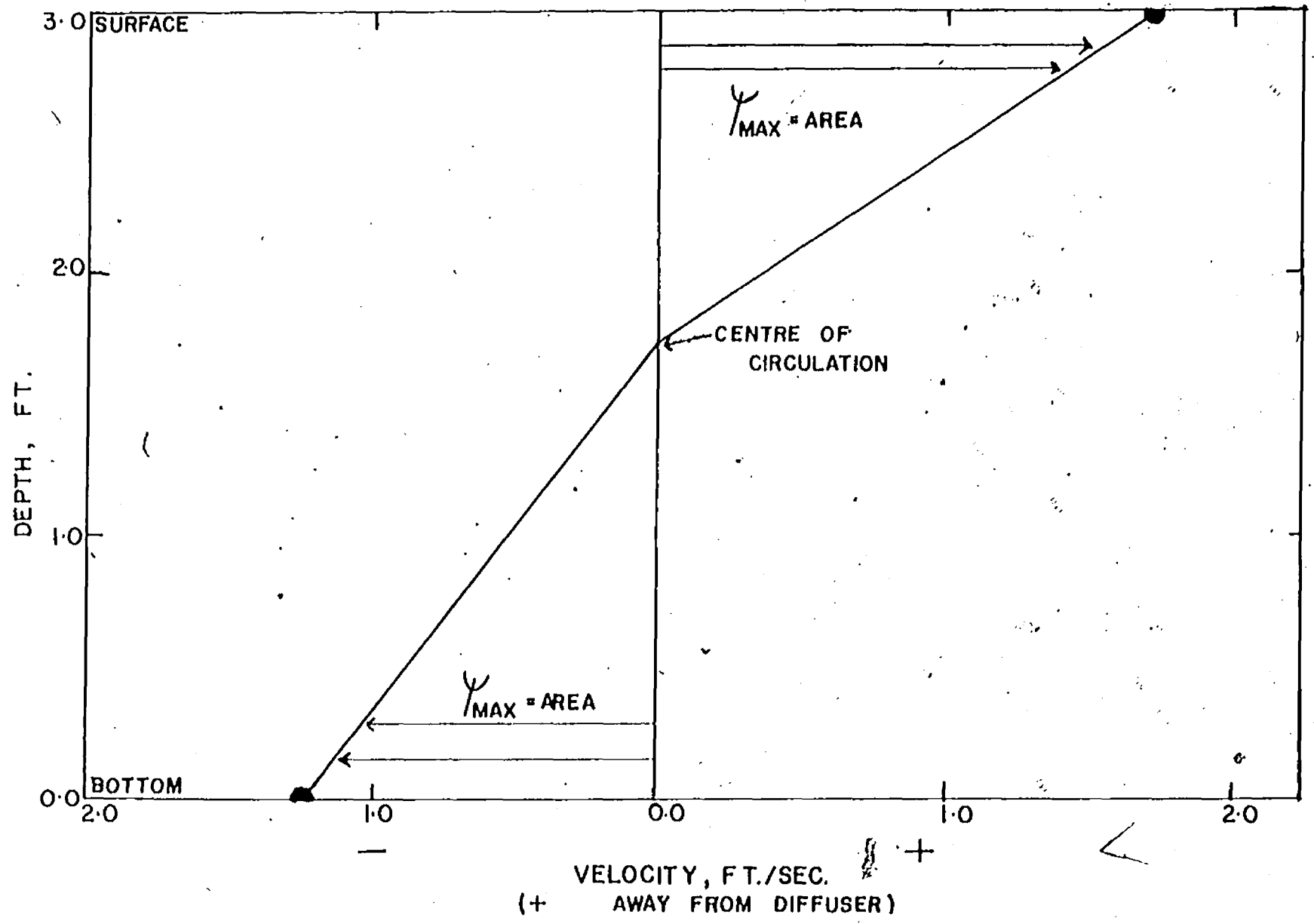


FIGURE 5-1 — DETERMINATION OF VELOCITY PARAMETERS, RUN 13

I. Tangential Turbulent Diffusion Coefficient ' E_t '

The tangential turbulent diffusion coefficient may be estimated directly from the corresponding correlations of longitudinal turbulent diffusion coefficients obtained for irrotational flow.

As discussed in Chapter II, the correlation is as follows:

$$E_t = \lambda H u^* \quad \dots 5.13$$

where

u^* = is shear velocity, ft/sec and H is the depth of the liquid flow, ft. λ is a non-dimensional longitudinal turbulent diffusion coefficient defined as E_t/Hu^*

It was pointed out in Chapter II that the numerical value of λ in equation 5.13 is reported to be different by various investigator. Typical values of λ are shown in Table 2.1. In this present work, λ is considered to be an adjustable model parameter and a tentative correlation for estimating its value has been obtained (discussed in section E of this chapter).

Equation 5.13 can be converted in terms of v_{max} . The shear velocity u^* can be written as

$$u^* = \bar{u} \sqrt{2f_f} \quad \dots 5.14$$

where

\bar{u} = average velocity, ft/sec

f_f = Fanning's friction factor

Substituting $f_f = 0.005$ for turbulent flow, equation 5.14 becomes

$$u^* = 0.1 \bar{u} \quad \dots 5.15$$

Substituting equation 5.15 into equation 5.13 and writing \bar{u} in term of ψ_{\max} , one gets

$$E_t = 0.1 \lambda \psi_{\max} = m \psi_{\max} \quad \dots 5.16$$

where

$$m = 0.1 \lambda$$

2. Normal Turbulent Diffusion Coefficient ' E_n '

The normal turbulent diffusion coefficient may be estimated directly from the corresponding correlation of vertical turbulent diffusion coefficients obtained for irrotational flow. As discussed in Chapter II, this correlation is as follows:

$$E_n = 0.067 Hu^* \quad \dots 5.17$$

Substituting equation 5.15 for u^* in correlation 5.17 one gets

$$E_n = 0.0067 \psi_{\max} \quad \dots 5.18$$

It should be noted here that the correlation 5.17 for the normal turbulent diffusion coefficients has been obtained theoretically by Vanoni (25) based on logarithmic profiles. Therefore correlation 5.18 is applicable only for logarithmic profiles. However, using

a similar analysis one may obtain a correlation for the normal turbulent diffusion coefficient using velocity profile obtained in this present work.

Using Reynolds analogy the normal diffusion coefficient may be defined as

$$E_n = \frac{\tau}{\rho \frac{d\bar{u}}{dz}} \quad \dots 5.19$$

where

τ = shear stress

ρ = density of the fluid

Writing the shear stress in terms of wall shear stress and substituting for \bar{u} from equation 5.8, one gets

$$E_n = \frac{\tau_0 z/B}{\rho(4/3 CA^2)} \quad \dots 5.20$$

where

τ_0 = wall shear stress = $u^{*2} \rho$

Replacing u^* by equation 5.15 and transforming in terms of ψ_{\max} yields

$$E_n = 0.0032 \psi_{\max} \quad \dots 5.21$$

Correlation 5.21 differs from correlation 5.18, which was based on logarithmic velocity profile, by a factor of 2.

D. Model Results

The model equation 5.1 with the help of equations 5.8 and 5.9 for velocity terms and equations 5.16 and 5.21 for turbulent diffusion coefficients was solved on a computer using an Alternating-Directions implicit technique. The details of the numerical solution of the model equation are given in Appendix D. A brief summary is given below.

To start the solution, a grid size of 0.5 x 0.5 feet and $\Delta t = 0.1$ second was selected and the finite difference approximation was applied to each grid point. This resulted in a number of simultaneous equations in terms of unknown concentration terms. These simultaneous equations were then solved using Gauss's elimination method to give a concentration profile. Figure 5.2 illustrates a typical result from the model for the concentration profile at the location where the sample was drawn for mixing time determination. This concentration profile is for run 5, for which the experimental profile is shown in Figure 4.3. On comparison of these two figures, it is apparent that the periodical oscillations

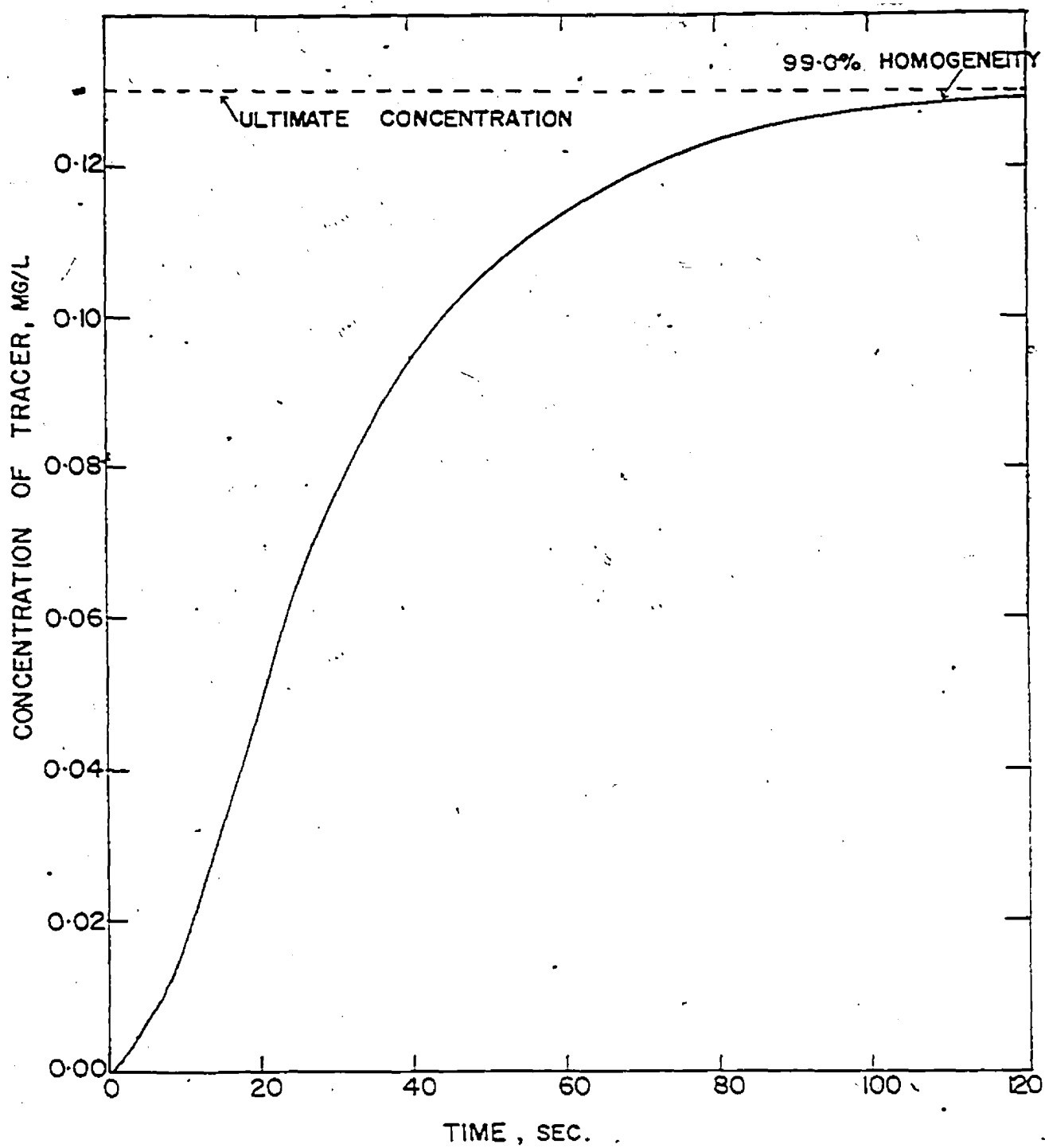


FIGURE 5.2— MODEL RESULT FOR RUN 5

of the concentration have been damped in the model results. According to McCorqudale (47), this is a common behaviour for the implicit technique of computation. In the implicit technique, the convective instability gets averaged which, in turn, averages out any periodic distribution. Fromm (48) has also solved a similar kind of equations for flood routing problem and his results lead to the same conclusion. Explicit technique for solving the proposed model equation did not work out since it gave a highly unstable results. Therefore, the implicit technique was used at the cost of damping out any periodical oscillation and the results, so obtained, seem reasonable, in that the end result, i.e the mixing time is reasonable.

The mixing times from the model equation are defined to be the times necessary to reach a certain degree of homogeneity of the contents in the tank. For each time step, concentration at the particular location from where the sample was drawn during the tracer work, was found and the extent of the homogeneity estimated from the following expression.

$$\text{Percent Homogeneity} = \frac{\text{concentration of the tracer at time } t}{\text{ultimate concentration of the tracer}} \times 100$$

A homogeneity of 99% was considered to correspond to complete mixing.

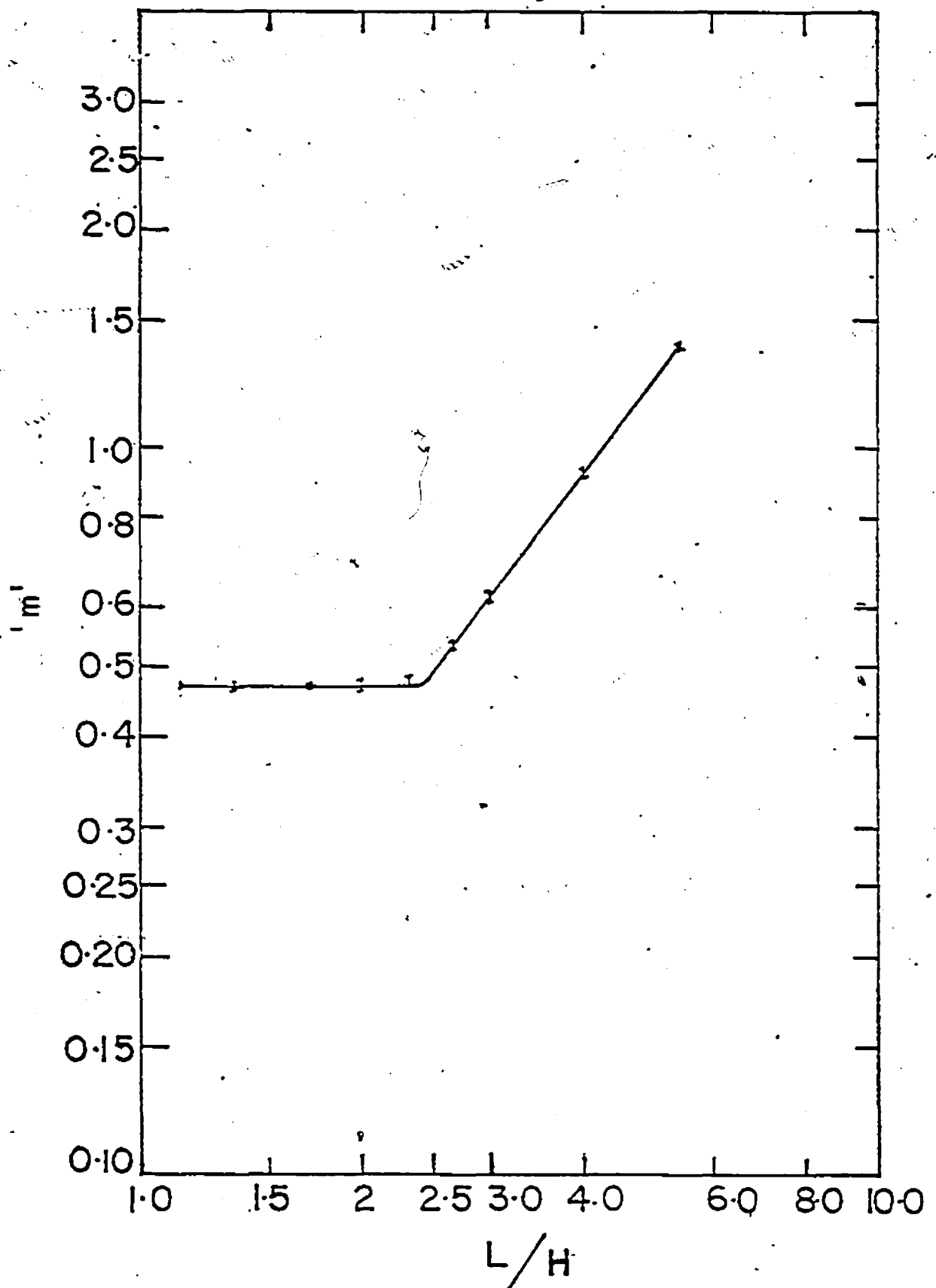
E. Comparison of Model Results to Experiments:

The calculated mixing times from model for achieving 99% homogeneity are compared with those obtained experimentally in Table 5.1. In order to obtain the mixing times from the model the tangential turbulent diffusion coefficient was estimated from equation 5.16 as a product of m and ψ_{\max} . The value of m was considered to be an adjustable parameter, in that for each run a value that gave a mixing time close to that obtained experimentally was selected. As shown in Table 5.1, the values of m vary from 0.46 to 1.39. These values correspond to λ values from 4.6 to 13.9 as defined by equation 5.16. It should be noted here that a similar range of values of λ has been reported by various investigators for open channel flows (Table 2.1).

A tentative correlation for calculating m may be obtained, based on the data of Table 5.1. On an intuitive basis, the tangential turbulent diffusion coefficient E_t may be expected to be a function of air flow rate Q_a , length L and depth H . Since ψ_{\max} is itself a function of air flow rate, as seen in Table 5.1, it was postulated that m should be a function of only L and H . On this basis, the values of m were plotted against the ratio $\frac{L}{H}$. In Figure 5.3, it is observed that for a length to depth ratio of less than 2.5, the m values remain constant but for a ratio higher than

TABLE 5.1
 Summary of Results
 (Line Diffuser at one side of the tank)

Run	H Depth Feet	L Length Feet	Ratio L/H	Air Flow scfm	Mixing Time from Experiments secs	ψ max cu.ft./sec.ft.	Value of m in equat- ion 5.16	Mixing Time From Model secs
1	3.5	8	2.28	17.82	121	1.39	0.465	120
2	3.5	8	2.28	9.45	141	1.06	0.475	140
3	3.5	8	2.28	3.85	197	0.84	0.460	195
4	3.0	8	2.67	15.28	98	1.17	0.525	98
5	3.0	8	2.67	8.10	110	0.81	0.530	112
6	3.0	8	2.67	3.30	187	0.64	0.510	187
7	2.0	8	4.00	15.28	65	0.52	0.925	64
8	2.0	8	4.00	10.18	79	0.41	0.920	77
9	2.0	8	4.00	5.40	83	0.36	0.925	83
10	2.0	8	4.00	2.2	111	0.27	0.925	111
11	1.5	8	5.33	15.28	63	0.28	1.390	60
12	3.5	6	1.71	13.37	100	1.41	0.465	100
13	3.0	6	2.0	11.46	91	1.09	0.475	90
14	2.0	6	3.0	7.64	74	0.52	0.62	74
15	3.5	4	1.14	8.91	91	1.55	0.465	91
16	3.0	4	1.33	7.64	85	1.26	0.46	84
17	2.0	4	2.0	5.09	76	0.57	0.48	79

FIGURE 5.3— $'m'$ VS RATIO L/H

2.5, the n or m values may be correlated linearly to L/H . Thus

$$m = 0.47 \frac{L}{H} < 2.5$$

$$m = 0.13 \left(\frac{L}{H}\right)^{1.41} \quad 2.5 < \frac{L}{H} < 5.33 \quad \dots 5.22$$

The correlation represented by equation 5.22 is applicable only for the range L and H covered in this investigation, and cannot at this stage be considered to be established beyond question.

F. Extension of Mixing Model:

In order to investigate possible use of the proposed mixing model for the cases in which the line diffuser is kept at mid length of the tank, three experimental runs were made. The results are summarized in Table 5.2. In these runs the line diffuser was kept at mid length of the tank, i.e., 4 feet from either side of the tank. This way the full tank was virtually divided into two sections separated by the cone of air - water mixture.

In Table 5.2, the mixing time data obtained experimentally are compared with those computed using the mixing model developed in the previous sections. It appears that the mixing model gives

TABLE 5.2

Summary of Results
(Line Diffuser at Mid.Length of the Tank)

Run	Diffuser Position	Depth of Tank ft	Length of Tank ft	Length Used in Model ft	Air Flow Rate		Surface Velocity ft/sec		Bottom Velocity ft/sec		Mixing Time From Experiments secs	Mixing Time From Model secs
					scfm	Per unit Width Per Section of The Tank scfs/ft	Sec. 1	Sec. 2	Sec. 1	Sec. 2		
42	Diffuser	3	8	4	16.28	0.0567	1.223	1.232	0.80	0.81	90	134
43	at Mid	3	8	4	8.1	0.0303	0.935	0.92	0.597	0.570	118	181
44	Length of the Tank	2	8	4	10.18	0.0378	0.796	0.774	0.535	0.495	75	160
16	Diffuser	3	4	4	7.64	0.0567	2.11		1.40		85	84
17	at one side of tank	2	4	4	5.09	0.0378	1.53		0.90		76	79

* = Section

higher mixing times than those observed experimentally. This could be due to the fact that lower surface and bottom velocities were observed in these runs as compared to those under similar condition of air flow rate for diffuser on the side runs. Lower velocities give rise to lower ψ_{max} and as a result lower values of longitudinal and lateral turbulent diffusion coefficients are estimated from correlations 5.16 and 5.21 respectively.

It should be noted here that the movement of the liquid in each section of the tank was observed to be quite different from that observed in cases in which the diffuser was placed at one side of the tank. It was observed that the cone of air water mixture was not still on the line diffuser but oscillated along the centre of the diffuser, as shown in Figure 5.4.

The frequency of oscillation was found to increase with airflow rates. Due to this oscillation the movement of the liquid in each section could be quite different from that established for the case where the line diffuser was kept at one side of the tank. One could describe this liquid agitation best by analogy to the washing action in a washing machine.

Based on these limited observations one can only conclude that further investigations with a wider variation of depth, length and air flow rates are necessary before a model procedure

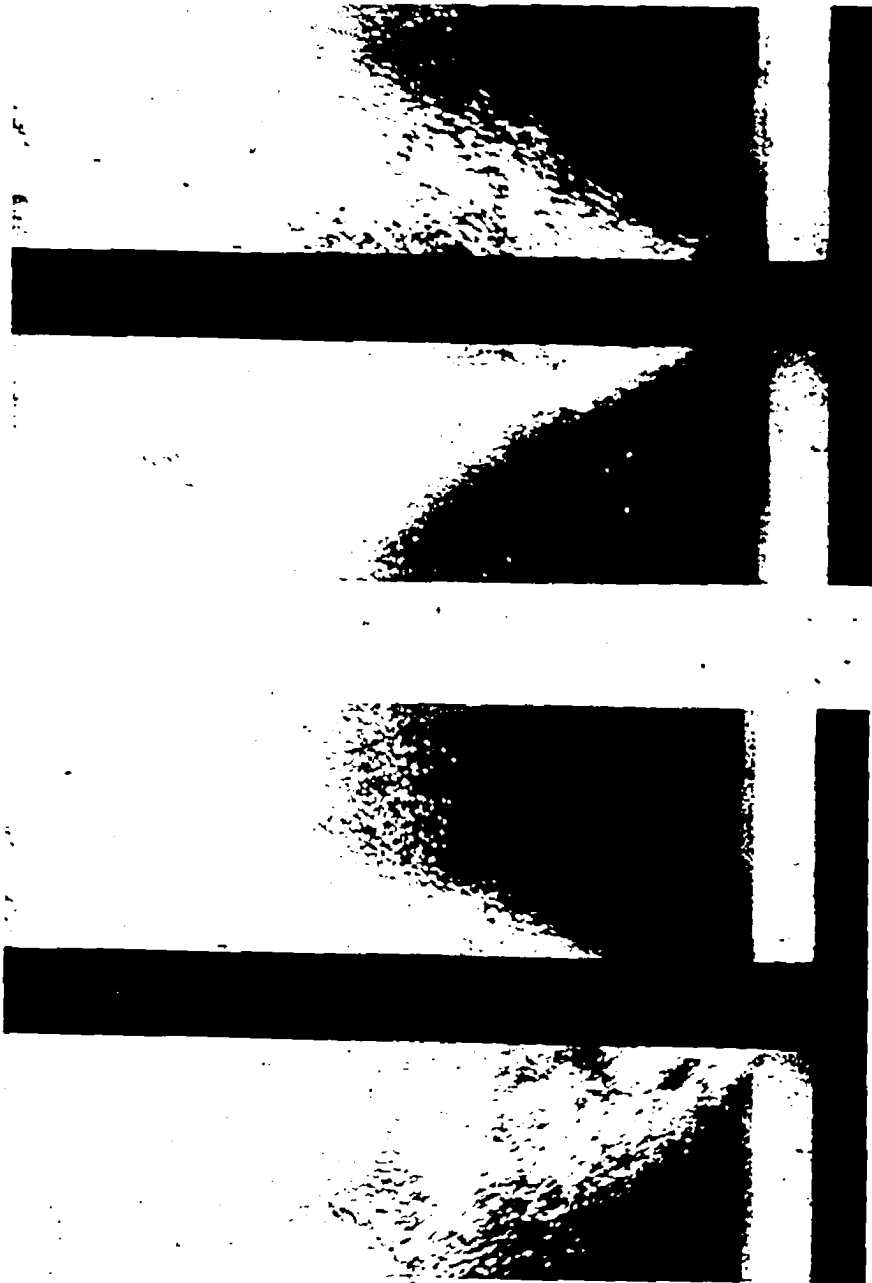


FIGURE 5.4 - Diffuser at Mid Length of the Tank

can be definitely recommended for this situation.

VI. USE OF MIXING MODEL IN DESIGN OF AIR AGITATED TANKS

A. The Design Problem

The design of air agitated mixing tanks involves the selection of the kind of diffuser, location of the diffuser, size and geometry of the tank and the air flow rate to be used. Generally three main kinds of diffusers, namely pipe, line and circular diffusers are used in the air agitated tanks of rectangular and circular shape. Since the mixing model developed in this work was based on studies done with line diffuser only, the design procedure developed will also apply only to tanks of rectangular shape with line diffusers located at or near the bottom of one side of the tank. However, as will be discussed in the next section, the circulation velocities induced in the tanks do not necessarily seem to depend upon the kind of diffuser as long as the diffuser is placed at one side of the tank.

In selecting the size and the geometry of the mixing tank, the conventional practices are the usual guide. Most air agitated tanks in North America are of rectangular geometry and have a liquid depth of about 15 feet, although tanks less than 9 feet deep have also been constructed (49). The selection of the depth of the tank

3

is governed in part by the foundation and construction costs and in part by power costs and mixing efficiency (1). Generally, for air agitated tanks, the ratios of width to depth, $\frac{W}{H}$, and length to depth, $\frac{L}{H}$, are maintained between 1 to 2 and 3 to 4 respectively (49). If the volume of the tank is fixed based on the amount of water to be treated, then decisions regarding $\frac{W}{H}$ and $\frac{L}{H}$ ratios are currently made using rules of thumb such as quoted above. There appears to be no information available relating geometry to mixing efficiency.

The decision on the air flow rate to be fed is an important one. The power requirement for the process is a function of the air flow rate. The selection of the air flow rate is also related to the objective of the water treatment in question. If the purpose is to mix the contents of the tank within a specified time, then the mixing time should be the basis for design. In other words, the mixing time would appear to be a suitable design criterion to determine whether a certain air flow rate would induce enough agitation to achieve homogeneity of the tank contents within a specified time. In water treatment, rapid mixing is an example of processes for which mixing time is an important parameter. The purpose of rapid mixing process is to insure uniform distribution of a coagulating agent within a short time. The mixing time in such a processes is recommended to be less than one minute (1).

For such processes, the design procedure should be based on the mixing time criterion. The information about mixing time may be obtained using the mixing model presented in Chapter V. As indicated in the model development, the mixing model requires the surface and bottom velocities in the tank for computing the mixing time. In a typical design problem, these velocities are of course not available. The design procedure developed in this Chapter relies on the correlations that relate surface and bottom velocities to tank geometry and air flow rate. The detailed design procedure is presented in section C.

In some treatment processes, the objective is mainly to induce a certain degree of agitation in the tank rather than to achieve a particular degree of homogeneity. Flocculation process, which involves aggregation of coagulated particles into flocs is an example of treatment where the degree of agitation is more important than a definite mixing time. The term 'degree of agitation', however, is difficult to define. In a series of papers in chemical engineering on design principles for liquid agitation, researchers from Chemineer Inc. (34) have proposed bulk velocity as a measure of degree of agitation in mechanically agitated tanks. The bulk velocity, measured at approximately 2/3 of total height of tank, is considered to be directly proportional to a scale of agitation.

Tables are presented that relate scale of agitation to different process results. In water treatment plant design handbooks, (1,2,36) information regarding recommended bulk velocities for some processes is available along with the desired detention times. For example, the flocculation process is said to require a degree of agitation corresponding to a bulk velocity ranging from 0.1 to 3 ft/sec and a detention time of 10 mins to 60 mins. It is to be noted that the values suggested cover a rather wide range indicating that the design problem is somewhat open ended.

For air agitated batch tanks, there appears to be no existing criterion parallel to those available for mechanically agitated tanks. There are some difficulties for example in identifying a proper location for measuring bulk velocity. Due to the vortex nature of velocity profile one possible way is to define a bulk velocity as the arithmetic average of velocities in the upper and lower section of the tank. This is the approach suggested in this work. Complete details of design procedure for this case are given in the following sections.

B. Velocity Correlations

Three types of correlations were obtained to relate surface, bottom, and bulk velocities in air agitated batch tank to tank

geometry and air flow rate. As discussed in the previous section, these correlations are needed to develop appropriate design procedures. The data used for these correlations are those obtained in the present experimental study and those obtained in a previous study by Bewtra and Rao (50). The data are plotted in Figures 6.1 and 6.2. Bulk velocity ' u_B ' data are calculated from Table 4.1 using the following expression which is an arithmetic average of average velocities in upper and lower section.

$$u_B = \frac{(u_s/2) + (u_b/2)}{2} \quad 6.1$$

The above definition is consistent with a calculation based on the circulation rate for the tank. In the top section, bulk velocity may be calculated from the circulation rate as ψ_{\max}/B , where B is the distance from centre of circulation to the top of the tank. This quantity is identically equal to $u_s/2$. Similarly, for the bottom section, one gets a bulk velocity of $u_b/2$. Averaging over the two sections yields equation 6.1. Bewtra and Rao data do not permit a calculation of the bulk velocity because the surface and bottom velocities data were not obtained at the same air flow rate. However, the present investigation measured both surface and bottom velocities simultaneously and therefore permits such a calculation.

The influence of tank geometry and air flow rates on the magnitude of the induced velocities can be seen from Figures 6.1 and 6.2. It is evident that the surface and bottom velocities increase with an increase in air flow rate and the depth of the liquid content. The surface and bottom velocities may be hypothesized to be functions of ratio L/H and a parameter

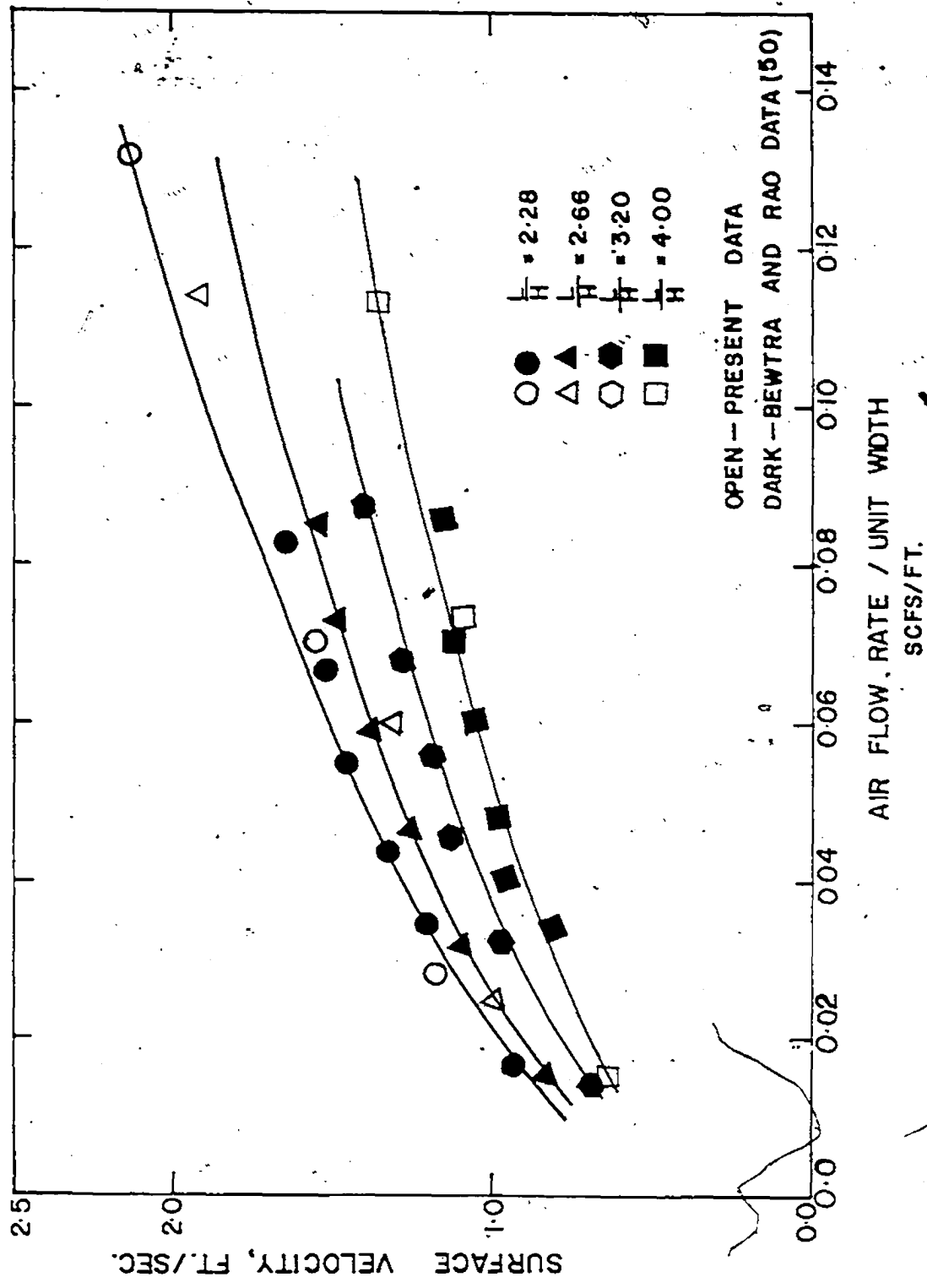


FIGURE 6-1 — SURFACE VELOCITY VS AIR FLOW RATE

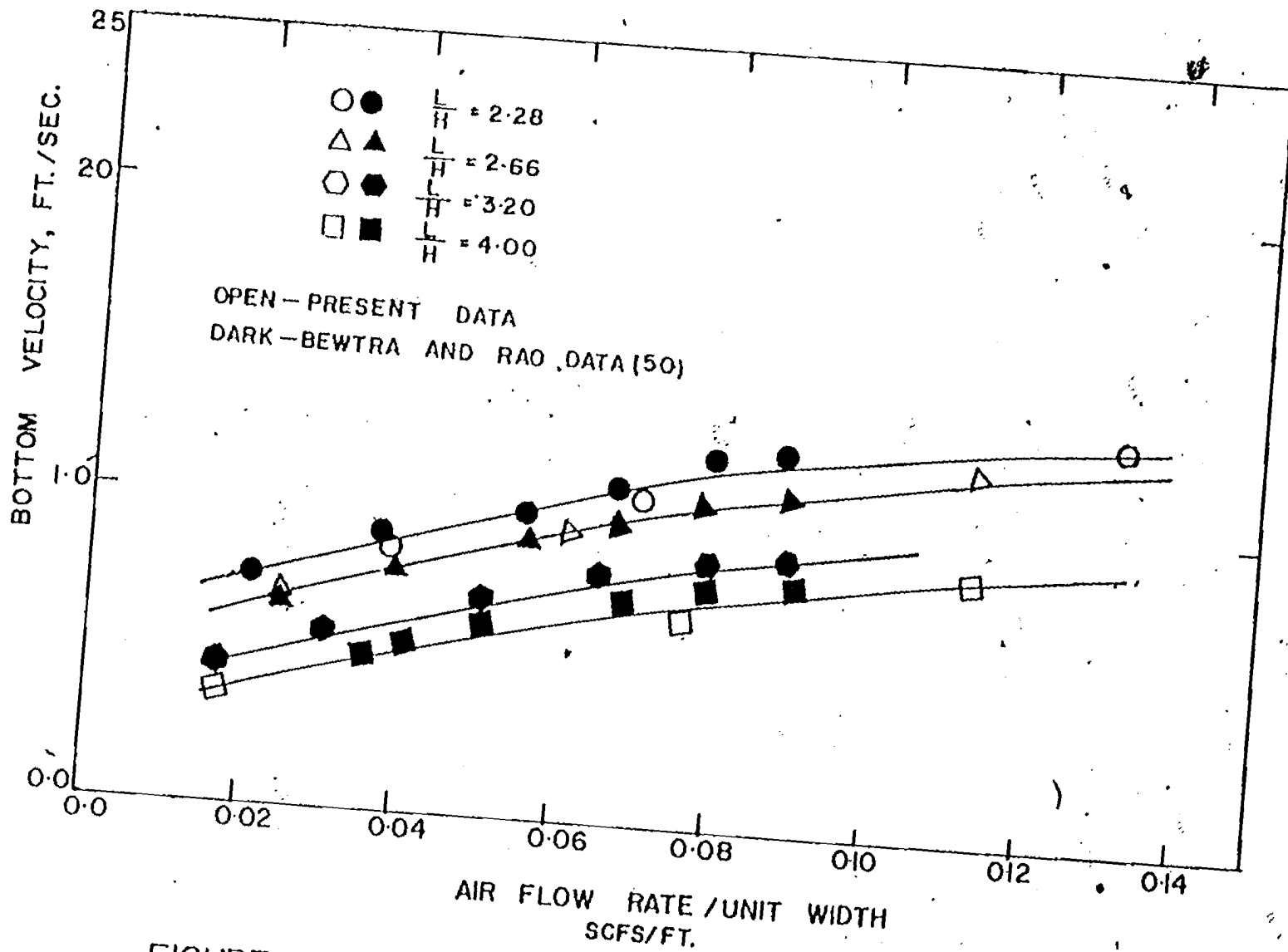


FIGURE 6-2 — BOTTOM VELOCITY VS AIR FLOW RATE

containing air flow rate. On this basis, following forms of correlations were tested for their goodness of fit to the surface, bottom and bulk velocity data using multiple linear regression (51).

$$u = A_1 \left(\frac{L}{H}\right)^{a_1} \xi^{b_1} \quad \dots 6.2$$

$$u = A_2 + A_3 \left(\frac{L}{H}\right)^{a_3} + A_4 \ln \xi \quad \dots 6.3$$

$$u = A_5 + A_6 \left(\frac{L}{H}\right)^{a_6} + A_7 \ln \xi + A_8 \left(\frac{L}{H}\right) \ln \xi \quad \dots 6.4$$

$$u = A_9 + A_{10} \ln \xi + A_{11} \left(\frac{L}{H}\right) \ln \xi \quad \dots 6.5$$

where

u = surface, bottom or bulk velocity, ft/sec

L = length of the tank, ft

H = depth of the liquid level, ft

ξ = parameter containing air flow rate, i.e., Q_a/W , Q_a/A' or Q_a/V

Q_a = air flow rate, ft³/sec at 70°F and 1 atmosphere

W = width of the tank, ft

A' = surface of the tank ($L \times W$), ft²

V = volume of the tank ($L \times W \times H$), ft³

$A_1, A_2, \dots, A_{11}, a_1$ and b_1 = correlation constants.

It was found that satisfactory correlations are obtained using either of the above variable sets (Q_a/W , Q_a/A' or Q_a/V). It was not possible to distinguish between the three possibilities on the basis of statistical fit alone. In order to check which combination is the most appropriate for scale up, several experimental runs were made in the small tank and results compared with those reported for a large scale tank in literature (52). Table 6.1 summarizes the details of the results. It appears the Q_a/W is the most appropriate parameter for scale up purposes.

All the above equations 6.2, 6.3, 6.4 and 6.5 with Q_a/W parameter were found to give statistically good fit with high correlation coefficients and low standard errors. Based on the goodness of fit and also due to its simple dimensional form, correlation 6.2 was chosen for use in the design procedure. The following equations were obtained for surface, bottom and bulk velocities.

$$u_s = 6.563 \left(\frac{Q_a}{W}\right)^{0.342} \left(\frac{L}{H}\right)^{-0.629} \quad \dots 6.6$$

TABLE 6.1

Results From Small and Large Tanks
 Large Scale Tank (24' x 4' x 14.4')
 Small Scale Tank (4' x 2.25 x 2.4)
 Ratio L/H = 1.66

W = width of the tank, A' = surface area of the tank (length x width), V = volume of the tank

Set No.	Tank Size	Air Flow Rate, Q_a Scfs	Surface Velocity ft/sec	Bottom Velocity ft/sec	Comment
1	Large	0.28	1.85	1.05	$Q_a/W = 0.07, Q_a/A' = 0.0029, Q_a/V = 0.0002$
	Small	0.157	2.00	1.20	$(Q_a/W)_{small} = (Q_a/W)_{large} = 0.07$
	Small	0.0261	1.02	0.73	$(Q_a/A')_{small} = (Q_a/A')_{large} = 0.0029$
	Small	0.00432	<0.50	<0.4	$(Q_a/V)_{small} = (Q_a/V)_{large} = 0.0002$
2	Large	0.52	2.33	1.62	$Q_a/W = 0.13, Q_a/A' = 0.0054, Q_a/V = 0.00038$
	Small	0.293	2.44	1.69	$(Q_a/W)_{small} = (Q_a/W)_{large} = 0.13$
	Small	0.0486	1.24	0.93	$(Q_a/A')_{small} = (Q_a/A')_{large} = 0.0054$
	Small	0.0082	0.67	0.50	$(Q_a/V)_{small} = (Q_a/V)_{large} = 0.00038$

$$u_{b \rightarrow} = 4.165 \left(\frac{Q_a}{W} \right)^{0.315} \left(\frac{L}{H} \right)^{-0.639} \dots\dots 6.7$$

$$u_B = 2.454 \left(\frac{Q_a}{W} \right)^{0.30} \left(\frac{L}{H} \right)^{-0.636} \dots\dots 6.8$$

Surface, bottom and bulk velocities calculated from above correlations are plotted against the experimental data in Figures 6.3, 6.4 and 6.5. In Table 6.2, predicted surface, bottom and bulk velocities are compared to experimental data obtained by Bewtra (52) for a larger scale tank. The first two runs are the same as reported in Table 6.1. These results suggest that the induced velocities are not affected by the kinds of diffuser as long as it is placed near one side of the tank. It should be noted that correlations 6.6-6.8 have been developed using air flow rates calculated at standard conditions (70°F and 1 atm.). An attempt was also made to develop correlations based on air flow rates calculated at the actual conditions existing at the bottom of the tank. This approach did not seem to result in improved correlations (see Appendix E).

The forms of equation 6.6-6.8 suggest that a dimensional explanation for these correlations may be possible. However, conventional dimensional analysis is not very helpful in providing more insight into the nature of velocity correlations, mainly because not all the variables of importance were examined fully in the present investigation. For example, effect of viscosity and density changes cannot be ascertained for these data. Nonetheless it is possible to come up with a dimensional formulation that is in agreement with the forms of equations 6.6 to 6.8 (see Appendix F).

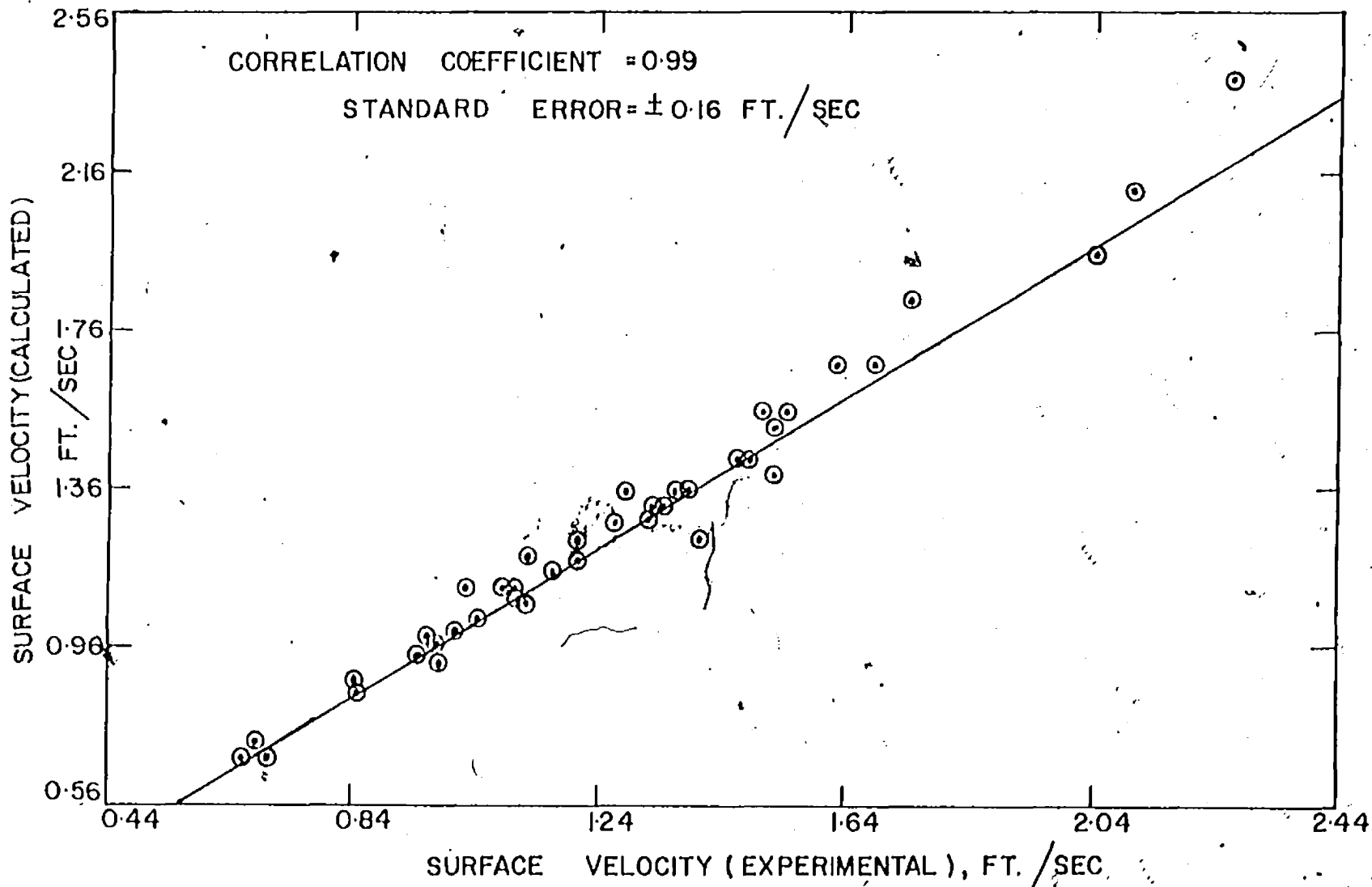


FIGURE 6.3 — SURFACE VELOCITY CORRELATION

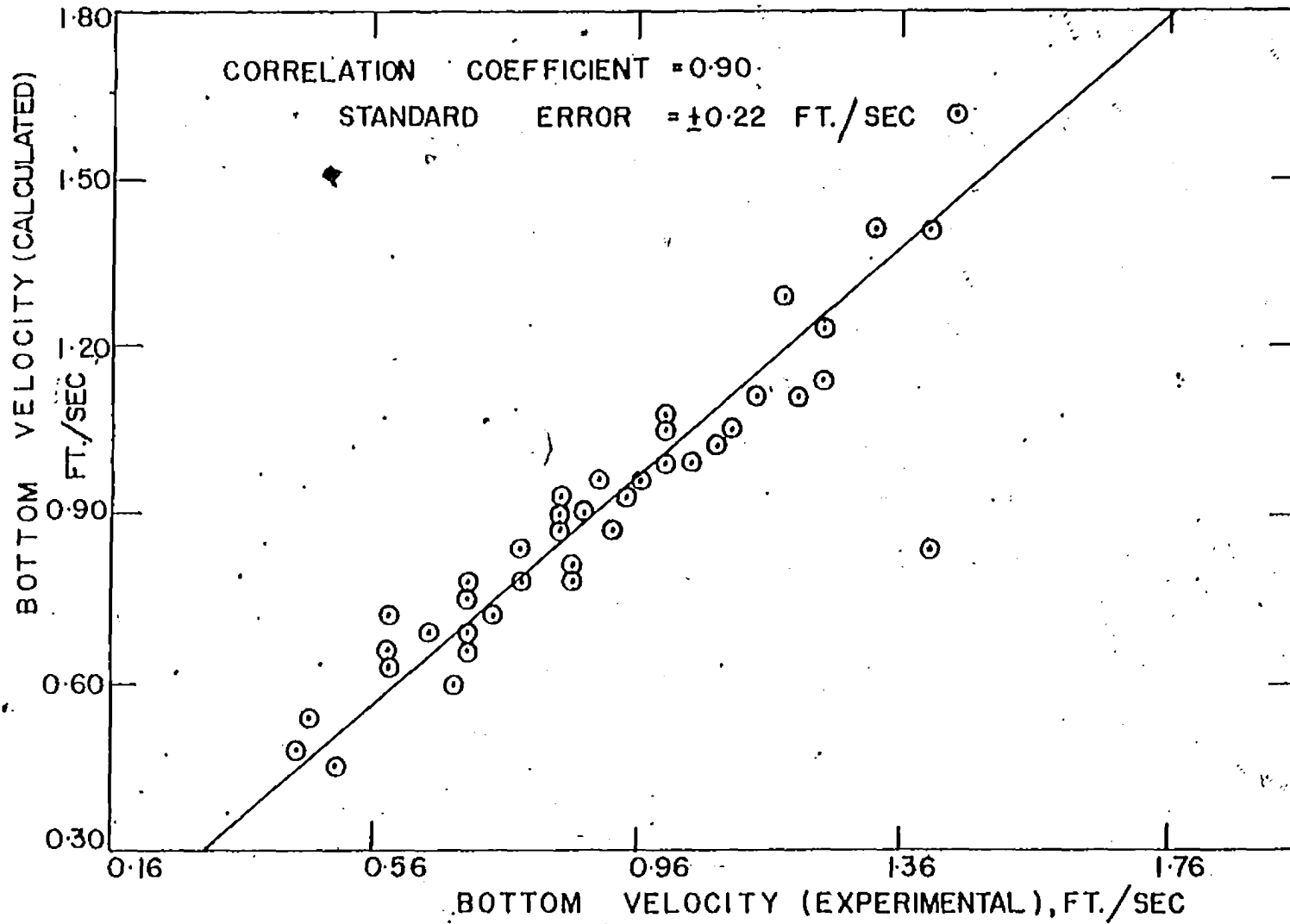


FIGURE 6.4 — BOTTOM VELOCITY CORRELATION

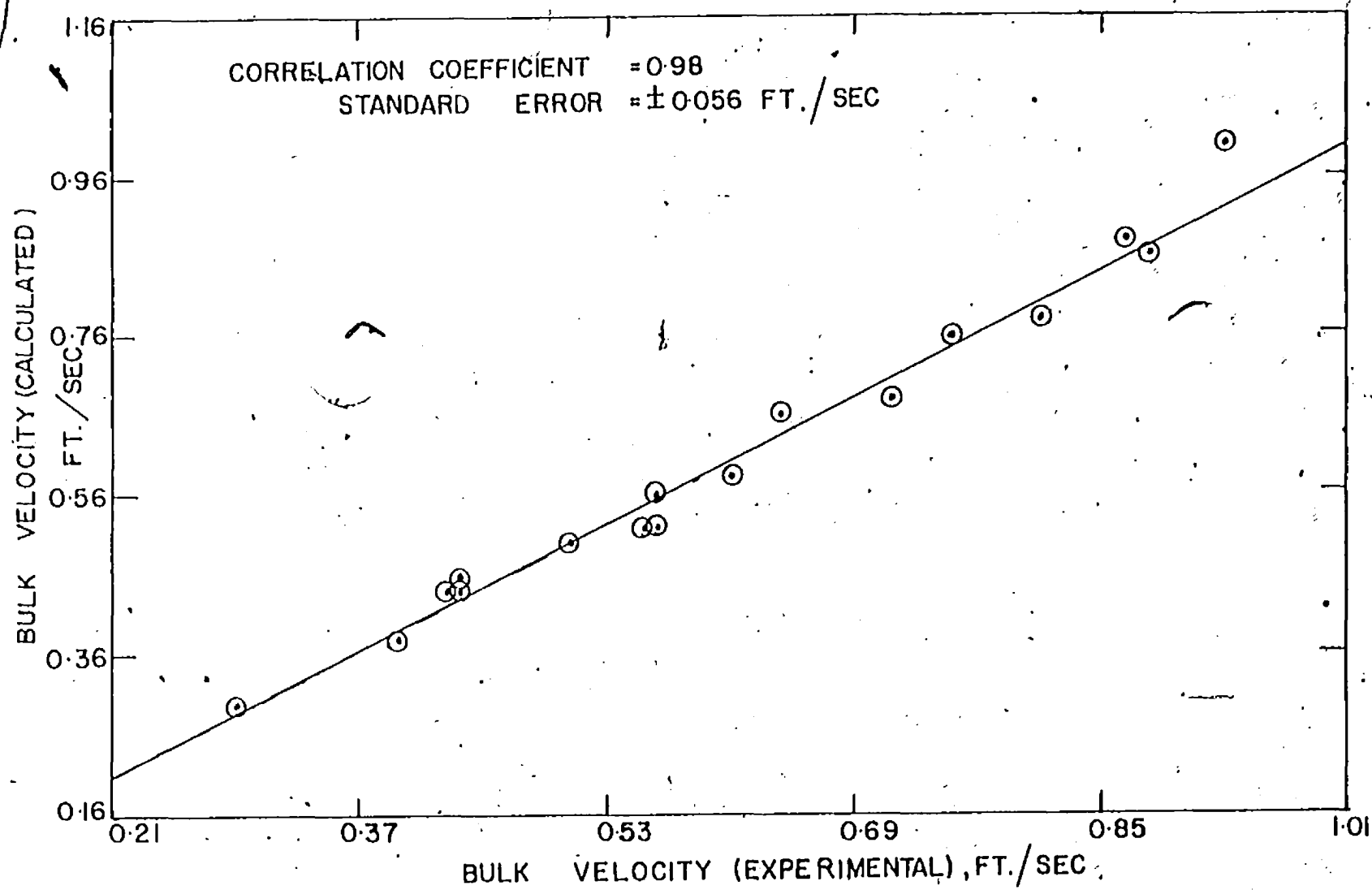


FIGURE 6.5 — BULK VELOCITY CORRELATION

TABLE 6.2

Predictions of Surface, Bottom and Bulk Velocities from Correlations
 Dimension of Tank = 24' x 4' x 14.4' and $\frac{L}{H} = 1.66$

Air Flow Rate/ Unit Width of Tank Q_a/W scfs/ft	Kind of Diffuser	Predictions from Correlations 6.6, 6.7 & 6.8			Experimental Results (52)		
		Surface Velocity ft/sec	Bottom Velocity ft/sec	Bulk Velocity ft/sec	Surface Velocity ft/sec	Bottom Velocity ft/sec	Bulk Velocity Estimated from Equation 6.1 ft/sec
0.07	1 sparger	1.91	1.30	0.79	1.85	1.05	0.72
0.13	2 saran tubes	2.36	1.58	0.96	2.33	1.62	0.98
0.085	2 saran "	2.05	1.38	0.85	2.15	1.42	0.89
0.225	6 saran "	2.85	1.89	1.13	3.11	2.00	1.27
0.35	6 saran "	3.33	2.16	1.30	3.41	1.64	1.26

C. The Design Procedure

On the basis of the correlation developed in section A & B, one may propose a design procedure for batch aerated tanks. The starting point of the procedure is a statement regarding the amount of liquid to be treated and the purpose of the air agitation. If the purpose of air agitation is simply to mix the tank contents, then the desired mixing time would be the obvious design criterion. If the purpose of air agitation is to induce a certain degree of agitation to meet a treatment objective, then a particular value of bulk velocity could be considered a suitable criterion (see Section A). The cases discussed below present design procedure for these two situations.

Case 1: Mixing Time Criterion

Step 1: Based on the volume of liquid to be treated choose a tank geometry. In selecting the tank dimensions, the comments made in section A regarding conventional practice are helpful. Note that the correlations developed in this work are applicable only over a range of $\frac{L}{H}$ from 1.14 to 5.33.

Step 2: Choose a value of air flow rate Q_a . Calculate power consumption using the following equation (3)

$$P = 81.5 Q_a' \log_{10} \left(\frac{H + 34}{34} \right) \quad \dots 6.11$$

where P = useful power dissipated by air,

ft-lb_f/sec

Q_a' = cubic feet per min of free air injected into the liquid from diffuser located H feet below the liquid surface.

Step 3: Estimate surface and bottom velocities using correlation 6.6 and 6.7 respectively. Obtain necessary parameters for mixing model such as ψ_{\max} and location of centre of circulation.

Step 4: Apply the mixing model to estimate the mixing time. If this mixing time is acceptable and the power consumption is also acceptable, then a suitable design has been arrived at. Otherwise go back to step 1 and start once again.

Case 2: Bulk Velocity Criterion

Step 1: Same as in Case 1

Step 2: Based on the desired value of bulk velocity, calculate the required airflow rate from the following correlation which is a rearranged version of correlation 6.8: $Q_a = 0.0502 u_B^{3.33} \left(\frac{L}{H}\right)^{2.12}$. Obtain power consumption from equation 6.11. If it is desired to have information regarding mixing time as well, then, steps 3 & 4 of Procedure 1 can be utilized for this purpose.

Step 3: In some treatments such as flocculation, a low magnitude of power consumption per unit volume is desired. For such cases, if the power consumption estimated in step 2 exceeds desired magnitude, then go back to step 1 and start once again.

In each of these cases it may also be necessary to maintain a certain minimum bottom velocity to keep particles in suspension. For examples, in activated sludge treatment, bottom velocity must be at least 0.5 ft/sec if sludge particles are not to settle out (3). In such cases, air flow rates must be so chosen to give the required minimum bottom velocity.

In order to illustrate the above design procedures, computations were made to design a large scale tank to treat 6912 cubic feet of water. For case 1, the required mixing time

was assumed to be 3 minutes. First a tank geometry of 48' x 12' x 12' was chosen on the basis of the conventional practices as indicated earlier. Different values for air flow rates were tried. Table 6.3 summarizes the results obtained from the computer runs. A low flow rate of 1.37 scfs was tried first and it gave a mixing time of 6.33 mins which is twice the stated criterion. An order of magnitude increase in the air flow rate to 11.38 scfs gave an acceptable mixing time of 2.98 mins. To illustrate the effect on the mixing time of air flow rate of another order of magnitude increase, a third run with air flow rate of 114.67 scfs was made. It can be seen from the Table 6.6, that this resulted in only 50% reduction in the mixing time. Having established the necessary air flow rate with one tank geometry the effect of variation in the geometry can be examined. Run 4 and 5 indicate that a higher L/H ratio gives a lower mixing time.

In order to illustrate the design procedure for case 2, the computations were made to design a large scale tank to treat 6912 cubic feet of water for flocculation objective. The bulk velocity requirement of 0.5 ft/sec corresponds to a typical flocculation process. In the flocculation process, too much power may sometimes break the flocs into fine particles which would

TABLE 6.3

Design Study - Case 1

Specified Mixing Time = 3.0 min, volume of liquid = 6912 ft³

Run No.	Dimensions of Tank Length x Width x Depth ft.	Length/Depth L/H	Air Flow Rate Q _a scfs	Power Consumption P HP	Surface Velocity ft/sec	Bottom Velocity ft/sec	Mixing Time mins
1	48 x 12 x 12	4	1.37	1.32	1.22	0.82	6.33
2	48 x 12 x 12	4	11.38	13.28	2.69	1.69	2.98
3	48 x 12 x 12	4	114.67	133.80	5.98	3.49	1.42
4	38.4 x 12 x 15	2.56	11.38	16.06	3.57	2.25	4.81
5	48 x 16 x 9	5.33	11.38	10.32	2.04	1.28	2.76

be difficult to settle in the settling tanks. Therefore, a magnitude of the power lower than 2.0×10^{-4} HP/ft³ is to be maintained in the tank in order to keep flocs unbroken (3). The detention time desired was assumed to be 10 minutes.

To start the design procedure for this situation a particular tank geometry was first chosen. Using bulk velocity value equal to 0.5 ft/sec, the appropriate amount of air flow rate was calculated from equation 6.8 as shown in Table 6.4. In order to estimate mixing time, surface and bottom velocities were calculated from equations 6.6 and 6.7 and then the model was applied to obtain a mixing time equal to 4.56 mins. This is less than detention time desired for the process. But the power consumption for this run is higher than that required. Therefore the L/H ratio is varied in order to obtain an acceptable power consumption as well as the mixing time. As shown in Table 6.4, run 2 with $\frac{L}{H}$ of 4 satisfies bulk velocity, detention time and power considerations.

TABLE 6.4

Design Study, Case 2

Specified Bulk Velocity = 0.5 ft/sec, Volume of Liquid = 6912 ft³

Run No.	Dimension of Tank Length x Width x Depth ft	Length/Depth L/H	Bulk Velocity u_b ft/sec	Air Flow Rate Q_a scfs	Power Consumption		Surface Velocity ft/sec	Bottom Velocity ft/sec	Mixing Time mins
					P HP	P/V HP/ft ³			
1	48 x 16 x 9	5.33	0.5	2.77	2.51	4.0×10^{-4}	1.26	0.82	4.56
2	48 x 12 x 12	4.00	0.5	1.13	1.32	1.7×10^{-4}	1.22	0.81	6.33
3	38.4 x 12 x 15	2.56	0.5	0.438	0.62	8.9×10^{-5}	1.17	0.80	14.06
4	32 x 12 x 18	1.77	0.5	0.202	0.33	4.8×10^{-5}	1.13	0.79	15.36

VII. CONCLUSIONS

The following conclusions may be drawn on the basis of the results obtained in the present investigations.

A. Mixing in Natural Streams

1. The dispersion process of the soluble wastes originating from continuous sources into a receiving natural stream can be formulated by steady state mass conservation equation of two or three dimensional form containing a convective flow term superimposed by the corresponding turbulent diffusion terms.
2. Both explicit and implicit schemes of computations are successful in solving the dispersion model equations. The results suggest that the explicit schemes have more potential in that their computation time is five to six times lower than that of the implicit schemes.
3. The model results indicate that the dispersion profile is relatively insensitive to the variations in the vertical diffusion coefficients but is quite sensitive to variations in the lateral diffusion coefficient.
4. Theoretical predictions from two dimensional model seem to agree well with the experimental work on the St. Clair river performed

by the Ontario Ministry of the Environment. However, it appears that a value of lateral coefficient higher than that proposed in literature for open channel flow gives a better agreement with the experimental results.

5. The effects of initial mixing zones and outfall locations on the dispersion of wastes in the river have been studied. The results show that a wider mixing zone can help reduce localized pollution substantially.

B. Mixing in Air Agitated Tanks

1. In an air-agitated batch tank of rectangular shape with a line diffuser placed at the bottom of one side of the tank, the rising bubbles generate a circulation pattern which resembles a forced vortex. This flow pattern can be correlated to the tank geometry and to the liquid circulation rate.
2. The mixing process in the batch air agitated tank can be adequately described in terms of a two dimensional unsteady state model. The resulting partial differential equation contains a convective term superimposed by longitudinal and vertical turbulent diffusion terms.
3. The mixing model proposed in this work has a strong appeal

in that its data requirements are minimal. In order to use the mixing model, information regarding the rate of liquid circulation and the location of the centre of circulation is needed for a particular airflow rate and tank geometry. It has been shown that only surface and bottom velocities at mid length of the tank need to be measured or specified to calculate the model parameters. The mixing model was satisfactory in predicting mixing times for rectangular tanks with line diffuser placed at one side, even though the attempted extension of the model to a different placement of the diffuser was not successful.

4. The mixing model has been shown to be directly usable for the design of batch air agitated tanks. Based on the existing practices, two distinct design situations have been identified. One used mixing time as the design criterion, the other used the bulk velocity as a measure of the induced degree of agitation. Stepwise procedures can be applied to different types of treatment and different volumes of tank.
5. The design equations that have been developed in this work relate surface, bottom and bulk velocities to tank geometry and a parameter containing airflow rate. Air flow rate per unit width of the tank has been shown to be the most appropriate parameter for scale up purposes. The following correlations have been developed for velocities induced in the tank by air agitation.

$$u_s = 6.563 \left(\frac{Q_a}{W}\right)^{0.343} \left(\frac{L}{H}\right)^{-0.629}$$

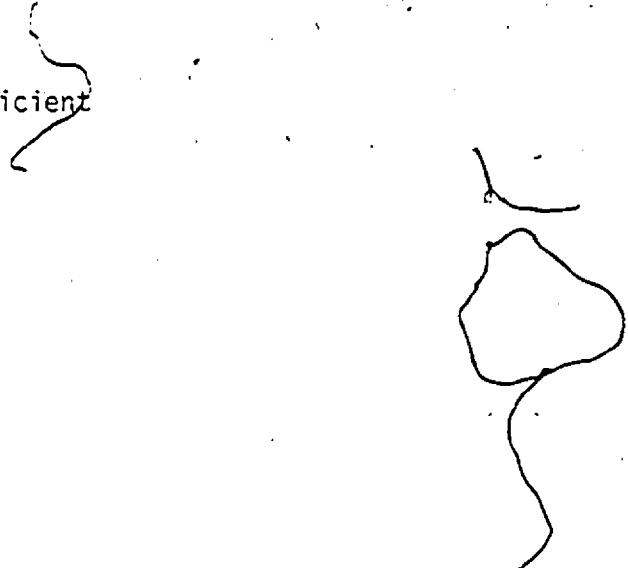
$$u_b = 4.165 \left(\frac{Q_a}{W}\right)^{0.315} \left(\frac{L}{H}\right)^{-0.639}$$

$$u_B = 2.454 \left(\frac{Q_a}{W}\right)^{0.30} \left(\frac{L}{H}\right)^{-0.636}$$

Though these correlations have been developed largely from the data obtained in a small scale tank, some confirmation of these correlations has been obtained for large scale tanks as well.

6. Further uses of the methodology developed in the present work can be envisaged for tank geometries other than rectangular and for continuous air agitated tanks.

NOMENCLATURE

- a = half of the length of the tank, ft
b = half of the liquid depth, ft
c = concentration of material, lbm/ft³
f_f = friction factor, Fanning
g = acceleration due to gravity, ft/sec²
k = von Karman Constant
k' = ratio of tangential fluid velocity at the periphery of an impeller
λ = dimensionless turbulent diffusion coefficient
p' = propeller pitch, ft
q = waste discharge rate, lbm/ft³
r = hydraulic radius, ft
t = time, sec
t_m = mixing time, sec
u = horizontal velocity, ft/sec
u* = shear velocity, ft/sec
v = lateral velocity, ft/sec
w = vertical velocity, ft/sec
x = longitudinal direction
- 

- x' = characteristic length defined as the distance from the point of maximum surface velocity to the most distant bank of the river, ft
- y = lateral direction
- z = vertical direction
- A = longitudinal distance from the point of zero velocity to either side of the tank, ft
- A' = cross sectional area of tank (Length x Width), ft²
- B = vertical distance from the point of zero velocity to either the liquid surface or the bottom of the tank, ft
- D_c = diameter of the tank, ft
- D_I = diameter of the propeller, ft
- E = turbulent diffusion coefficient, ft²/sec
- H = depth of the liquid content, or depth of the river, ft
- L = length of the tank, ft
- M = total mass of the material, lbm
- N = impeller speed, revolutions/sec
- P = power consumption, ft-lb_f/sec
- Q = discharge rate of river, ft³/sec
- Q_a = volumetric air flow rate, ft³/sec at 70°F. and 1 atmosphere
- Q_a' = volumetric air flow rate, ft³/sec at a temperature and pressure existing at the bottom of the tank.
- Q_m = pumping capacity of an impeller, ft³/sec

V = volume of the tank, ft^3

W = width of the tank, ft

X = the distance from the source of pollutant, ft

α = angle of pitch of the blade face

ρ = density of liquid, lbm/ft^3

μ = viscosity of liquid, $\text{lbm}/\text{ft sec}$

τ_0 = wall shear stress, lb_f/ft^2

Subscripts:

a = air

b = bottom

B = bulk

l = liquid

m = molecular

n = normal

s = surface

t = tangential

x = longitudinal

y = lateral

z = vertical

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APPENDIX A

ST. CLAIR RIVER FLOW SURVEY

4

TABLE A1

ST. CLAIR RIVER FLOW SURVEY

SECTION A - November 16, 1972

Q = 211,000 cfs

Distance From Shore (ft).	50	100	250	500
Velocity at 5' Depth u_5 ft. (ft./sec)	-*	0.79	3.02	3.69
Mean River Velocity \bar{u} (ft/sec)	0	0.66	2.70	3.49
River Depth (ft)	4.9	7.0	29.7	37.5

SECTION B - November 16, 1972

Q = 211,000 cfs

Distance From Shore (ft)	50	100	250	500
Velocity at 5' Depth u_5 ft. (ft/sec)	-*	0**	2.61	4.25
Mean River Velocity \bar{u} (ft/sec)	0	0	2.66	3.82
River Depth (ft)	4.9*	6.1	30.0	34.6

* Depth less than 5 ft. Measurements taken - no revolutions of blade.
Lower limit of equipment = 0.03 feet-per second.

** No revolutions of blade - below lower limit.

TABLE A 1 (cont'd)

SECTION C - November 16, 1972

Q = 211,000 cfs

Distance From Shore (ft)	50	100	250	500
Velocity at 5' Depth u_5 ft (ft/sec)	1.79	1.98	3.85	4.17
Mean River Velocity \bar{u} (ft/sec)	1.45	2.00	3.32	3.90
River Depth (ft)	8.8	21.9	33.3	34.0

SECTION D - November 7, 1972

Q = 213,000 cfs

Distance From Shore (ft)	50	100	250	500
Velocity at 5' Depth u_5 ft (ft/sec)	1.68	2.23	3.54	4.02
Mean River Velocity \bar{u} (ft/sec)	1.55	2.06	3.24	3.72
River Depth (ft)	12.1	23.8	31.1	36.7

TABLE A 1 (Cont'd)

SECTION E - November 7, 1972

Q = 213,000 cfs

Distance From Shore (ft)	50	100	250	500
Velocity at 5' Depth u_5 ft (ft/sec)	1.05	1.90	3.93	4.21
Mean River Velocity \bar{u} (ft/sec)	1.17	1.84	3.38	3.67
River Depth (ft)	10.2	24.6	33.7	36.8

SECTION F - November 6, 1972

Q = 216,000 cfs

Distance From Shore (ft)	50	100	250	500
Velocity at 5' Depth u_5 ft (ft/sec)	1.53	2.12	3.37	3.93
Mean River Velocity \bar{u} (ft/sec)	1.70	1.83	3.16	3.86
River Depth (ft)	6.0	20.2	30.9	36.2

APPENDIX B

NUMERICAL SOLUTION OF THE MIXING MODEL

EQUATIONS FOR THE ST. CLAIR RIVER

Numerical Solution of the Mixing Model Equations for the St. Clair River

Numerical approximation to the solutions of equation 3.1 and 3.4 may be obtained by stepwise solution of the associated finite difference equation. In this present work, two numerical methods i.e., implicit (Crank-Nicholson's scheme) and explicit (Forward Marching scheme) have been used to solve the model equations. A summary of the procedures is given below.

A. Numerical Scheme For Two Dimensional Model

Equation 3.1 of two dimensional model along with its boundary conditions 3.2 and 3.3 was solved numerically using both implicit and explicit methods.

Using indices i, j to define mesh quantities such that $x = i\Delta x$, $y = j\Delta y$, equation 3.1 may be written in two alternate finite difference forms (53).

a) Forward Marching Scheme (Explicit)

1. With convective term in central difference form --

$$c(i+1, j) = c(i-1, j) + 2A(i, j+\frac{1}{2}) c(i, j+1) + 2B(i, j-\frac{1}{2})$$

$$c(i, j-1) - 2[A(i, j+\frac{1}{2}) + B(i, j-\frac{1}{2})] c(i, j) \dots B1$$

2. With convective term in forward difference form --

$$c(i+1, j) = [1 - A(i, j+\frac{1}{2}) - B(i, j-\frac{1}{2})] c(i, j) + A(i, j+\frac{1}{2}) c(i, j+1) + B(i, j+\frac{1}{2}) c(i, j-1) \quad \dots B2$$

b) Crank-Nicholson's Scheme (Implicit)

With convective term in forward difference form --

$$[1 + A(i+1, j+\frac{1}{2}) + B(i+1, j-\frac{1}{2})] c(i+1, j) - \frac{1}{2} A(i+1, j+\frac{1}{2}) c(i+1, j+1) - \frac{1}{2} B(i+1, j-\frac{1}{2}) c(i+1, j-1) = [1 - \frac{1}{2} A(i, j+\frac{1}{2}) - \frac{1}{2} B(i, j-\frac{1}{2})] c(i, j) + \frac{1}{2} A(i, j+\frac{1}{2}) c(i, j+1) + \frac{1}{2} B(i, j-\frac{1}{2}) c(i, j-1) \quad \dots B3$$

where

$$A(i, j+\frac{1}{2}) = \frac{\Delta x E_y(i, j+\frac{1}{2})}{(\Delta y)^2 u(j)}, \quad B(i, j-\frac{1}{2}) = \frac{\Delta x E_y(i, j-\frac{1}{2})}{(\Delta y)^2 u(j)}$$

$$A(i+1, j+\frac{1}{2}) = \frac{\Delta x E_y(i+1, j+\frac{1}{2})}{(\Delta y)^2 u(j)}, \quad B(i+1, j-\frac{1}{2}) = \frac{\Delta x E_y(i+1, j-\frac{1}{2})}{(\Delta y)^2 u(j)}$$

Boundary condition 3.2 becomes

$$\left. \begin{aligned} \frac{\partial c}{\partial y} &= \frac{c(i, 1) - c(i, -1)}{2\Delta y} = 0 \quad \text{at } y = 0 \\ \frac{\partial c}{\partial y} &= \frac{c(i, J+1) - c(i, J-1)}{2\Delta y} = 0 \quad \text{at } y = 500 \\ &\text{where } J = 500/\Delta y \end{aligned} \right\} \dots B4$$

Equation B3 uses implicit formulation for lateral direction, but such formulation for x-direction is not feasible in the present case since there is no finite boundary in longitudinal direction. Implicit method involves solving a number of simultaneous equations to evaluate unknown terms on (i+1)-plane using known terms on i-plane.

In order to account for the variation in depth of the river in lateral and downstream directions, equations B1, B2 and B3 were modified in the following forms.

Forward Marching Scheme:

$$c(i+1, j) = c(i-1, j) \left(\frac{H(i-1, j)}{H(i+1, j)} \right) + 2A(i, j+\frac{1}{2}) c(i, j+1) \left(\frac{H(i, j+1)}{H(i+1, j)} \right) + 2B(i, j-\frac{1}{2}) c(i, j-1) \left(\frac{H(i, j-1)}{H(i+1, j)} \right) - 2[A(i, j+\frac{1}{2}) + B(i, j-\frac{1}{2})] c(i, j) \left(\frac{H(i, j)}{H(i+1, j)} \right) \quad \dots B5$$

$$c(i+1, j) = [1 - A(i, j+\frac{1}{2}) - B(i, j-\frac{1}{2})] c(i, j) \left(\frac{H(i, j)}{H(i+1, j)} \right) + A(i, j+\frac{1}{2}) c(i, j+1) \left(\frac{H(i, j+1)}{H(i+1, j)} \right) + B(i, j-\frac{1}{2}) c(i, j-1) \left(\frac{H(i, j-1)}{H(i+1, j)} \right) \quad \dots B6$$

Crank-Nicholson's Scheme:

$$\begin{aligned}
 & [1 + A(i+1, j+\frac{1}{2}) + B(i+1, j-\frac{1}{2})] c(i+1, j) H(i+1, j) - \frac{1}{2} A(i+1, j+\frac{1}{2}) \\
 & c(i+1, j+1) H(i+1, j+1) - \frac{1}{2} B(i+1, j-\frac{1}{2}) c(i+1, j-1) H(i+1, j-1) \\
 & = [1 - \frac{1}{2} A(i, j+\frac{1}{2}) - \frac{1}{2} B(i, j-\frac{1}{2})] c(i, j) H(i, j) + \frac{1}{2} A(i, j+\frac{1}{2}) \\
 & c(i, j+1) H(i, j+1) + \frac{1}{2} B(i, j-\frac{1}{2}) c(i, j-1) H(i, j-1) \quad \dots\dots B7
 \end{aligned}$$

where $H(i, j)$ = depth of the river at i th and j th point of the mesh, ft

The modified equations B5, B6 and B7 result in getting the concentrations of material at each grid point of $i+1$ th plane averaged over the entire depth.

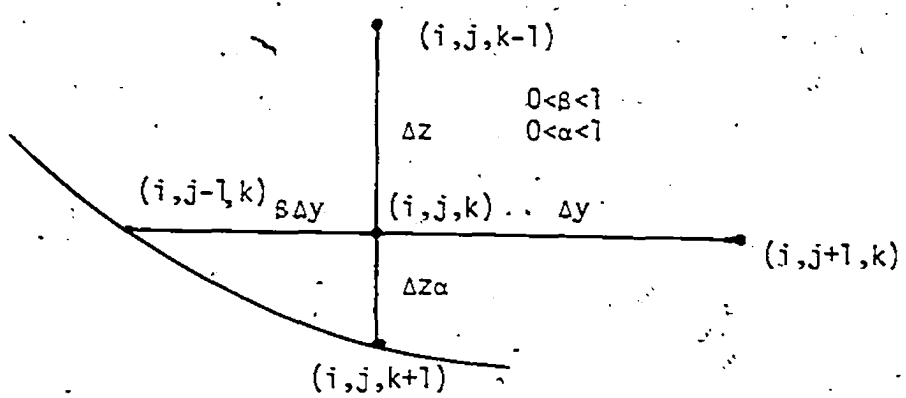
B. Numerical Scheme For Three Dimensional Model:

Using a three dimensional grid $x=i\Delta x$, $y=j\Delta y$ and $z=k\Delta z$ finite difference form of equation 3.4 of three dimensional model is written in forward marching scheme, with convective term in forward difference form.

$$\begin{aligned}
 c(i+1, j, k) = & [1 - A_y(j+\frac{1}{2}) - B_y(j-\frac{1}{2}) - A_z(k+\frac{1}{2}) - B_z(k-\frac{1}{2})] \\
 & c(i, j, k) + A_y(j+\frac{1}{2}) c(i, j+1, k) + B_y(j-\frac{1}{2}) c(i, j-1, k) \\
 & + A_z(k+\frac{1}{2}) c(i, j, k+1) + B_z(k-\frac{1}{2}) c(i, j, k-1) \quad \dots\dots B8
 \end{aligned}$$

Equation B8 is suitable for evaluating the concentration at the intersection of full rectangular mesh, but in the present case,

with a river having irregular cross sections, it is not always possible to reach the bottom with a full mesh. For such cross sections, expressions for curved boundaries are used. Three kinds of irregular meshes may appear in a given cross section, the most general being that shown in the following figure.



For such cases, the modified forms of equation B8 can be written as follows. The method of formulations is presented elsewhere (53).

$$\begin{aligned}
 c(i+1, j, k) = & \left[1 - \frac{Ay(j+\frac{1}{2})}{\beta} - \frac{By(j-\frac{1}{2})}{\beta} - \frac{Az(k+\frac{1}{2})}{\alpha} \right. \\
 & - \left. \frac{Bz(k-\frac{1}{2})}{\alpha} \right] c(i, j, k) + 2 \frac{Ay(j+\frac{1}{2})}{(1+\beta)} c(i, j+1, k) \\
 & + 2 \frac{By(j-\frac{1}{2})}{\beta(\beta+1)} c(i, j-1, k) + 2 \frac{Az(k+\frac{1}{2})}{(1+\alpha)} c(i, j, k+1) \\
 & + 2 \frac{Bz(k-\frac{1}{2})}{(1+\alpha)} c(i, j, k-1) \dots\dots B9
 \end{aligned}$$

where

$$A_y(j+\frac{1}{2}) = \frac{\Delta x E_y(i, j+\frac{1}{2}, k)}{(\Delta y)^2 u(j, k)}, \quad B_y(j-\frac{1}{2}) = \frac{\Delta x E_y(i, j-\frac{1}{2}, k)}{(\Delta y)^2 u(j, k)}$$

$$A_z(k+\frac{1}{2}) = \frac{\Delta x E_z(i, j, k+\frac{1}{2})}{(\Delta z)^2 u(j, k)}, \quad B_z(k-\frac{1}{2}) = \frac{\Delta x E_z(i, j, k-\frac{1}{2})}{(\Delta z)^2 u(j, k)}$$

Boundary condition 3.5 becomes in finite difference form as:

$$\frac{\partial c}{\partial y} = \frac{c(i, 1, k) - c(i, -1, k)}{2\Delta y} = 0 \quad \text{at } y = 0$$

$$\frac{\partial c}{\partial y} = \frac{c(i, J+1, k) - c(i, J-1, k)}{2\Delta y} = 0 \quad \text{at } y = 500 \text{ feet}$$

$$\frac{\partial c}{\partial z} = \frac{c(i, j, 1) - c(i, j, -1)}{2\Delta z} = 0 \quad \text{at } z = 0$$

$$\frac{\partial c}{\partial z} = \frac{c(i, j, K+1) - c(i, j, K-1)}{2\Delta z} = 0 \quad \text{at } z = H(j)$$

$$\text{where } K = \frac{H(j)}{\Delta z}$$

B10

B. Stability and Convergence of Numerical Schemes

Several preliminary runs were made to study numerical stability and convergence of the numerical formulations. Two dimensional equation B5, in which central difference form of

convective term is used, was found to be numerically unstable. Though different combinations of mesh sizes were tried, all solutions showed an unbounded oscillation of concentrations values. However, equation B6 with convective term in forward difference form yielded stable results for a number of different mesh sizes. The criteria for the stability of the equation B6 may be established rather simply. Looking at equation B6, it is obvious that the coefficient of $c(i,j)$, generally termed the 'modulus' of the equation, must be positive to yield numerically stable results. Hence,

$$\gamma = \frac{\Delta x (E_y(i, j+\frac{1}{2}) + E_y(i, j-\frac{1}{2}))}{(\Delta y)^2 u(j)} \geq 0 \quad \dots B11$$

Assuming $E_y(i, j+\frac{1}{2}) + E_y(i, j-\frac{1}{2}) = 2E_y(i, j)$, and substituting the relation 3.7 with $\lambda = 0.23$ for E_y , equation B11 reduces to

$$\frac{\Delta x}{(\Delta y)^2} \leq \frac{25}{(H(j))^{5/6}} \quad \dots B12$$

where $H(j)$ is local depth of the river at mesh point j in lateral direction.

Thus, in order to get stable results from equation B6 a variable condition depending upon the particular region in the river has to be met. This could be achieved either by using different

grid systems at different regions so as to follow the depth dependent condition B12, or by choosing a grid system such that it fulfills the least value of the condition estimated for the deepest region. To avoid unnecessary complexity in the programme, the second method was used in the present work. The deepest region of the St. Clair River, studied presently, was of 36 feet depth; the condition for stability was

$$\frac{\Delta x}{(\Delta y)^2} \leq 1.26 \quad \dots B13$$

Several preliminary runs verified the condition B13; however, to remain on the safe side, condition of

$$\frac{\Delta x}{(\Delta y)^2} < 1$$

was used. Though the equation B6 could be solved by using a number of sets of large mesh sizes, in these the discretization error would be very high. It is generally assumed that this error decreases as the mesh lengths are reduced. To search for the appropriate grid set several runs were made, the results of which are plotted in Figure B1. Figure B1 clearly illustrates how the results converge with decrease in the mesh lengths. Keeping in mind about the round off error and computation time which act in

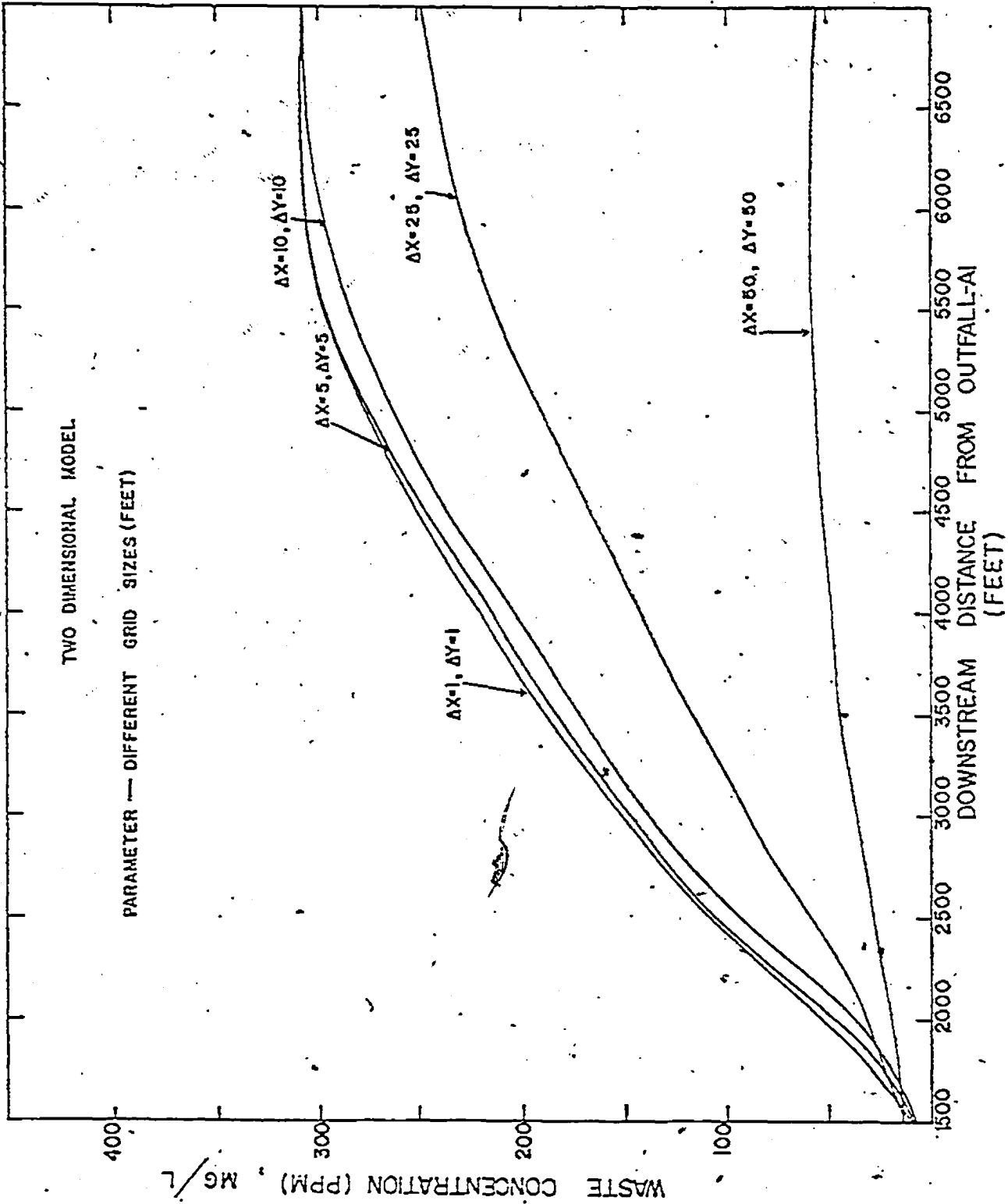


FIGURE B1.—LONGITUDINAL CONCENTRATION PROFILE (SURFACE—50 FEET OFF CANADIAN SHORE)

reverse direction, a grid system of $\Delta x = 10$, $\Delta y = 10$ was selected for further studies.

The forward marching method, though very simple, is generally considered less accurate than other implicit methods such as Crank-Nicholson method. Taking this into consideration the Crank-Nicholson's equation B7 for two-dimensional model was programmed using a number of different grid sizes. In the present work, the results were found to be not very different from those obtained using forward marching equation B6. Figure B2 illustrates the comparisons of solutions obtained from two techniques. The computation time for a particular terminal condition was five to six times greater than that for forward marching equation. This suggests that the use of this numerical method for the present particular problem is not desirable, because of substantially higher computation times. Therefore, this technique was not employed for the three dimensional model.

To determine the criteria for the stability of three dimensional forward marching equation B8, the technique used was similar. The coefficient of $c(i,j,k)$ in equation B8 must be positive. This could be achieved if

$$\frac{\Delta x [E_y(i, j + \frac{1}{2}, k) + E_y(i, j - \frac{1}{2}, k)]}{(\Delta y)^2 u(j, k)} + \frac{\Delta x [E_z(i, j, k + \frac{1}{2}) + E_z(i, j, k - \frac{1}{2})]}{(\Delta z)^2 u(j, k)} \leq 1 \quad \dots B14$$

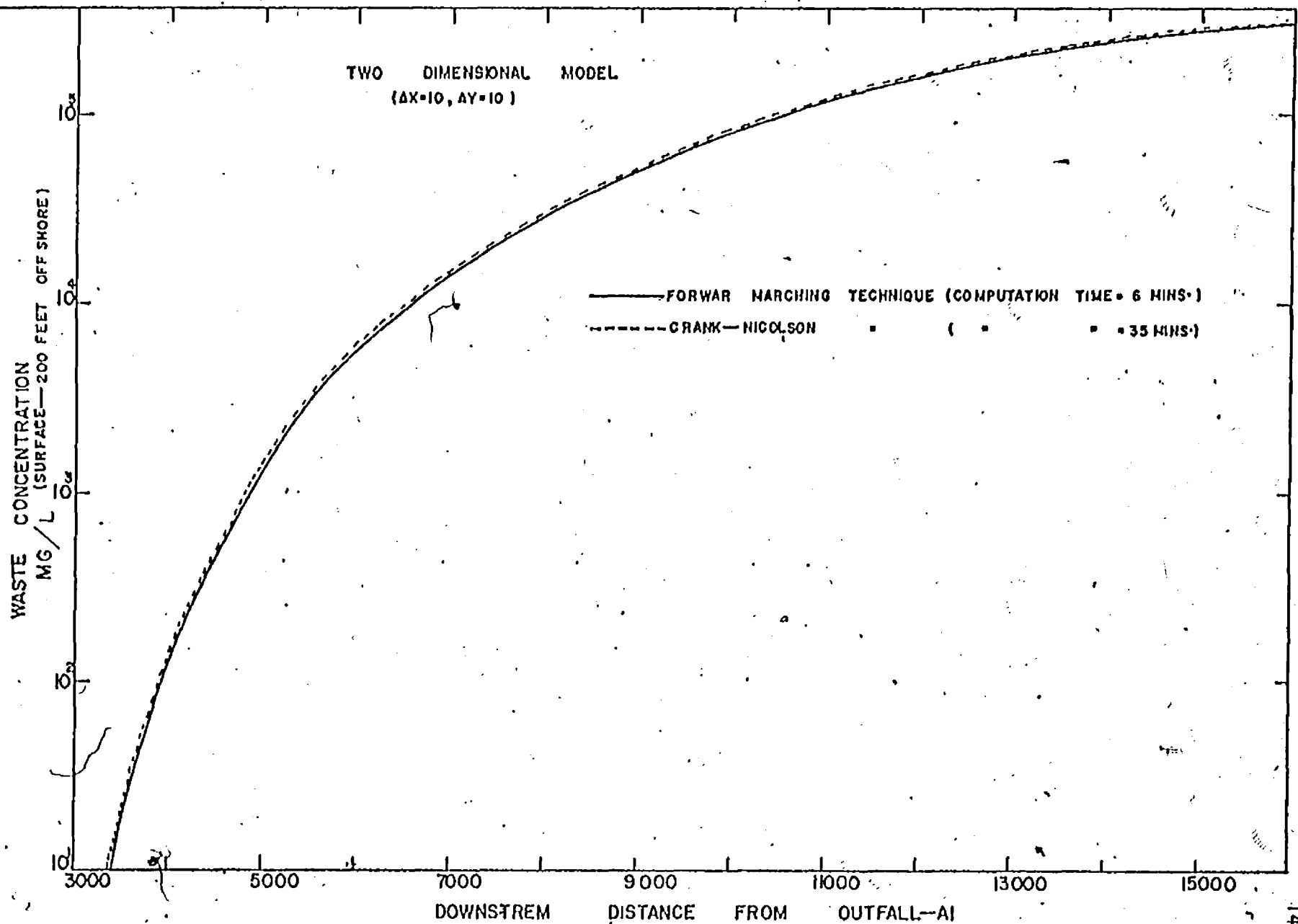


FIGURE B2—COMPARISON BETWEEN LONGITUDINAL CONCENTRATION PROFILES OBTAINED USING FORWARD MARCHING & CRANK—NICOLSON TECHNIQUES

Again, to get a rough estimate for the stability condition, equation B14 was simplified by applying the same assumptions as employed in two dimensional case and by substituting the values of E_y and E_z

$$0.04(H(j))^{5/6} \frac{\Delta x}{(\Delta y)^2} + 0.07 \left(1 - \frac{z}{H(j)}\right) \frac{z \Delta x}{(H(j))^{1/6} (\Delta y)^2} \leq 1 \quad \dots B15$$

A maximum value of the function on left side obtained at $z = 0.5 H(j)$,

$$0.04(H(j))^{5/6} \frac{\Delta x}{(\Delta y)^2} + 0.018(H(j))^{5/6} \frac{\Delta x}{(\Delta y)^2} \leq 1 \quad \dots B16$$

For the deepest region $H(j) = 36$ feet,

$$0.79 \frac{\Delta x}{(\Delta y)^2} + 0.35 \frac{\Delta x}{(\Delta z)^2} \leq 1 \quad \dots B17$$

Equation B17 may be modified for the curved boundaries by introducing function α and β ,

$$0.79 \frac{\Delta x}{(\Delta y)^2 \beta} + 0.35 \frac{\Delta x}{(\Delta z)^2 \alpha} \leq 1 \quad \dots B18$$

The difficulty in sorting out an appropriate grid size which suits the conditions of the type B18 is apparent, since α and β are dependent upon the river geometry and grid size as well.

Several runs were made to solve equation B9 with curved boundaries, but all the results obtained were found to be numerically unstable. Consequently, the curved boundaries equations were abandoned and instead, equation B8 was used alone ignoring the curved boundaries. The results thus obtained are stable, and error due to ignoring fractional grids may be suspected not to be significant.

To search for an appropriate set of grid, a number of runs were made for different grid sizes. As shown in Figure B3, the solutions converge for smaller grids. For further studies, a grid system of $\Delta x = 10$, $\Delta y = 10$, $\Delta z = 4$ (feet) employed in three dimensional model.

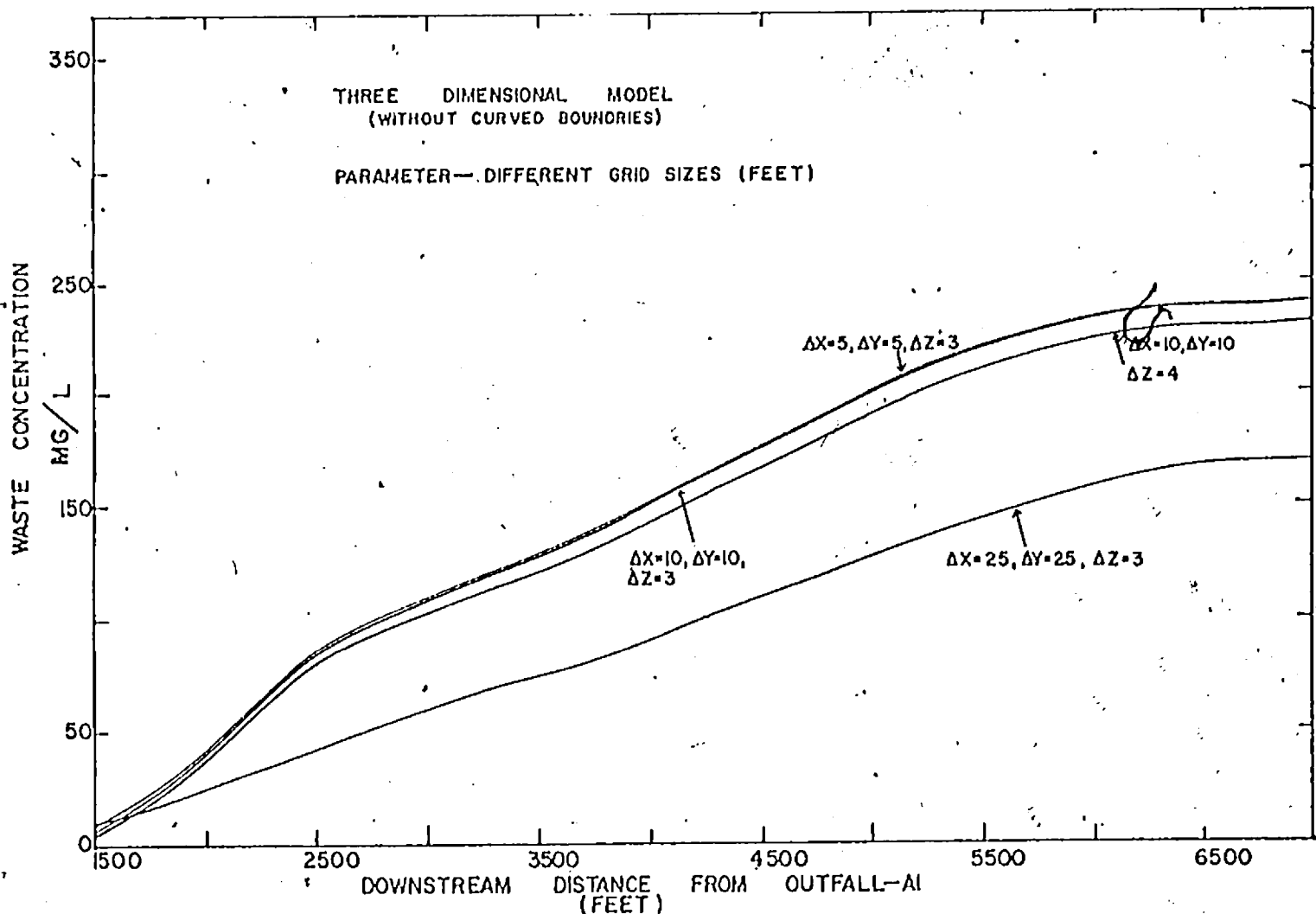


FIGURE B3—LONGITUDINAL CONCENTRATION PROFILE (SURFACE—50 FEET OFF CANADIAN SHORE)

APPENDIX C

CALCULATION FOR INTEGRATED VELOCITIES
USED IN AIR AGITATED TANK MODEL

Calculation For Integrated Velocities

In Table C1, the details of the velocity data obtained in the tank for run 4 are given. A typical profile using velocity data for a distance of four feet from the diffuser is shown in Figure 4.4 (Chapter IV). In order to calculate stream functions at different points along the liquid depth, the velocity profile is divided into a number of strips as shown in Figure C1. The area of each strip is obtained using trapezoid rule. Starting from point of zero velocity, the integrated velocities at each point are estimated by adding the areas of strips. From Figure C1, the following data are obtained for stream functions.

Liquid Depth ft	Total Area of Strips ft ² /sec	Integrated Velocities ft ² /sec
Surface 3.0	0.80 + 0.45 + 0.0	1.25
2.5	0.45	0.45
1.7	0.0	0.0
1.0	0.26	0.26
0.5	0.43 + 0.26	0.68
Bottom 0.0	0.56 + 0.43 + 0.26	1.25

TABLE C1
Velocity Data for Run 4

(+ → Flow away from Diffuser, - → Flow towards Diffuser)

Liquid Depth from Bottom ft	Distance from one side of the tank ft	Velocity 'u' ft/sec - 0.5 ft from Diffuser					Average Velocity ft/sec	Direction of Flow
		0.125	0.625	1.125	1.625	2.125		
3.0		2.10	2.35	2.30	2.30	2.20	2.25	+
2.5		0.45	0.45	0.35	0.39	0.41	0.41	+
2.0		-	-	-	-	-	-	Random
1.5		-	-	-	-	-	-	Random
1.0		0.34	0.39	0.51	0.39	0.37	0.40	-
0.5		0.43	0.51	0.58	0.54	0.44	0.50	-
0.0		0.33	0.38	0.41	0.42	0.44	0.40	-
		Velocity 'u' ft/sec - 1.0 ft from Diffuser						
3.0		2.87	3.12	2.96	3.15	2.90	3.0	+
2.5		0.50	0.70	0.75	0.60	0.45	0.60	+
2.0		-	-	-	-	-	-	Random
1.5		-	-	-	-	-	-	Random
1.0		0.42	0.52	0.64	0.51	0.45	0.51	-
0.5		0.48	0.64	0.68	0.67	0.50	0.60	-
0.0		0.53	0.57	0.61	0.56	0.66	0.58	-

TABLE C1
Velocity Data for Run 4
(Continued)

Liquid Depth from Bottom ft	Distance from one side of the tank ft	Velocity 'u' ft/sec - 1.5 feet from Diffuser					Average Velocity ft/sec	Direction of Flow
		0.125	0.625	1.125	1.625	2.125		
3.0		2.05	2.15	2.11	2.20	2.04	2.11	+
2.5		0.53	0.84	0.85	0.92	0.64	0.76	+
2.0		-	-	-	-	-	-	Random
1.5		-	-	-	-	-	-	Random
1.0		0.43	0.61	0.68	0.57	0.44	0.55	-
0.5		0.53	0.69	0.63	0.69	0.54	0.62	-
0.0		0.76	0.72	0.73	0.76	0.78	0.75	-
		Velocity 'u' ft/sec - 2.0 ft from Diffuser						
3.0		2.37	2.38	2.50	2.42	2.33	2.40	+
2.5		0.90	1.00	1.28	0.95	0.72	0.97	+
2.0		-	-	-	-	-	-	Random
1.5		-	-	-	-	-	-	Random
1.0		0.51	0.62	0.82	0.74	0.66	0.67	-
0.5		0.68	0.83	0.85	0.79	0.69	0.77	-
0.0		0.82	0.89	0.83	0.85	0.86	0.85	-

TABLE C1
Velocity Data for Run 4
(Continued)

Liquid Depth from Bottom ft	Distance from one side of the tank ft	Velocity 'u' ft/sec - 3.0 ft from Diffuser					Average Velocity ft/sec	Direction of Flow
		0.125	0.625	1.125	1.625	2.125		
3.0		2.10	2.25	2.49	2.15	2.12	2.22	+
2.5		0.90	1.20	1.40	0.90	0.87	1.05	+
2.0		-	-	-	-	-	-	Random
1.5		-	-	-	-	-	-	Random
1.0		0.53	0.73	0.79	0.74	0.55	0.67	-
0.5		0.85	0.93	1.04	0.89	0.80	0.90	-
0.0		1.10	0.12	1.12	1.09	1.09	1.10	-
		Velocity 'u' ft/sec - 5.0 ft from Diffuser						
3.0		1.70	1.73	2.08	1.75	1.73	1.79	+
2.5		0.98	1.20	1.35	0.92	0.89	1.07	+
2.0		-	-	-	-	-	-	Random
1.5		-	-	-	-	-	-	Random
1.0		0.70	0.68	0.67	0.67	0.69	0.68	-
0.5		0.98	1.01	1.07	1.00	0.95	1.00	-
0.0		1.26	1.24	1.26	1.25	1.24	1.25	-

TABLE C1
Velocity Data, for Run 4
(Continued)

Distance from one side of the tank ft	Velocity 'u' ft/sec - 6.0 ft from Diffuser				Average Velocity ft/sec	Direction of Flow
	0.125	0.625	1.125	1.625		
3.0	1.40	1.42	1.60	1.44	1.41	+
2.5	0.87	0.90	1.12	0.93	0.87	+
2.0	-	-	-	-	-	Random
1.5	-	-	-	-	-	Random
1.0	0.60	0.51	0.48	0.53	0.55	-
0.5	0.90	0.86	0.82	0.86	0.87	-
0.0	1.20	1.22	1.25	1.23	1.22	-
	Velocity 'u' ft/sec - 7.0 ft from Diffuser					
3.0	1.00	1.10	1.21	1.08	0.94	+
2.5	0.71	0.85	0.94	0.82	0.70	+
2.0	-	-	-	-	-	Random
1.5	-	-	-	-	-	Random
1.0	0.58	0.40	0.37	0.36	0.45	-
0.5	0.69	0.56	0.55	0.54	0.61	-
0.0	1.09	0.99	0.78	0.90	0.96	-

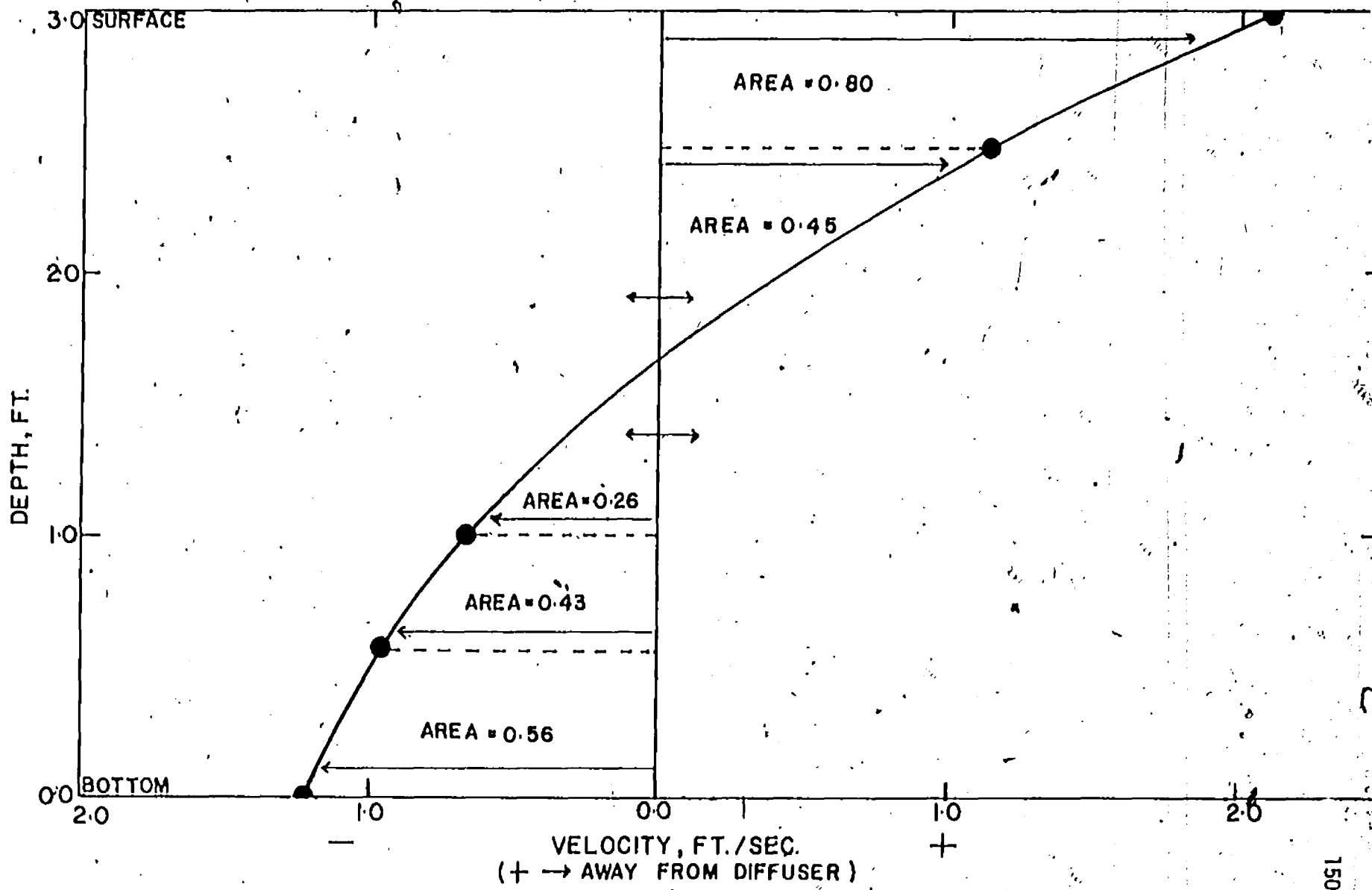


FIGURE C1 — VELOCITY PROFILE, 4.0 FEET FROM DIFFUSER (RUN 4)

These data are plotted in Figure 4.5 (Chapter IV). Similar data have been computed from the velocity profiles obtained for a distance for 0.5, 1, 1.5, 2.0, 3.0, 5.0, 6.0 and 7.0 feet from the diffuser. Integrated velocities, thus obtained are plotted in Figure 4.5 (Chapter IV) and Figure C2. From these two figures, data are obtained to plot a two dimensional flow pattern in terms of streamlines as illustrated in Figure 4.6 (Chapter IV).

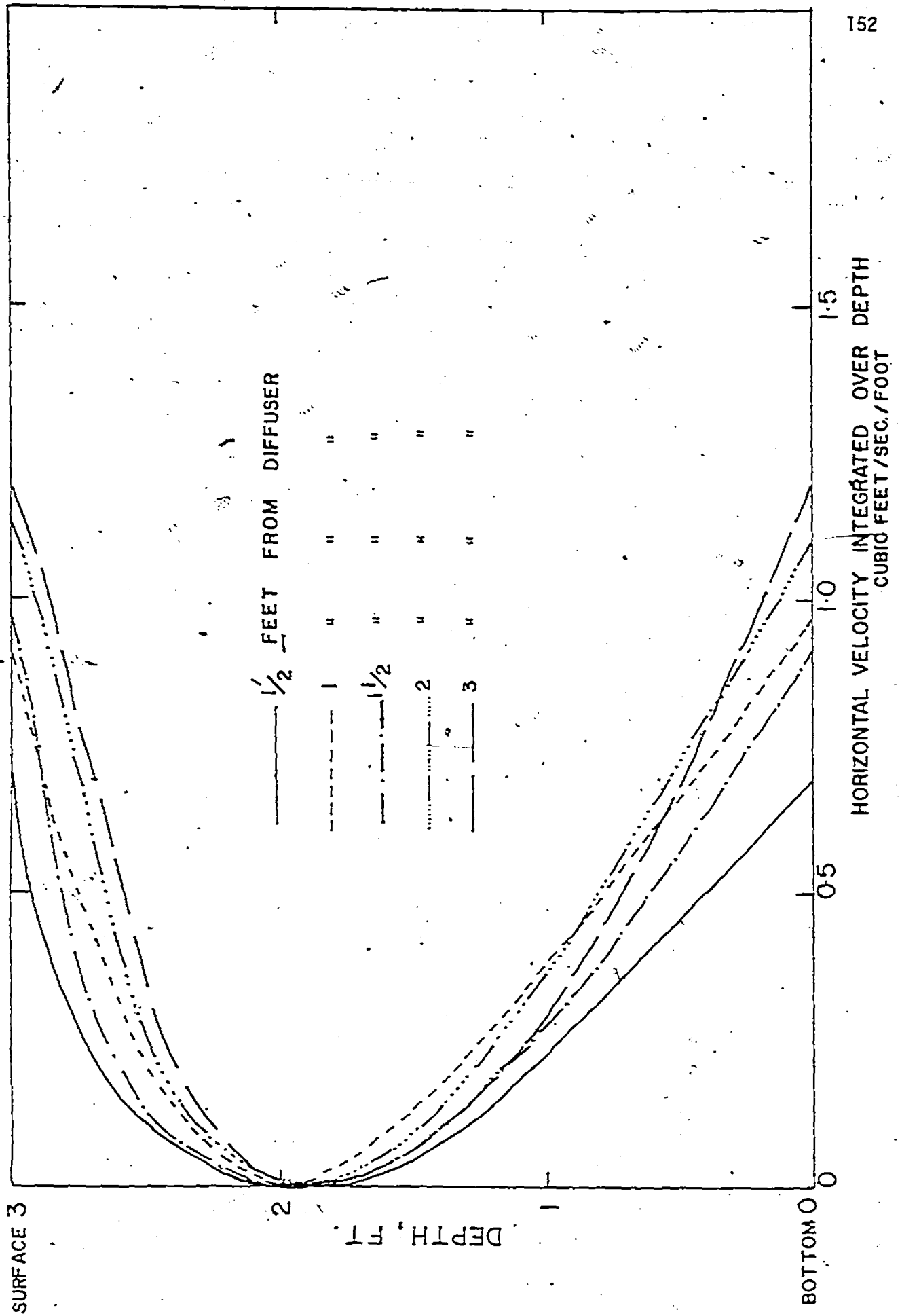


FIGURE C2 — INTEGRATED HORIZONTAL VELOCITY VS DEPTH

APPENDIX D

NUMERICAL SOLUTION OF THE MIXING MODEL

EQUATION FOR AN AIR AGITATED TANK

D

Numerical Scheme For Model Equation

Numerical approximation to the solutions of equation 5.1 may be obtained by stepwise solution of the associated finite difference equation. An efficient method for rectangular regions is the one proposed by Peaceman and Rachford, sometimes also called alternating-direction implicit method (53,54). This method is simple and reportedly requires less computation time than the Crank-Nicholson method. A summary of the procedure used for solving equation 5.1 is given below.

The model equation 5.1 was written in a finite difference approximation such that it was implicit with respect to the x-direction terms and explicit with respect to the z-direction terms. The x-directional implicit form of model equation 4.5 may be written as follows:

$$\begin{aligned}
 & - [EB(i,j) + AU(i,j)] c(i,j,k+1) + [1+EB(i,j)+EF(i,j)] c(i,j,k) \\
 & - [EF(i,j) - AU(i,j)] c(i+1,j,k) = [FB(i,j)+BW(i,j)] c(i,j-1,k) \\
 & - [FB(i,j) + FF(i,j) - 1] c(i,j,k) + [FF(i,j)-BW(i,j)] c(i,j+1,k) \\
 & \dots\dots D1
 \end{aligned}$$

where

$$EB(i,j) = \frac{E_x(i - \frac{1}{2}, j) \cdot \Delta t}{\Delta x^2}, \quad EF(i,j) = \frac{E_x(i + \frac{1}{2}, j) \cdot \Delta t}{\Delta x^2}$$

$$FB(i,j) = \frac{E_z(i,j - \frac{1}{2}) \cdot \Delta t}{\Delta z^2}, \quad FF(i,j) = \frac{E_z(i,j + \frac{1}{2}) \cdot \Delta t}{\Delta z^2}$$

$$AU(i,j) = \frac{u(i,j) \cdot \Delta t}{2\Delta x}, \quad BW(i,j) = \frac{w(i,j) \cdot \Delta t}{2\Delta z}$$

$\Delta x, \Delta z$ = Grid size

Δt = time interval

and

i = represents columns

j = represents rows

k = represents time

To start the computation, a grid size and Δt were selected and the finite difference approximation was applied to each grid point. This resulted in a number of simultaneous equations in terms of unknown concentration terms. These simultaneous equations were then solved using Gauss's elimination method.

The advancement of the solution to the next time level was achieved by repeating the above procedure once again but this time the z-direction terms were written in an implicit form and the x-direction terms were in an explicit form. The time interval Δt was the same for each advancement. The z-directional implicit form of model equation may be written as follows:

$$\begin{aligned}
& - [FB(i,j)+BW(i,j)] c(i,j-1,k+2) + [1+FB(i,j)+FF(i,j)] c(i,j,k+2) \\
& - [FF(i,j)-BW(i,j)] c(i,j+1,k+2) = [EB(i,j)+AU(i,j)] c(i-1,j,k+1) \\
& - [EB(i,j)+EF(i,j)-1] c(i,j,k+1) + [EF(i,j)-AU(i,j)] c(i+1,j,k+1)
\end{aligned}$$

.....D2

The following boundary conditions in finite differences forms were used with equations D1 and D2

At $x = 0, x = L$ for all t :

$$\frac{\partial c}{\partial x} = 0, \text{ or in finite difference form } \frac{c(i+1,j,k) - c(i-1,j,k)}{\Delta x} = 0$$

$$\text{or } c(i+1,j,k) = c(i-1,j,k)$$

At $z = 0, z = H$ for all t

$$\frac{\partial c}{\partial z} = 0, \text{ or in finite difference form } \frac{c(i,j+1,k) - c(i,j-1,k)}{\Delta z} = 0$$

$$\text{or } c(i,j+1,k) = c(i,j-1,k)$$

B. Stability and Convergence of Numerical Scheme:

The stability of the numerical procedure was found to be satisfactory. Several runs were made with different grid sizes in order to check the stability criteria. The Peaceman and Rachford scheme has been reported to be stable for all grid sizes (54). However, in the present case, due to the presence of convective terms, the stability of the scheme was found to be

dependent on the grid size and time interval. The conditions for stable results were found to be as follows:

$$E_x(i+\frac{1}{2},j) > u(i,j) \Delta x/2$$

$$E_z(i,j+\frac{1}{2}) > w(i,j) \Delta z/2$$

$$E_x(i,j) < \Delta x^2/\Delta t$$

$$E_z(i,j) < \Delta z^2/\Delta t$$

All these conditions were satisfied during the numerical solution of equation D1 and D2.

The main problem encountered in solving the model equation was the failure of the numerical procedure to satisfy the continuity condition. It is a physical requirement that the tracer be conserved at each Δt . Several runs were made to check the reasons for the violation of this condition. It was concluded that the convective terms were responsible for giving rise to this problem. The problem could be related to the size of steps for Δt . For example, it was found that by decreasing Δt , the problem was reduced. However, computer time required with small Δt was extremely long. Two other techniques were tried in an effort to overcome the problem. They involve the use of (a) Yotsukura method (b) Imposed continuity condition.

Yotsukura (18) treated convective terms in a different way. By his method the finite difference approximation of the equation 5.1 is written in such a way that the convective terms are implicit. A characteristic method is used directly to solve the convective terms. However, using Yotsukura's method yielded no improvement of results for the present case.

The second method, in which the continuity condition is imposed at each time step, worked well. At each time step before the advancement of the solution, the average concentration in the tank was estimated. If this estimated average concentration was not the same as the required average concentration per continuity condition, then the concentration at each grid point was multiplied by the factor

$$\frac{\text{required average concentration}}{\text{estimated average concentration}}$$

It was found that after a few time steps the multiplication factor tended to one of its own accord.

APPENDIX E

CORRELATIONS FOR SURFACE
BOTTOM AND BULK VELOCITIES
BASED ON ACTUAL AIR FLOW RATES

Correlations for Surface, Bottom and Bulk Velocities-Based on Actual Air Flow Rates

In order to compute air flow rate based on the actual conditions existing at the bottom of the tank, a correction must be made to air flow rates calculated at standard conditions (70°F and 1 atm). The following correction for temperature and pressure existing at the bottom of tank is applied

$$Q_a' = Q_a \left(\frac{34.0}{34.0+H} \right) \left(\frac{460+T}{530} \right) \quad E1$$

where

Q_a' = air flow rate at the temperature and pressure existing at the bottom of the tank, ft³/sec

Q_a = air flow rate at 70°F and 1 atmosphere, ft³/sec

H = depth of liquid content, ft

T = temperature at the bottom of the tank, °F

The values of air flow rates given in Table 4.2, and Figures 6.1 and 6.2 were converted using expression E1. Based on new values of air flow rate Q_a' , the following correlations were obtained for surface, bottom and bulk velocities.

$$u_s = 6.841 \left(\frac{Q_a'}{W} \right)^{0.341} \left(\frac{L}{H} \right)^{-0.643} \quad E2$$

$$u_b = 4.192 \left(\frac{Q_a'}{W} \right)^{0.311} \left(\frac{L}{H} \right)^{-0.646} \quad E3$$

$$u_B = 2.543 \left(\frac{Q_a}{W} \right)^{0.30} \left(\frac{L}{H} \right)^{-0.646} \quad E4$$

Correlations E2, E3 and E4 are similar to those obtained previously with air flow rates calculated at standard conditions. In Table E1, predicted surface, bottom and bulk velocities are compared to experimental data obtained by Bewtra (52) for a large scale tank. A comparison of the results given in Table E1 to those in Table 6:2 indicates that the predicted values of velocities are lower from correlations based on bottom air flow rates. A use of standard flow rates yields better predictions for the conditions investigated in this work.

TABLE E 1

Predictions of Surface, Bottom and Bulk Velocities from Correlations Based on Actual Air Flow Rates.
 Dimension of Tank = 24' x 4' x 14' 4" and $\frac{L}{H} = 1.66$

Air Flow Rate/ Unit Width of Tank Q_s/W acfs/ft	Kind of Diffuser	Predictions from Correlations E2, E3 & E4			Experimental Results (52)		
		Surface Velocity ft/sec	Bottom Velocity ft/sec	Bulk Velocity ft/sec	Surface Velocity ft/sec	Bottom Velocity ft/sec	Bulk Velocity Estimated from Equation 6.1 ft/sec
0.0513	1 sparger	1.79	1.20	0.75	1.85	1.05	0.72
0.0953	2 saran tubes	2.21	1.45	0.91	2.33	1.62	0.98
0.0623	2 saran "	1.91	1.27	0.79	2.15	1.42	0.89
0.1649	6 saran "	2.67	1.72	1.06	3.11	2.00	1.27
0.256	6 saran "	3.10	1.98	1.21	3.41	1.64	1.26

APPENDIX F

DIMENSIONAL ANALYSIS

Dimensional Analysis

$$u = F (Pg_c, L, W, H, g, \rho_l, u_l)$$

where P is useful power dissipated by air as defined by equation 6.11

$$u = F (Pg_c, L, W, H, g, \rho_l, u_l)$$

$$u = A_{12} (Pg_c)^a L^b W^c H^d g^e \rho_l^f u_l^h \quad F 1$$

$$\frac{L}{T} = A_{12} \left(\frac{ML^2}{T^3}\right)^a L^b L^c L^d \left(\frac{L}{T^2}\right)^e \left(\frac{M}{L^3}\right)^f \left(\frac{M}{LT}\right)^h$$

$$LT^{-1} = A_{12} L^{2a+b+c+d+e-3f-h} T^{-3a-2e-h} M^{a+f+h} \quad F 2$$

Comparing the exponents of each side of equation F 2

$$2a+b+c+d+e-3f-h = 1 \quad F 3$$

$$-3a-2e-h = -1 \quad F 4$$

$$a+f+h = 0 \quad F 5$$

From equation F 19, we have

$$h = 1-3a-2e \quad F 6$$

Substituting equation F 6 in equation F 5, we have

$$f = -1+2a+2e \quad F 7$$

Substituting equations F 6 and F 7 in equation F 3 we get

$$-a+b+c+d-3e = -1 \quad F 8$$

Writing equation F 8 in terms of d, we get

$$d = -1+a-b-c+3e \quad F 9$$

Substituting values of h, f and d from equations F 6, F 7, & F 9 in equation F 1, we get

$$u = A_{12} (Pg_c)^a L^b W^c H^{-1+a-b-c+3e} g^e \rho_\ell^{-1+2a+2e} \mu_\ell^{1-3a-2e} \quad \text{F. 10}$$

Arranging in groups

$$\left(\frac{uH\rho_\ell}{\mu_\ell} \right) = A_{12} \left(\frac{Pg_c H\rho_\ell^2}{\mu_\ell^3} \right)^a \left(\frac{L}{H} \right)^b \left(\frac{W}{H} \right)^c \left(\frac{H^3 g \rho_\ell^2}{\mu_\ell^2} \right)^e \quad \text{F. 11}$$

In equation F 11, the group on the left hand side is a Reynolds number for the liquid. The first group on the right hand side may be termed as a Power number, since it has a power term in it. The last group is a combination of gravitational and viscous forces. Correlation F 11 was tested for the data plotted in Figures 6.1 and 6.2 using multiple variable linear correlation scheme and gave the following results.

Surface Velocity

$$\left(\frac{u_s H \rho_\ell}{\mu_\ell} \right) = 0.125 \left(\frac{Pg_c H \rho_\ell^2}{\mu_\ell^3} \right)^{0.34} \left(\frac{L}{H} \right)^{-0.68} \left(\frac{W}{H} \right)^{0.021} \left(\frac{H^3 g \rho_\ell^2}{\mu_\ell^2} \right)^{0.089} \quad \text{F. 12}$$

Correlation coefficient = 0.99

Bottom Velocity

$$\left(\frac{u_b H \rho_\ell}{\mu_\ell} \right) = 2.96 \left(\frac{Pg_c H \rho_\ell^2}{\mu_\ell^3} \right)^{0.31} \left(\frac{L}{H} \right)^{-0.677} \left(\frac{W}{H} \right)^{-0.30} \left(\frac{H^3 g \rho_\ell^2}{\mu_\ell^2} \right)^{0.0021} \quad \text{F. 13}$$

Correlation coefficient = 0.96

APPENDIX G

Computer Program for Two Dimensional Mixing Model

(St. Clair River)

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KJOB  KATFIV  XXXXXXXXXXXX NAME=JASEEM AKHTAR
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCCCCPOLLUTANTS DISPERSION MODEL FOR ST. CLAIR RIVER. . SARINIA, ONTARIO
CC==C--T40 DIMENSIONAL DISPERSION MODEL FOR ST. CLAIR RIVER
CCCCCFORWARD MARCHING METHOD
CCCCC.....X=LONGITUDINAL DISTANCE
CCCCC.....Y=LATERAL DISTANCE
CCCCC.....XX=GRID SIZE X-DIRECTIONAL
CCCCC.....YY=GRID SIZE Y-DIRECTIONAL
CCCCC.....FX=LONGITUDINAL DIFFUSION COEFFICIENT
CCCCC.....FY=LATERAL DIFFUSION COEFFICIENT
CCCCC.....JA TO JL=DISCHARGE RATE OF OUTFALLS
CCCCC.....C =CONCENTRATION OF POLLUTANT
CCCCC.....YYYY= ZONE WIDTH

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DIMENSION A(510),U(510),D(510),U(510),H(510),E(510),C(3,510),C(11,
1510)
DIMENSION FH(3,510)
DEFINING GRIDS AND GIVING INITIAL VALUES FOR CONCENTRATIONS
PRINT 34
14 FORMAT(10X,5AHX=LUNGITUDINAL DISTANCE FROM FIRST POLYMER FALL*020
IN*.5X,3BH=LATCHAL DISTANCE FROM CANADIAN SHORE )
PRINT 35
15 FORMAT(10X,6X,3H*X*,11X,5HY=0.0,3X,6HY=50.0,3X,7HY=100.0,2X,7HY=15
10.0,2X,7HY=200.0,2X,7HY=250.0,2X,7HY=300.0,2X,7HY=350.0,2X,7HY=400
2.0,2X,7HY=450.0,2X,7HY=500.0 )
G=1.0
MCM=0
ZAZ=4.0
FAC=3.13
FAC=1.0
JL=0
MM=1
L=0
AYAZ=10.0
AYAZ=50.0
Z=0.0
ZZ=0.0
ZZZ=0.0
Y1=500.0
Y=500.0
XX=5.0
YY=5.0
YY=1.0
XX=1.0
XX=25.0
YY=25.0
YY=50.0
XX=50.0
XX=10.0
YY=10.0
M=Y/YY
M=M*2
Q=(1.0/(0.24+C.36))
Q2=0
QA=(Q/62.5)*550.0
QB=(Q/62.5)*150.0
QC=(Q/62.5)*510.0
QD=(Q/62.5)*60.0
QE=(Q/62.5)*310.0
QF=(Q/62.5)*120.0
QG=(Q/62.5)*5.0
QH=(Q/62.5)*1.333
QI=(Q/62.5)*120.0
QJ=(Q/62.5)*740.0
QA=(Q/62.5)*250.0
QL=(Q/62.5)*13.333
C(3,M+1)=0.0
C(1)=0.0
AXA=15021.0
DO 1 J=1,N
C(2,J+1)=0.0
C(3,J)=0.0
X=2700.0
X=3950.0
X=5400.0
X=4750.0
X=0.0
DEPC=X
MLA=0
Y=YY/2.0

```

```

62      18  YYYY/2.0
CC      80  IF(X-1720.0) 19.19.3
67      19  K=1.0
68      S=0.0
69      T=0.0
70      GO TO 2
71      3  IF(X-2620.0) 20.20.21
72      20  R=0.0
73      S=1.0
74      T=0.0
75      GO TO 2
76      21  R=0.0
77      S=0.0
78      T=1.0
79      C  CALCULATIONS FOR DEPTH VELOCITY OF RIVER AT GRID POINTS
80      7  DO 4 J=2,M
81      IF(Y-50.0) 5,5.6
82      5  H(J)=R*(4.9+S*((0.005422*X)-4.4262))+T*0.780
83      U(J)=R*(0.03+0.00046802*X)*(Y-50.)/50.)+J*((0.005550*
84      1*X)-0.3550)*(Y-50.)/50.)+(0.0015444*X)-2.6264))+T*((0.50*(Y-50.)/5
85      20.))+1.42)
86      GO TO 7
87      6  IF(Y-100.0) 8,9.3
88      8  H(J)=R*((1.03*(Y-50.)/50.)+4.9)+S((((0.013003*X)-20.7100)*(Y-50.)
89      1/50.))+((0.005422*X)-4.4262))+T*((13.35*(Y-50.)/50.))+J.78)
90      U(J)=R*((0.005-0.00046802*X)*(Y-50.)/50.)+J*((0.005550*
91      1*X)-0.3550)*(Y-50.)/50.)+(0.0015444*X)-2.6264))+T*((0.50*(Y-50.)/5
92      20.))+1.42)
93      GO TO 7
94      9  IF(Y-250.) 10,10.11
95      10 H(J)=R*((24.57*(Y-100.)/150.))+6.55)+S((((0.018422*(Y-100.)/150.))+
96      110.))+((0.018422*X)-25.1362))+T*((7.99*(Y-100.)/150.))+J.13)
97      U(J)=R*((2.255+(0.00046802*X))*(Y-100.)/150.)+(0.035-(0.00046802*
98      1*X))+S((((0.00720-(0.0021009*X))*(Y-100.)/150.))+((0.0021000*X)-3.58
99      220))+T*((1.17*(Y-100.)/150.))+1.92)
100     GO TO 7
101     11 H(J)=(4.77*(Y-250.)/250.))+31.12
102     U(J)=(0.70*(Y-250.)/250.))+3.00
103     7  Y=Y+YY
104     4  CONTINUE
105     Z=Z+1.0
106     IF(Z=1.0) 12, 12, 13
107     C  CALCULATIONS FOR LATERAL DISPERSION COEFFICIENTS AT DIFFERENT GRID POINTS
108     12  DO 14 J=2,M
109     E(J)=0.0115*H(J)*U(J) *FAC
110     14  CONTINUE
111     Y=0.0
112     X=X+XX
113     GO TO 80
114     13  MCV=MCV+1
115     IF(MCV.EQ.2) GO TO 81
116     DO 82 J=2,M
117     MH(J,J)=H(J)
118     42  CONTINUE
119     Y=0.0
120     X=X+XX
121     GO TO 80
122     81  Z=0.0
123     MCV=0
124     DO 83 J=2,M
125     MH(2,J)=H(J)
126     IF(X.EQ.DEPC) MH(1,J)=H(J)
127     83  CONTINUE
128     C  CHECKING A NEW WASTE FALL
129     SUMA=0.0
130     SUMU=0.0
131     YYYY=0.0
132     YYYY=0.0
133     YYYY=100.0
134     YYYY=200.0
135     YYYY=50.0
136     MMM=1
137     LCC=0.0
138     LCC=(YYYY/YY)+2.0
139     LLC=LCC-1
140     DO 23 J=2,LCC
141     IF(X-330.0) 300,300.23
142     300 IF(X) 301,301.23
143     301 IF(MMM.GT.1) GO TO 300
144     CALL RIVER(AC,LLC,U,MH,C,YYYY,YY,SUMA,SUMU,AVE(U),TAVEC)

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```

131      ASA=1.0/((SUMA*AVERU)+3A)
132      SA=0.350.0 *ASA
133 9000  MMM=MMM+1
134      C(2,J)=C(2,J)+SA
135      C(2,J)=C(2,J)+AC
136      59 IF(X=300.0) 23,24,25
137      24 IF(MMM.EQ.1) PRINT 37
138      37 FORMAT('0',25HPOLYMER WASTE FALL '08055' )
139      IF(MMM.GT.1) GO TO 9001
140      CALL RIVER(AC,LLC,U,H,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
141      ASA=1.0/((SUMA*AVERU)+0B)
142      SD=0.100.0 *ASA
143 9001  MMM=MMM+1
144      C(2,J)=(TAVEC+(SUMA*AVERU)*ASA)+SD
145      C(2,J)=C(2,J)+AC
146      MUA=0
147      GO TO 23
148      25 IF(X=1800.0) 23,26,27
149      26 IF(MMM.EQ.1) PRINT 38
150      38 FORMAT('0',25HPOLYMER WASTE FALL '17905' )
151      IF(MMM.GT.1) GO TO 9002
152      CALL RIVER(AC,LLC,U,H,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
153      ASA=1.0/((SUMA*AVERU)+0C)
154      SC=0.010.0 *ASA
155 9002  MMM=MMM+1
156      C(2,J)=(TAVEC+(SUMA*AVERU)*ASA)+SC
157      C(2,J)=C(2,J)+AC
158      MUA=0
159      GO TO 23
160      27 IF(X=1850.0) 23,29,45
161      28 IF(MMM.EQ.1) PRINT 39
162      39 FORMAT('0',25HPOLYMER WASTE FALL '10505' )
163      IF(MMM.GT.1) GO TO 9003
164      CALL RIVER(AC,LLC,U,H,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
165      ASA=1.0/((SUMA*AVERU)+0D)
166      SD=0.000.0 *ASA
167 9003  MMM=MMM+1
168      C(2,J)=(TAVEC+(SUMA*AVERU)*ASA)+SD
169      C(2,J)=C(2,J)+AC
170      MUA=0
171      GO TO 23
172      45 IF(X=2100.0) 23,46,47
173      46 IF(MMM.EQ.1) PRINT 48
174      48 FORMAT('0',53HDOW CHEMICALS WASTE FALL -- DISCHARGE RATE (14+17)MG
175      )
176      IF(MMM.GT.1) GO TO 9004
177      CALL RIVER(AC,LLC,U,H,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
178      ASA=1.0/((SUMA*AVERU)+2E)
179      SE=0.310.0*ASA
180 9004  MMM=MMM+1
181      C(2,J)=(TAVEC+(SUMA*AVERU)*ASA)+SE
182      C(2,J)=C(2,J)+AC
183      MUA=0
184      GO TO 23
185      47 IF(X=2150.0)23,49,50
186      49 IF(MMM.EQ.1) PRINT 51
187      51 FORMAT('0',53HDOW CHEMICALS WASTE FALL -- DISCHARGE RATE ( 2+10)MG
188      )
189      IF(MMM.GT.1) GO TO 9005
190      CALL RIVER(AC,LLC,U,H,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
191      ASA=1.0/((SUMA*AVERU)+0F)
192      SF=0.120.0 *ASA
193 9005  MMM=MMM+1
194      C(2,J)=(TAVEC+(SUMA*AVERU)*ASA)+SF
195      C(2,J)=C(2,J)+AC
196      MUA=0
197      GO TO 23
198      50 IF(X=2600.0) 23,52,53
199      52 IF(MMM.EQ.1) PRINT 54
200      54 FORMAT('0',4GHDO# CHEMICALS WASTE FALL -- DISCHARGE RAT 1/2MGD )
201      IF(MMM.GT.1) GO TO 9006
202      CALL RIVER(AC,LLC,U,H,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
203      ASA=1.0/((SUMA*AVERU)+0G)
204      SG=0.5.0 *ASA
205 9006  MMM=MMM+1
206      C(2,J)=(TAVEC+(SUMA*AVERU)*ASA)+SG
207      C(2,J)=C(2,J)+AC
208      MUA=0
209      GO TO 23
210      53 IF(X=2700.0) 23,55,56

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206 55 IF(MMM.EQ.1) PRINT 57
210 57 FORMAT('0',49HDOW CHEMICALS WASTE FALL -- DISCHARGE PAT 1/3MGD )
211 IF(MMM.GT.1) GO TO 9007
212 CALL RIVER(AC,LLC,U,M,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
213 ASA=1.0/((SUMA+AVERU)+DH)
214 SHQ=J.333 *ASA
215 9007 MMM=MMM+1
216 C(2,J)=(TAVEC*(SUMA+AVERU)*ASA)+SH
217 C(2,J)=C(2,J)+AC
218 MUA=0
219 GO TO 23
220 59 IF(X-3150.0) 23,58,59
221 58 IF(MMM.EQ.1) PRINT 60
222 60 FORMAT('0',49HDOW CHEMICALS WASTE FALL -- DISCHARGE RATE 12MGD )
223 IF(MMM.GT.1) GO TO 9008
224 CALL RIVER(AC,LLC,U,M,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
225 ASA=1.0/((SUMA+AVERU)+OI)
226 SI=Q2*120.0 *ASA
227 9008 MMM=MMM+1
228 C(2,J)=(TAVEC*(SUMA+AVERU)*ASA)+SI
229 C(2,J)=C(2,J)+AC
230 MUA=0
231 GO TO 23
232 59 IF(X-3950.0) 23,61,62
233 61 IF(MMM.EQ.1) PRINT 63
234 63 FORMAT('0',49HDOW CHEMICALS WASTE FALL -- DISCHARGE RATE 74MGD )
235 IF(MMM.GT.1) GO TO 9009
236 CALL RIVER(AC,LLC,U,M,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
237 ASA=1.0/((SUMA+AVERU)+QJ)
238 SJ=Q2*740.0 *ASA
239 9009 MMM=MMM+1
240 C(2,J)=(TAVEC*(SUMA+AVERU)*ASA)+SJ
241 C(2,J)=C(2,J)+AC
242 MUA=0
243 GO TO 23
244 62 IF(X-4950.0) 23,64,65
245 64 IF(MMM.EQ.1) PRINT 66
246 66 FORMAT('0',49HDOW CHEMICALS WASTE FALL -- DISCHARGE RATE 25MGD )
247 IF(MMM.GT.1) GO TO 9010
248 CALL RIVER(AC,LLC,U,M,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
249 ASA=1.0/((SUMA+AVERU)+QK)
250 SK=Q2*250.0 *ASA
251 9010 MMM=MMM+1
252 C(2,J)=(TAVEC*(SUMA+AVERU)*ASA)+SK
253 C(2,J)=C(2,J)+AC
254 MUA=0
255 GO TO 23
256 65 IF(X-5300.0) 23,67,68
257 67 IF(MMM.EQ.1) PRINT 68
258 68 FORMAT('0',53HDOW CHEMICALS WASTE FALL -- DISCHARGE RATE(1+1/3)MGD
259 )
260 IF(MMM.GT.1) GO TO 9011
261 CALL RIVER(AC,LLC,U,M,C,YYYY,YY,SUMA,SUMU,AVERU,TAVEC)
262 ASA=1.0/((SUMA+AVERU)+UL)
263 SL=Q2*12.333 *ASA
264 9011 MMM=MMM+1
265 C(2,J)=(TAVEC*(SUMA+AVERU)*ASA)+SL
266 C(2,J)=C(2,J)+AC
267 MUA=0
268 23 YYY=YYY+YY
269 9999 AYAX=0.0
270 HH(2,M+1)=H(M)
271 HH(3,M+1)=H(M)
272 CALL SMASS(MDA,C,HH,XX,YY,M)
273 DO 34 J=2,M
274 34 CONTINUE
275 DO 115 J=2,M
276 115 C(1,J)=C(2,J)*16021.0
277 N=X/AYAZ
278 IF(N-L) 41,43,40
279 40 PRINT 33,X,(C(1,J),J=2,M,5)
280 33 FORMAT('0',F9.1,10X,11(F9.2))
281 L=L+1
282 41 C(2,J)=C(2,J)
283 H(1)=H(2)
284 H(M+1)=H(M)
285 70 DJ 15 J=2,M
286 A(J)=(1.0+XX*C(J))/((YY**2.0)+U(J))
287 U(J)=1.0+XX*C(J-1)/((YY**2.0)+U(J))

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```

298      D(J)=A(J)+E(J)
299      C(3,J)=C(2,J)*(1.0-D(J))*H(J)+A(J)*H(J+1)+C(2,J+1)+B(J)+H(J-1)*C
300      (2,J-1)/HH(3,J)
301      15 CONTINUE
302      DO 200 J=2,M
303      IF (C(3,J).LE.1.0E-10) C(3,J)=0.0
304      C(2,J)=C(3,J)
305      X=X+XX
306      IF (X-100000.0) 18,18,20
307      20 STOP
308      END

```

```

278      SUBROUTINE RIVER(AC,LLC,U,M,C,YYYY,YY,SUMA,SUMZ,AVERU,TAVEC)
279      DIMENSION U(S10),H(S10),C(3,S10)
300      TSUMC=0.0
301      LCC=LLC+1
302      DO 600 K=2,LLC
303      SUMU=SUMU+(((U(K)+U(K+1))/2.0)*YY)
304      600 SUMA=SUMA+(((H(K)+H(K+1))/2.0)*YY)
305      SUMU=SUMU+((3.0*U(LLC+1)+U(LLC+2))/4.0)*YY/2.0
306      SUMA=SUMA+((3.0*H(LLC+1)+H(LLC+2))/4.0)*YY/2.0
307      TSUMC=TSUMC+C(2,2)*YY/2.0*H(2)
308      DO 3 J=3,LCC
309      TSUMC=TSUMC+C(2,J)*YY*H(J)
310      3 CONTINUE
311      AVERU=SUMU/(YYYY+YY/2.0)
312      TAVEC=TSUMC/SUMA
313      CCCCCC :.. BRINGING THE TOTAL MASS EQUAL TO ONE IN THREE DIMEN. MODEL
314      Z7A=4.0
315      SUMH=0.0
316      SUMZ=0.0
317      DO 4 J=2,LCC
318      SUMH=SUMH+H(J)
319      LSUMZ=H(J)/Z7A
320      SUMZ=SUMZ+LSUMZ*Z7A
321      4 CONTINUE
322      SUMH=SUMH/LLC
323      SUMZ=SUMZ/LLC
324      AC=SUMZ/SUMH
325      RETURN
326      END

```

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326      SUBROUTINE SMASS(MBA,C,HI,XX,YY,M)
327      DIMENSION MH(3,510),C(3,510)
328      MA=0
329      TMASS=0.0
330      5 MA=MA+1
331      TMASS=C(2,2)*(YY/2.0)*XX*((MH(1,21)+MH(3,21)+MH(2,51))+3.0*MH(2,21)/M)
332      DO 1 J=3,M
333      TMASS=TMASS+C(2,J)*YY*XX*((MH(1,J)+MH(3,J)+MH(2,J-1)+MH(2,J+1))+4.0
1=MH(2,J)/M)
334      1 CONTINUE
335      MBA=MBA+1
336      IF(MBA.EQ.1) AMASS=TMASS
337      AFAC=AMASS/TMASS
338      IF(MA.EQ.3) GO TO 6
339      DO 2 J=2,M
340      C(2,J)=C(2,J)*AFAC
341      2 CONTINUE
342      IF(MA.EQ.1) GO TO 5
343      6 RETURN
344      END

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SENTRY

APPENDIX H

Computer Program For Three
Dimensional Mixing Model
(St. Clair River)

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1004 WATFIV ***** NAME--ASEEM AKHTAR
CC***C--THREE DIMENSIONAL DISPERSION MODEL FOR ST. CLAIR RIVER
CC***C--FORWARD MARCHING FINITE DIFFERENCE METHOD
CC***C--DEFINING GRID DIMENSIONS AND GIVING INITIAL VALUES
CCCCC.....X=LONGITUDINAL DISTANCE
CCCCC.....Y=LATERAL DISTANCE
CCCCC.....Z=VERTICAL DISTANCE
CCCCC.....XX=GRID SIZE X-DIRECTIONAL
CCCCC.....YY=GRID SIZE Y-DIRECTIONAL
CCCCC.....ZZ=GRID SIZE Z-DIRECTIONAL
CCCCC.....CX=LONGITUDINAL DIFFUSION COEFFICIENT
CCCCC.....CY=LATERAL DIFFUSION COEFFICIENT
CCCCC.....CZ=VERTICAL DIFFUSION COEFFICIENT
CCCCC.....CA TO CL=DISCHARGE RATE OF OUTFALLS
CCCCC.....ZM=MAXIMUM DEPTH OF THE RIVER SECTION
CCCCC.....C=CONCENTRATION OF POLLUTANT
1 DIMENSION C(2,40,105),C(140,105),V(1,210),AH(1,210),EY(1,210),EZ(
12,210),U(310),H(210),W(50),A(105),AA(210),B(105),JU(210),D(105),D
20(210),E(105),EE(210),F(105),FF(210),G(105),GG(210),J(210),P(210),
JMH(105),SLMC(105),AVEC(105),TUG(105)
2 DIMENSION LU(105)
3 PRINT 34
4 34 FORMAT(10X,54HX=LONGITUDINAL DISTANCE FROM FIRST POLYMER FALL*0020
5 IN*5X,26HY=LATERAL DISTANCE FROM CANADIAN SHORE )
6 PRINT 1030
7 1030 FORMAT(10X,51HZ=VERTICAL DISTANCE MEASURED FROM THE RIVER SURFACE
8 )
9 X=2700.0
10 X=2950.0
11 X=3400.0
12 X=C.0
13 MUA=0
14 LNA=0
15 JL=0
16 ZM=J0.C
17 Y=500.0
18 YY=10.0
19 XX=10.0
20 ZZ=0.C
21 AGA=1.0
22 AAGA=1.0
23 M=(Y/YY)+2
24 N=(ZM/ZZ)+2
25 M1=(2*Y/YY)+2
26 N1=(2*ZM/ZZ)+2
27 N2=N1+1
28 M2=M1+1
29 M3=M-1
30 N3=N-1
31 DO 1 I=1,N
32 DO 1 J=1,M
33 1 C(I,1,J)=0.0
34 DO 100 J=1,M
35 EY(1,J)=0.0
36 EZ(1,J)=0.0
37 AH(1,J)=0.0
38 V(1,J)=0.0
39 U=1.0/(0.20+C.24)
40 U2=0
41 CA=(U/62.5)*550.0
42 CB=(U/62.5)*160.0
43 CC=(U/62.5)*610.0
44 CD=(U/62.5)*50.0
45 CE=(U/62.5)*310.0
46 CF=(U/62.5)*120.0
47 CG=(U/62.5)*5.0
48 CH=(U/62.5)*1.333
49 CI=(U/62.5)*120.0
50 CJ=(U/62.5)*740.0
51 CK=(U/62.5)*220.0
52 CL=(U/62.5)*12.333
53 CC CHECKING SECTIONS
54 Z=0.0
55 Y=0.0
56 IF(X=1720.0) 19,19,3
57 19 N=1.0
58 S=C.0
59 T=0.0
60 GU TO 2
61 3 IF(X=2620.0) 20,20,21

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56 20 R=C.0
57 S=1.0
58 T=C.0
59 GU TO 2
60 21 R=C.0
61 S=0.0
62 T=1.0
63 CC**CC--CALCULATIONS FOR ESTIMATING DEPTH AND VELOCITY OF RIVER AT GRID POINTS
64 2 DU 4 J=2,K2
65 IF(Y-50.0) E.2.2
66 S H(J)=R*(1.003422*X)-4.4262)+T*9.780
67 U(J)=R*(0.001647C*X)-2.83281*Y/50.0)+0.0J)+T*((1.48*Y750
68 1.0)+0.0J)
69 U(J)=0.2325
70 P(J)=(10.0*(U(J)/D(J)))/H(J)
71 GO TO 7
72 3 IF(Y-100.0) E.0.3
73 8 H(J)=R*((1.003422*(Y-50.)/50.)+4.9)+S*((((0.013000*X)-20.7100)*(Y-50.)
74 1/50.))+((0.003422*X)-4.4262))+T*((13.35*(Y-50.)/50.)+1.78)
75 U(J)=R*((0.001647C*X)-2.83281*Y/50.0)+0.0J)+T*((0.003422*X)-4.4262)
76 1X)+T*((0.003422*(Y-50.)/50.))+((0.001647C*X)-2.83281)+T*((0.003422*(Y-50.)/5
77 20.))+1.5123)
78 C(J)=R*((0.000077093*X)+(Y-50.0)/50.0)+2.2325)+S*((0.003422*(
79 Y-50.0)/50.0)+0.2325)+T*((0.003422*(Y-50.0)/50.0)+0.2325)
80 P(J)=(10.0*(U(J)/D(J)))/H(J)
81 GO TO 7
82 9 IF(Y-250.) 1C.10.11
83 10 H(J)=R*((24.57*(Y-100.)/150.))+6.45)+S*((50.2502-(0.013422*X)+1*(Y-
84 1100.)/150.))+((0.013422*X)-25.1362))+T*((17.59*(Y-100.)/150.))+2J.13)
85 U(J)=R*((2.650+(0.0004660C*X))*(Y-100.)/150.))+0.0J)+T*((0.0004660C*
86 1X))+S*((0.0004660C*(Y-100.)/150.))+((0.0004660C*X)-J.42
87 280))+T*((1.44*(Y-100.)/150.))+2.048E)
88 U(J)=R*((0.5816+0.000077093*X)*(Y-100.0)/150.0)+J.4415-0.0000770
89 193*X)+S*((0.7142*(Y-100.0)/150.0)+0.2289)+T*((0.7142*(Y-100.0)/15
90 20.0)+0.2289)
91 P(J)=(10.0*(U(J)/D(J)))/H(J)
92 GO TO 7
93 11 H(J)=(4.77*(Y-250.)/250.))+31.12
94 U(J)=(0.7269*(Y-250.)/250.))+3.4881
95 Q(J)=(0.1822*(Y-250.)/250.0))+1.0431
96 P(J)=(10.0*(U(J)/D(J)))/H(J)
97 7 Y=Y+(YY/2.C)
98 4 CONTINUE
99 C CHECKING A NEW WASTE FALL
100 YYY=50.0
101 LC=(YYYY/YY)+2.0
102 LLC=LC-1
103 SUMU=0.0
104 SUMA=0.0
105 MM=1.0
106 UU(2)=U(2)
107 MM(2)=H(2)
108 DO 5555 K=2,K3
109 UU(K+1)=U(K+2)
110 MM(K+1)=H(K+2)
111 YYY=0.0
112 DO 5556 J=2,LC
113 KK=(MM(J)/ZZ)+2
114 DO 23 I=2,KK
115 IF(X-500.C) 304,304,23
116 304 IF(X) 305,305,69
117 305 IF(MMM.GT.1) GO TO 5000
118 CALL RIVER(LC,LLC,UU,MM,C,ZZ,YYYY,YY,SUMA,AVERU,TAVEC)
119 ASA=1.0/((SUMA*AVERU)+2A)
120 SA=0.50.C*ASA
121 5000 MM=MM+1
122 C(1.1,J)=C(1.1,J)+SA
123 GO TO 23
124 69 IF(X-300.C) 23,24,25
125 24 IF(MMM.EQ.1) PRINT 17
126 17 FORMAT('0',25PCLYMEK WASTE FALL 020555 )
127 IF(MMM.GT.1) GO TO 301
128 CALL RIVER(LC,LLC,UU,MM,C,ZZ,YYYY,YY,SUMA,AVERU,TAVEC)
129 ASA=1.0/((SUMA*AVERU)+2B)
130 SB=J*100.C*ASA
131 5001 MM=MM+1
132 C(1.1,J)=(TAVEC*(SUMA*AVERU)+ASA)+SB
133 MHA=0
134 GO TO 23
135 25 IF(X-1000.C) 23,26, 27

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127      26 IF(MMM.EC.1) PRINT 26
128      38 FORMAT('0'.23#POLYMER WASTE FALL*17905' )
129      IF(MMM.GT.1) GO TO 3032
130      CALL RIVER(LC,LLC,UU,MM,C.22.YYYY.YY,SUMA,AVERU,TAVEC)
131      ASA=1.0/((SUMA+AVERU)*QC)
132      SG=0*10.C *ASA
133      MYN=MM+1
134      C(I,I,J)=(TAVEC*(SUMA+AVERU)*ASA)*SC
135      MJA=0
136      GO TO 23
137      27 IF(X=1550.C) 23.28.45
138      28 IF(MMM.EC.1) PRINT 30
139      30 FORMAT('0'.23#POLYMER WASTE FALL*18505' )
140      IF(MMM.GT.1) GO TO 3033
141      CALL RIVER(LC,LLC,UU,MM,C.22.YYYY.YY,SUMA,AVERU,TAVEC)
142      ASA=1.0/((SUMA+AVERU)*QD)
143      SD=0*10.C *ASA
144      MYN=MM+1
145      C(I,I,J)=(TAVEC*(SUMA+AVERU)*ASA)*SD
146      MJA=0
147      GO TO 23
148      45 IF(X=2100.C) 23.46.47
149      46 IF(MMM.EC.1) PRINT 40
150      48 FORMAT('0'.23#DU# CHEMICALS WASTE FALL -- DISCHARGE RATE (14*17)MG
151      1D )
152      IF(MMM.GT.1) GO TO 3034
153      CALL RIVER(LC,LLC,UU,MM,C.22.YYYY.YY,SUMA,AVERU,TAVEC)
154      ASA=1.0/((SUMA+AVERU)*QE)
155      SE=0*10.C *ASA
156      MYN=MM+1
157      C(I,I,J)=(TAVEC*(SUMA+AVERU)*ASA)*SE
158      MJA=0
159      GO TO 23
160      47 IF(X=2150.C) 23.49.50
161      49 IF(MMM.EC.1) PRINT 51
162      51 FORMAT('0'.23#DU# CHEMICALS WASTE FALL -- DISCHARGE RATE ( 2*10)MG
163      1D )
164      IF(MMM.GT.1) GO TO 3035
165      CALL RIVER(LC,LLC,UU,MM,C.22.YYYY.YY,SUMA,AVERU,TAVEC)
166      ASA=1.0/((SUMA+AVERU)*JF)
167      SF=0*10.C *ASA
168      MYN=MM+1
169      C(I,I,J)=(TAVEC*(SUMA+AVERU)*ASA)*SF
170      MJA=0
171      GO TO 23
172      50 IF(X=2600.C) 23.52.53
173      52 IF(MMM.EC.1) PRINT 54
174      54 FORMAT('0'.4#DU# CHEMICALS WASTE FALL -- DISCHARGE RAT 1/3MCD )
175      IF(MMM.GT.1) GO TO 3036
176      CALL RIVER(LC,LLC,UU,MM,C.22.YYYY.YY,SUMA,AVERU,TAVEC)
177      ASA=1.0/((SUMA+AVERU)*JG)
178      SG=0*5.C *ASA
179      MYN=MM+1
180      C(I,I,J)=(TAVEC*(SUMA+AVERU)*ASA)*SG
181      MJA=0
182      GO TO 23
183      53 IF(X=2700.C) 23.55.56
184      55 IF(MMM.EC.1) PRINT 57
185      57 FORMAT('0'.4#DU# CHEMICALS WASTE FALL -- DISCHARGE RAT 1/3MCD )
186      IF(MMM.GT.1) GO TO 3037
187      CALL RIVER(LC,LLC,UU,MM,C.22.YYYY.YY,SUMA,AVERU,TAVEC)
188      ASA=1.0/((SUMA+AVERU)*JH)
189      SH=0*3.333 *ASA
190      MYN=MM+1
191      C(I,I,J)=(TAVEC*(SUMA+AVERU)*ASA)*SH
192      MJA=0
193      GO TO 23
194      56 IF(X=2150.C) 23.58.59
195      58 IF(MMM.EC.1) PRINT 60
196      60 FORMAT('0'.4#DU# CHEMICALS WASTE FALL -- DISCHARGE RATE 12MCD )
197      IF(MMM.GT.1) GO TO 3038
198      CALL RIVER(LC,LLC,UU,MM,C.22.YYYY.YY,SUMA,AVERU,TAVEC)
199      ASA=1.0/((SUMA+AVERU)*JI)
200      SI=0*120.C *ASA
201      MYN=MM+1
202      C(I,I,J)=(TAVEC*(SUMA+AVERU)*ASA)*SI
203      MJA=0
204      GO TO 23
205      59 IF(X=2250.C) 23.61.62
206      61 IF(MMM.EC.1) PRINT 63

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205 63 FORMAT('0',4#D00# CHEMICALS WASTE FALL -- DISCHARGE RATE 74MCO )
206 IF(MMM.GT.1) GO TO 900
207 CALL RIVER(LC,LLC,UU,MM,C,ZZ,YYYY,YY,SUMA,AVERU,TAVEC)
208 ASA=1.07*(SUMA*AVERU)*JJ
209 SJ=Q2*740.C *ASA
210 MVA=MM+1
211 C(1,1,J)=(TAVEC*(SUMA*AVERU)*ASA)*SJ
212 MVA=0
213 GO TO 23
214 62 IF(X=9500.C) 23.04.05
215 64 IF(MMM.EQ.1) PRINT 68
216 64 FORMAT('0',4#D00# CHEMICALS WASTE FALL -- DISCHARGE RATE 25MCO )
217 IF(MMM.GT.1) GO TO 9010
218 CALL RIVER(LC,LLC,UU,MM,C,ZZ,YYYY,YY,SUMA,AVERU,TAVEC)
219 ASA=1.07*(SUMA*AVERU)*JK
220 SK=Q2*250.C *ASA
221 MVA=MM+1
222 C(1,1,J)=(TAVEC*(SUMA*AVERU)*ASA)*JK
223 MVA=0
224 GO TO 23
225 65 IF(X=9300.C) 23.07.23
226 67 IF(MMM.EQ.1) PRINT 68
227 68 FORMAT('0',4#D00# CHEMICALS WASTE FALL -- DISCHARGE RATE(1+1/3)MCO
228 )
229 IF(MMM.GT.1) GO TO 9011
230 CALL RIVER(LC,LLC,UU,MM,C,ZZ,YYYY,YY,SUMA,AVERU,TAVEC)
231 ASA=1.07*(SUMA*AVERU)*KL
232 SL=Q2*13.222 *ASA
233 MVA=MM+1
234 C(1,1,J)=(TAVEC*(SUMA*AVERU)*ASA)*SL
235 MVA=0
236 23 CONTINUE
237 5555 YYYYYYYYYY
-CALL SMASE(MEA,C,MM,XX,YY,ZZ,M,N)
CC**CC--CALCULATIONS FOR ESTIMATING LATERAL AND VERTICAL TURBULENT MIXING
CC**CC--COEFFICIENTS .....
CCCCC CALCULATIONS OF CONCENTRATION PROFILES
238 Z=0.0
239 VK=50.0/YY
240 VKEVK=1.0
241 ZZZ=0.0
242 AAAZ=0.0
243 JLL=1
244 DU 200 1=2.N
245 ZZZ=0.0
246 AAAZ=AAAZ+ZZ
247 Z=AAAZ-ZZ
248 DU 700 J=2.W2.2
249 AH(1,J)=F(J)-1
250 AH(1,J-1)=F(J-1)-2
251 IF(AH(1,J)) 212,212,2013
252 AH(1,J)=0.0
253 2213 IF(AH(1,J-1)) 2212,2212,213
254 AH(1,J-1)=0.0
255 4007 V(1,J-1)=C(J-1)*ALU/10*(F(J-1)*Q-10)
256 GO TO 1006
257 213 IF(AH(1,J-1)=0.1) 1007,1006,100A
258 100A V(1,J-1)=C(J-1)*ALU/10*(P(J-1)*AH(1,J-1))
259 1006 IF(V(1,J-1))1005,1005,213
260 1005 V(1,J-1)=0.0
261 216 EY(1,J)=0.2110*H(J) *L(J) *ASA
262 AA(J-1)=EY(1,J)*XX/((YY**2.0)+V(1,J-1))
263 DB(J-1)=EY(1,J-2)*XX/((YY**2.0)+V(1,J-1))
264 DB(J-1)=AA(J-1)+DB(J-1)
265 700 CONTINUE
266 DU 100 J=2.W2.2
267 AH(1,J)=F(J)-2-(ZZ/2.0)
268 IF(AH(1,J)) 1212,1212,1210
269 1212 AH(1,J)=0.0
270 1216 E2(2,J)=0.03*AH(1,J)*(2*(ZZ/2.0))*U(J)/H(J)*ASA
271 EC(J)=E2(2,J)*XX/(ZZ**2.0)*V(1,J)
272 FF(J)=E2(1,J)*XX/(ZZ**2.0)*V(1,J)
273 GS(J)=EE(J)+FF(J)
274 100 CONTINUE
275 A(2)=AA(2)
276 J(2)=AR(2)
277 D(2)=A(2)+E(2)
278 C(2)=CF(2)
279 F(2)=FF(2)
280 G(2)=E(2)+F(2)

```

```

231      TDC(2)=D(2)+C(2)
232      DO 221 K=2,M
233      A(K+1)=AA(K+1)
234      B(K+1)=BB(K+1)
235      C(K+1)=CC(K+1)
236      D(K+1)=DD(K+1)
237      E(K+1)=EE(K+1)
238      F(K+1)=FF(K+1)
239      G(K+1)=A(K+1)+B(K+1)
240      H(K+1)=C(K+1)+D(K+1)
241      TDC(K+1)=G(K+1)+H(K+1)
242      CONTINUE
243      L22=C
244      DO 100 J=2,M
245      CHEZEMH(J)=AAZ
246      CHEJEMH(J)=Z
247      IF(CHEJ) 124,223,22J
248      IF(CHEZ) 112,113,113
249      C(2,1,J)=0.0
250      GO TO 103
251      113 C(1,1,J)=C(1,1,J)
252      C(1,1,1)=C(1,1,3)
253      C(1,1,M+1)=C(1,1,M-1)
254      C(1,N+1,J)=C(1,N-1,J)
255      C(2,1,J)=C(1,1,J)+A(J)*C(1,1,J+1)+B(J)*C(1,1,J-1)-D(J)*C(1,1,J)+
256      E(J)*C(1,1,J)+F(J)*C(1,1-1,J)-G(J)*C(1,1,J)
257      GO TO 103
258      112 C(1,1,1)=C(1,1,1)
259      C(1,1,M+1)=C(1,1,M-1)
260      C(1,N+1,J)=C(1,N-1,J)
261      C(2,1,J)=C(1,1,J)+A(J)*C(1,1,J+1)+B(J)*C(1,1,J-1)-D(J)*C(1,1,J)+
262      F(J)*C(1,1-1,J)-F(J)*C(1,1,J)
263      GO TO 103
264      103 GO TO 100
265      100 CONTINUE
266      DO 2000 J=2,M,2
267      L2(1,J)=E2(2,J)
268      CONTINUE
269      NLN=KX50.0
270      IF((NLN-LNN) 41,40,40)
271      Z=0.0
272      PRINT 250,Y
273      FORMAT('*.5*.2HXB=.F5.1)
274      PRINT 35
275      FORMAT('C'. 20X,5HY=0.0,3X,6HY=50.0,3X,7HY=100.0,2X,7HY=15
276      10.0,2X,7HY=200.0,2X,7HY=250.0,2X,7HY=300.0,2X,7HY=350.0,2X,7HY=400
277      4.0,2X,7HY=450.0,2X,7HY=500.0 )
278      DO 600 I=2,N
279      DO 550 J=2,M
280      CC(1,J)=C(1,1,J)+10C21.C
281      PRINT 251 ,Z,(CC(1,J),J=2,M,5)
282      FORMAT('0*.3X,2HZ=.F5.2,3X,12(E3.2))
283      Z=2+Z
284      LNN=LNN+1
285      DO 252 I=2,N
286      DO 252 J=2,M
287      IF(C(2,1,J).LL.1.0E-07) C(2,1,J)=0.0
288      C(1,1,J)=C(2,1,J)
289      XXX+XX
290      IF(IX-2100.0) 253,253,254
291      STOP
292      END

```

```

347 SUBROUTINE RIVER(LC,LLC,UU,PH,C,ZZ,YYYY,YY,SUAA,AVLRO,TAVEC)
348 DIMENSION LU(105),PH(105),C(2,40,105)
349 DIMENSION MZ(2)
350 SUMU=0.0
351 TMASS=0.0
352 MZ(1)=PH(2)/ZZ+2
353 DO 1 J=2,LC
354 MZ1=1
355 MZ=MIN(J)/ZZ+2
356 MZ(2)=MZ
357 DO 4 I=2,MZ
358 IF(MZ(1)-I) 3,2,2
359 IF(MZ(1)-MZ) 3,2,2
360 2 IF(U,LC-2,AND,I,EU-2)TMASS=TMASS+C(1,I,J)* YY*ZZ/4.0
361 IF(U,EU-2,AND,I,GT-2,AND,I,LT,MZ)TMASS=TMASS+C(1,I,J)* YY*ZZ/2.0
362 IF(U,EU-2,AND,I,EU,MZ)TMASS=TMASS+C(1,I,J)* YY*ZZ/4.0
363 IF(U,GT-2,AND,I,EU-2)TMASS=TMASS+C(1,I,J)* YY*ZZ/2.0
364 IF(U,GT-2,AND,I,GT-2,AND,I,LT,MZ)TMASS=TMASS+C(1,I,J)* YY*ZZ
365 IF(U,GT-2,AND,I,GT-2,AND,I,EU,MZ)TMASS=TMASS+C(1,I,J)* YY*ZZ/2.0
366 GO TO 4
367 5 IF(MZ1,EU,1) GO TO 6
368 IF(I,LT,MZ) TMASS=TMASS+C(1,I,J)* YY*ZZ/2.0
369 IF(I,EU,MZ) TMASS=TMASS+C(1,I,J)* YY*ZZ/4.0
370 GO TO 4
371 6 TMASS=TMASS+C(1,I,J)* YY*ZZ*3.0/4.0
372 MZ1=MZ1+1
373 4 CONTINUE
374 MZ(1)=MZ(2)
375 1 CONTINUE
376 DO 6660 IK=2,LLC
377 SUMU=SUMU+(((UU(IK)+UU(IK+1))/2.0)*YY)
378 6660 SUMA=SUMA+(((PH(IK)+PH(IK+1))/2.0)*YY)
379 SUMU=SUMU+((J,0*UU(LLC+1)+UU(LLC+2))/4.0)*YY/2.0
380 SUMA=SUMA+((J,0*PH(LLC+1)+PH(LLC+2))/4.0)*YY/2.0
381 AVEU=SUMU/(YYYY+YY/2.0)
382 TAVLC=TMASS/SLMA
383 RETURN
384 END

```

```

378 SUBROUTINE SPASS(MGA,C,PH,XX,YY,ZZ,M,N)
379 DIMENSION C(2,40,105),PH(105),MZ(2)
380 MA=0
381 12 MA=MA+1
382 TMASS=0.0
383 MZ(1)=PH(2)/ZZ+2
384 DO 1 J=2,M
385 MZ1=1
386 MZ=MIN(J)/ZZ+2
387 MZ(2)=MZ
388 DO 4 I=2,MZ
389 IF(MZ(1)-I) 3,2,2
390 IF(MZ(1)-MZ) 3,2,2
391 2 IF(U,EU-2,AND,I,EU-2)TMASS=TMASS+C(1,I,J)*XX*YY*ZZ/4.0
392 IF(U,EU-2,AND,I,GT-2,AND,I,LT,MZ)TMASS=TMASS+C(1,I,J)*XX*YY*ZZ/2.0
393 IF(U,EU-2,AND,I,EU,MZ)TMASS=TMASS+C(1,I,J)*XX*YY*ZZ/4.0
394 IF(U,GT-2,AND,I,EU-2)TMASS=TMASS+C(1,I,J)*XX*YY*ZZ/2.0
395 IF(U,GT-2,AND,I,GT-2,AND,I,LT,MZ)TMASS=TMASS+C(1,I,J)*XX*YY*ZZ
396 IF(U,GT-2,AND,I,GT-2,AND,I,EU,MZ)TMASS=TMASS+C(1,I,J)*XX*YY*ZZ/2.0
397 GO TO 4
398 5 IF(MZ1,EU,1) GO TO 6
399 IF(I,LT,MZ) TMASS=TMASS+C(1,I,J)*XX*YY*ZZ/2.0
400 IF(I,EU,MZ) TMASS=TMASS+C(1,I,J)*XX*YY*ZZ/4.0
401 GO TO 4
402 6 TMASS=TMASS+C(1,I,J)*XX*YY*ZZ*3.0/4.0
403 MZ1=MZ1+1
404 4 CONTINUE
405 MZ(1)=MZ(2)
406 1 CONTINUE
407 MA=MA+1
408 IF(MGA,EU,1)TMASS=TMASS
409 AFAC=AFAC/TMASS
410 IF(MA,EU-2) GO TO 13
411 DO 7 I=2,M
412 DO 7 J=2,N
413 C(1,I,J)=C(1,I,J)*AFAC
414 IF(MA,EU-1) GO TO 12
415 13 RETURN
416 END

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APPENDIX I

Computer Program For Mixing Model

(Air Agitated Tank)


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$JOB WATFIV XXXXXXXXXX NAME=WASEEM AKHTAR
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCCC...STUDY OF MIXING IN AIR-AGITATED BATCH TANKS
CCCCC...PFACEMAN=RACHFORD'S ALTERNATING DIRECTION IMPLICIT METHOD
CCCCC YYY=DEPTH OF TANK
CCCCC XXX=LENGTH OF TANK
CCCCC TT=TIME OF MIXING
CCCCC XX=LENGTH GRID
CCCCC N0=COUNTER FOR NUMBERS OF RESULTS NOT PRINTED FOR EACH TIME STEP
CCCCC YY=DEPTH GRID
CCCCC TT=TIME GRID
CCCCC XD=DISTANCE OF CENTRE OF CIRCULATION FROM DIFFUSER SIDE
CCCCC AAA=HALF OF THE LENGTH
CCCCC YD=DISTANCE OF CENTRE OF CIRCULATION FROM SURFACE OF LIQUID CONTENT
CCCCC BDB=SAME AS Y
CCCCC BCU=DISTANCE OF CENTRE OF CIRCULATION FROM BOTTOM OF THE TANK
CCCCC SIM=S1-MAX RATE OF LIQUID CIRCULATION FT3/SEC PER FOOT OF WIDTH
CCCCC ET=TANGENTIAL TURBULENT DIFFUSION COEFFICIENT
CCCCC EN=NORMAL TURBULENT DIFFUSION COEFFICIENT
CCCCC EX=LONGITUDINAL TURBULENT DIFFUSION COEFFICIENT
CCCCC CY=VERTICAL TURBULENT DIFFUSION COEFFICIENT
CCCCC FAC1=MULTIPLE FACTOR IN ET EXPRESSION
CCCCC FAC2=MULTIPLE FACTOR IN EN EXPRESSION
CCCCC U=HORIZONTAL VELOCITY
CCCCC V=VERTICAL VELOCITY
CCCCC SC=LOCATION OF THE POINT CONCENTRATION FROM WHERE THE SAMPLE BEING DRAWN
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
DIMENSION U(40,20),V(40,20),TH(40,20),EX(40,20),EY(40,20)
COMMON C(40,20,2),A(40,20),J(40,20),EP(40,20),FP(40,20),EB(40,20)
1,FB(40,20),N,N
COMMON KA
COMMON XXX,YYY,XX,YY ,T
COMMON NA,NS
COMMON UNIFORM
KA=1
T=0.0
XXX=30.0
AAA=10.5
X=-14.5
YYY=15.0
TT=1.0
TTT=0.5
NA=1
NH=1
NAA=0
NDB=NS
TT=1.0
XX=3.0
YY=3.0
XT=XX
YT=YY
N=(XXX/XX)+2
M=(YYY/YY)+2
XX=1.5
YY=1.5
NT=(XXX/XX)+2
MT=(YYY/YY)+2
AV=0.09
SIM=3.56
THAY
BBD=AY
RDB=AY-YYY
FAC1=0.49
FAC2=1.0
ET=FAC1*SIM
EN=FAC2*0.00325*SIM
DO 7 I=1,N
DO 7 J=1,M
C(I,J,1)=0.0
7 CONTINUE
C(2,2,1)=50.0
DO 1 I=2,NT
DO 2 J=2,MT
IF(Y.L.C-0.00)RDB=RDB*8
AC=SIM/(AAA*AAA*RDB*BDB)
U(I,J)=-2.0*Y*AC*(X-X*AAA*AAA)
V(I,J)=2.0*X*AC*(Y-Y*BDB*BDB)
IF(U(I,J).EQ.0.0.AND.V(I,J).EQ.0.0) GO TO 8

```

```

0001 IF(U(I,J).EQ.0.0.AND.V(I,J).NE.0.0) GO TO 16
0002 TH(I,J)=ATAN(V(I,J)/U(I,J))
0003 GO TO 9
0004 16 TH(I,J)=11.0/7.0
0005 GO TO 9
0006 8 TH(I,J)=0.0
0007 9 EX(I,J)=ET=cos(TH(I,J))-EN*SIN(TH(I,J))
0008 EY(I,J)=EY=SIN(TH(I,J))+EN*cos(TH(I,J))
0009 EX(I,J)=ABS(EX(I,J))
0010 EY(I,J)=ABS(EY(I,J))
0011 YV=Y
0012 W CONTINUE
0013 X=X+XX
0014 TRAY
0015 RRR=AY
0016 1 CONTINUE
0017 IF(NAA.EQ.NB8) GO TO 52
0018 GO TO 53
0019 52 TT=1.0
0020 TT=0.1
0021 NABO
0022 53 KX=XT
0023 YY=YT
0024 KI=1
0025 DO 31 I=2,N
0026 KJ=1
0027 DO 32 J=2,M
0028 U(I,J)=U(2*KI,2*KJ)
0029 V(I,J)=V(2*KI,2*KJ)
0030 A(I,J)=U(I,J)*TT/(2.0*XX)
0031 B(I,J)=V(I,J)*TT/(2.0*YY)
0032 IF(I=KI+1).GT.NT EX(NT+1,2*KJ)=EX(NT-1,2*KJ)
0033 FF(I,J)=EX(2*KI-1,2*KJ)*TT/(XX*XX)
0034 IF(KI.EQ.1) EX(1,2*KJ)=CX(1,2*KJ)
0035 EB(I,J)=EX(2*KI-1,2*KJ)*TT/(XX*XX)
0036 IF(2*KJ+1).GT.NT EY(2*KI,NT+1)=EY(2*KI,NT-1)
0037 FF(I,J)=EY(2*KI,2*KJ-1)*TT/(YY*YY)
0038 IF(KJ.EQ.1) EY(2*KI,1)=EY(2*KI,3)
0039 FB(I,J)=EY(2*KI,2*KJ-1)*TT/(YY*YY)
0040 KJ=KJ+1
0041 32 CONTINUE
0042 KI=KI+1
0043 31 CONTINUE
0044 DO 20 J=2,M
0045 20 PRINT 30 ,(U(I,J),I=2,N)
0046 DO 21 J=2,M
0047 21 PRINT 30 ,(V(I,J),I=2,N)
0048 DO 25 J=2,M
0049 25 PRINT 30 ,(A(I,J),I=2,N)
0050 DO 26 J=2,M
0051 26 PRINT 30 ,(B(I,J),I=2,N)
0052 DO 27 J=2,M
0053 27 PRINT 30 ,(FF(I,J),I=2,N)
0054 DO 28 J=2,M
0055 28 PRINT 30 ,(EB(I,J),I=2,N)
0056 DO 33 J=2,M
0057 33 PRINT 30 ,(FF(I,J),I=2,N)
0058 DO 34 J=2,M
0059 34 PRINT 30 ,(FB(I,J),I=2,N)
0060 30 FORMAT('0',5X,10(F11.4))
0061 6 CALL AVERC
0062 CALL LCNGI
0063 DO 3 I=2,N
0064 DO 3 J=2,M
0065 C(I,J,1)=C(I,J,2)
0066 3 CONTINUE
0067 T=TT+TT
0068 NAA=NAA+1
0069 CALL AVENG
0070 CALL VERTI
0071 DO 4 I=2,N
0072 DO 4 J=2,M
0073 C(I,J,1)=C(I,J,2)
0074 4 CONTINUE
0075 T=TTT
0076 NAB=NAA+1
0077 IF((9.2-UNIFCR).GE.0.010) GO TO 6
0078 STOP
0079 END

```

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130 SUBROUTINE LONGI
131 CCC GAUSS ELIMINATION...LONGITUDINAL DIRECTION
132 DIMENSION BB(40),AA(40),CC(40), D(40),V(40),S(40)
133 COMMON C(40,20),A(40,20),B(40,20),EF(40,20),FF(40,20),EB(40,20)
134 I=FB(40,20),M=N
135 COMMON KA
136 COMMON XXX,YYY,XX,YY ,T
137 COMMON NA,NB
138 COMMON UNIFORM
139 DO 1 J=2,M
140 DO 2 I=2,N
141 AA(I)=EB(I,J)+A(I,J)
142 BB(I)=1.0+EF(I,J)+EB(I,J)
143 CC(I)=EF(I,J)-A(I,J)
144 C(I,J-1)=C(I,J-1)
145 C(I,M-1)=C(I,M-1)
146 C(I,J-1)=C(I,J-1)
147 C(N+1,J-1)=C(N+1,J-1)
148 D(I)=FB(I,J)-B(I,J)+C(I,J-1)-(FB(I,J)+FF(I,J)-1)*C(I,J-1)+(FF
149 I(I,J)-B(I,J))*C(I,J-1)
150 2 CONTINUE
151 AA(N)=EF(N,J)+EB(N,J)
152 CC(2)=EF(2,J)+EB(2,J)
153 V(2)=D(2)
154 S(2)=0(2)
155 DO 3 J=3,M
156 V(J)=D(J)-((AA(J)+CC(J-1))/W(J-1))
157 S(J)=D(J)-((AA(J)+S(J-1))/W(J-1))
158 3 CONTINUE
159 C(I,N-2)=S(N)/W(N)
160 NN=N-1
161 DO 4 I=1,NN
162 C(N-I,J-2)=(S(N-I)+CC(N-I)*C(N-I+1,J-2))/W(N-I)
163 4 CONTINUE
164 1 CONTINUE
165 RETURN
166 END

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164 SUBROUTINE VERTI
165 CCC GAUSS ELIMINATION...VERTICAL DIRECTION
166 DIMENSION BB(40),AA(40),CC(40), D(40),V(40),S(40)
167 COMMON C(40,20),A(40,20),B(40,20),EF(40,20),FF(40,20),EB(40,20)
168 I=FE(40,20),M=N
169 COMMON KA
170 COMMON XXX,YYY,XX,YY ,T
171 COMMON NA,NB
172 COMMON UNIFORM
173 DO 1 J=2,M
174 DO 2 J=2,M
175 AA(J)=FB(I,J)+B(I,J)
176 BB(J)=1.0+FF(I,J)+FB(I,J)
177 CC(J)=FF(I,J)-B(I,J)
178 C(I,J-1)=C(I,J-1)
179 C(N+1,J-1)=C(N+1,J-1)
180 C(I,1)=C(I,1)
181 C(I,M-1)=C(I,M-1)
182 D(J)=EB(I,J)-A(I,J)+C(I-1,J-1)-(EB(I,J)+EF(I,J)-1)*C(I,J-1)+(EF
183 I(I,J)-A(I,J))*C(I-1,J-1)
184 2 CONTINUE
185 AA(M)=FF(I,M)+FB(I,M)
186 CC(2)=FF(I,2)+FB(I,2)
187 V(2)=D(2)
188 S(2)=0(2)
189 DO 3 J=3,M
190 V(J)=D(J)-((AA(J)+CC(J-1))/W(J-1))
191 S(J)=D(J)-((AA(J)+S(J-1))/W(J-1))
192 3 CONTINUE
193 C(I,M-2)=S(M)/W(M)
194 MM=M-1
195 DO 4 J=1,MM
196 C(I,M-J,2)=(S(M-J)+CC(M-J)*C(I,M-J+1,2))/W(M-J)
197 4 CONTINUE
198 1 CONTINUE
199 RETURN
200 END

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- 1945 Born in Saharanpur
- 1963 Received the degree of Bachelor of Science (Hons) in Chemistry from University of Karachi, Pakistan.
- 1964 Received the degree of Master of Science in Chemistry from University of Karachi, Pakistan.
- 1964-67 Chemist with Dawood Chemical Industries (Hydrogen Peroxide Plant), Karachi, Pakistan.
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- 1972 Received the degree of Master of Applied Science in Chemical Engineering from the University of Windsor, Windsor, Ontario, Canada.
- 1976-77 Sessional Instructor with the Department of Chemical Engineering, University of Windsor, Windsor, Ontario, Canada.
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