A 2-D STUDY OF DISPERSION OF POLLUTANTS THROUGH POROUS MEDIA

THESIS

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By

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CANDIDATE'S DECLARATION

I hereby certify that the work which is being presented in the thesis entitled ''A 2-D Study of Dispersion of Pollutants Through Porous Media'' in fulfilment of the requirement for award of the Degree of Doctor of Philosophy, submitted in the Department of Civil Engineering of the University is an authentic record of my own work carried out during a period from August 1977 to August 1982 under the supervision of Prof. R.P. Mathur and Prof. P.K.Pande.

The matter embodied in this thesis has not been submitted by me for the award of any other degree.

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This is to certify that the above statement made by the candidate is correct to the best of my knowledge.

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SYNOPSIS

A 2-D study of dispersion of pollutants through porous media.

The ever increasing magnitude of deliberate or inadvertent subsurface discharge of wastes poses a threat to the quality of ground waters, which often constitute important resources of fresh water supplies. Considerable research has been done on the dispersion of pollutants through porous media. Yet a satisfactory method for the prediction of dispersion of pollutants, underground, is still elusive. Hence there is a good need for extensive laboratory and field studies, as well as development of theoretical models.

In this study, the two dimensional dispersion of pollutants through a uniform flow field in a homogeneous, isotropic, porous medium has been taken up. The pollutants for this study have been Sodium chloride, often considered to be an ideal tracer for such studies, and a pure bacterial culture, Echerichia coli Var. I, which is a popular indicator of sewage pollution. The organisms have an inherent decay and are also absorbed on the soil matrix.

The experimental facility comprised of a 77.5 cm long, 80 cm high, and 5 cm wide perspex box with suitable inlet and outlets and a supporting structure. The box was filled with sand (d_{50} = 0.055 cm, U_c = 1.3) to a porosity of 0.46. Horizontal uniform seepages were maintained within a Reynold

number range of 0.6 to 2.0, for different runs. Pollutants were injected at constant rates, with step function inputs, at a point, into the model, and the concentrations were monitored with time, from samplings at selected tapping points. The concentrations of Sodium chloride were measured on a conductivity meter, while E.coli concentrations were estimated by the standard M.F. technique. Steady state concentrations and break through curves (concentration vs. time) were obtained at selected tapping points.

The available analytical solutions for 2-D dispersion have been used for evaluation of apparent dispersivities for the two pollutants, studied. Theoretical break through curves have been computed with the evaluated dispersivities.

Numerical solutions have been obtained by a fortran algorithm, developed with the adoption of ADIP (alternating direction implicit procedure), which ensured good convergence. Solutions have also been worked out from discretized pulse technique.

The experimental, analytical and numerical solutions for the two dimensional dispersion of the pollutants have been compared, for the selected parameters of this study.

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CONTENTS

NOTATION*

Symbol	Meaning	Dimensions
B	Function defined by eqn. 3.5	L
$B_{i,j}$	Concentration at a nodal point (i,j) at the previous time level of a time step in a finite difference grid	-
C	Concentration of the pollutant,mass/mass in case of chemical and number/volume in the case of bacteria	- (L^{-3})
C_o	Initial concentration	-
$C_{i,j}$	Concentration at a nodal point (i,j) at the new time level of a time step, in a finite difference grid	-
D_x, D_y, D_z:	Dispersion coefficients in the x,y,z directions respectively	L^2T^{-1}
D'_x, D'_y, D'_z:	D_x/R_d, D_y/R_d, D_z/R_d respectively	L^2T^{-1}
d_{50}	The particle size of the porous medium for which 50% of the particles, by weight, are finer	L
$E_{i,j}$	Concentration at a nodal point (i,j) during the middle of a time step in a finite difference grid	-
F	Function defined by eqn. 4.3	
K	Darcy's coefficient of permeability	LT^{-1}
m	Mass of pollutant injected per unit length in Z-direction	ML^{-1}

*Not applicable for Chapter 2.

Symbol	Meaning	Dimensions
M	Equivalent mass of injection, in a pulse of discretization, per unit length in z-direction	ML^{-1}
n	Porosity of the porous medium	-
P	Coefficient in eqn. 3.20 as defined there under	-
Q	Coefficient in eqn. 3.20 as defined there under	-
	Also the rate of flow through the experimental model.	L^3T^{-1}
	(The context is clear enough to preclude confusion)	
q	Volumetric rate of injection of the pollutant	L^3T^{-1}
q'	Volumetric rate of injection of the pollutant per unit length in Z-direction	L^2T^{-1}
R	Coefficient in eqn. 3.20 as defined thereunder	-
R_d	Retardation factor ($\geq$ 1) which slows down the travel of pollutant due to adsorption	-
r	Function defined by eqn. 3.8	
S	Coefficient in eqn. 3.20 as defined there under	-
T	Coefficient in eqn. 3.20 as defined there under	-
t	Time	T
U	Pore velocity of the fluid (= Gross velocity/porosity) in the x-direction	LT^{-1}

Symbol	Meaning	Dimensions
U'	U/R_d	LT^{-1}
U_1	Function defined by eqn. 3.7	-
V	Coefficient in eqn. 3.21 as defined there under	-
W	Coefficient in eqn. 3.21 as defined there under	-
x, y, z	Cartesian coordinates	L
α_x, α_y	Dispersivities of the porous medium in the x and y directions respectively	L
γ	Function defined by eqn. 3.6	-
ρ	Density of the fluid	ML^{-3}
No. in superscript	Number in the list of references	-

Abbreviations

ADIP	Alternating Direction Implicit Procedure
IBT	Inverse Break Through
TDMA	Tri Diagonal Matrix Algorithm

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CHAPTER I

INTRODUCTION

CONTENTS

1.1 GENERAL

Ground water resources are facing ever increasing threats of qualitative deterioration, due to deliberate or inadvertent sub-surface disposal and dispersion of pollutants. The potential of soil matrix as an absorber of natural and man-made pollutants, and also, the role of soil in the recycling of materials in the ecosystem are quite alluring to the environmentalist. Hence, there is a need to exploit subsurface waste disposal potential, without causing undue deterioration of ground water quality, at the places of it's withdrawl. This objective necessitates the knowledge of various transformations, occurring in a polluted soil system. For successful engineering applications, such a knowledge should include the laws governing (i) the dynamics of the movement of pollutants (ii) the retention of pollutants in the soil matrix by clogging, adsorption and microsedimentation and (iii) the physical, chemical, biological and biochemical interactions of the pollutants and the soil components.

1.2 PROBLEMS OF DISPERSION

The need for understanding the dispersion phenomena arises from the following human activities.

(i) Liquid wastes are injected into the subsoil either for their disposal or for ground water recharge.

(ii) Partially treated sewage is used for irrigation, causing leaching of pollutants into the soil.

(iii) Pesticides and fertilizers are applied on agricultural lands. These substances are likely to enter into the soil system.

(iv) Garbage dumps, waste water ponds and polluted rivers contribute pollutants to the soil.

Under the present activities, the ground water quality should be controlled at the points of withdrawl. In addition, modeling the salt water intrusion into coastal aquifers, oil mining by displacement with brines, and using porous media reactors in industries and water treatment plants, also necessitate the understanding of dispersion phenomena within porous media.

The multiplicity of relevent parameters with complex and often non-linear functional relationships, render the solution, of practical field problems of subsurface pollutant dispersion, very difficult. The option left to the engineer is to split up a complex problem into simpler hypothetical components, each amenable to a theoretical solution or an empirical laboratory study. These solutions of the component problems may, suitably, be superposed to obtain a solution, of tolerable inaccuracy, for the original problem. Some compromise with the degree of accuracy is inevitable.

1.2.1 Movement of Pollutants

The movement of a pollutant in an aquifer is the result of (i) advective dispersion, in which the seepage fluid is the vehicle for the pollutant and (ii) molecular diffusion, wherein the pollutant gets scattered along the concentration gradient due to molecular motions. For general field problems the magnitudes of molecular diffusions are negligible in contrast to advective dispersion.

1.2.2 Classification of Pollutants

In dispersion phenomena, the pollutants are classified as 'non-conservative pollutants' and 'conservative pollutants'. The former are subjected to phenomena like clogging, adsorption, microsedimentation and inherent decay while a conservative pollutant undergoes none of the above.

1.3 EARLIER WORKS

Considerable work has been reported in the field of dispersion of substances in flow through porous media. The basic approaches have been

(i) theoretical work, mostly based on heat transfer analogy or statistical methods

(ii) numerical modeling for the solution of the mass balance partial differential equation and

(iii) simulation study on either laboratory experimental set up or in the field itself.

1.3.1 The available theoretical solutions are extremely limited in scope, because of the numerous assumptions involved, which are difficult to obtain in any real problem. For instance the available analytical solution to predict dispersion pattern, requires homogeneous, isotropic and inert porous media of infinite areal extent with saturated, unidirectional steady seepage and an instantaneous mass injection of pollutant or a steady and continuous injection after a sudden start, known as step function input.

1.3.2 With the advent of numerical techniques on fast computers, some of the implied limitations of the analytical methods can, now, be circumvented. The numerical technique has, essentially, the partial differential equation, governing the pollutant mass balance, as the starting point. Finite difference and finite element methods, with the appropriate initial and boundary conditions, are being improved, availing digital computer services. Yet, the numerical techniques have their own limitations, like 'numerical dispersion', 'numerical overshoot' and problems of stability and convergence. A workable numerical procedure of the desired degree of accuracy, has to be developed for each individual case and the technique has to be proved by comparing it with analytical or experimental values.

1.3.3 A large part of the simulation study on the laboratory models has been, hitherto, confined to the dispersion of conservative pollutants, mostly Sodium chloride, because of it's advantages as a 'tracer' in pollution study. Reports on investigations with bacterial pollutants are scanty and are also inconsistent in their findings.

In view of the above limitations in the different approaches, a need for further investigations in this area is still very large.

1.4 PRESENT STUDY

For the present study, a 2-D solution domain has been chosen, due to it's relevence in many field problems, where confined aquifers are often encountered. Extension of 2-D solutions to 3-D cases is possible, where necessary. A pulse technique, based on the time discretization of the pollutant input, has been explored, using the analytical solution for instantaneous mass injection of pollutant at a point. Further, the numerical method by the Alternating Direction Implicit Procedure is modified to suit concentration predictions at exactly down stream points in the aquifer. A model, for the concentration decay on the cessation of the pollutant inputs, during a steady state pollution, has also been presented. This concentration decay, termed as Inverse Break Through (IBT), needs to be predicted, to assess the recovery of an aquifer from inadvertent subsurface spillages of a pollutant, or the recovery after the termination of pollutant inputs, during a steady state pollution of the aquifer.

Sodium chloride has been employed as a conservative pollutant in this study because of the ease of monitoring, it's concentration and it's noninterference with the density or viscosity of water to significant levels, if it's concentration is kept down below 0.1 percent by weight. As a non-conservative pollutant *Escherichia coli*, Var. I (*E. coli*) has been chosen for the following reasons

(i) *E. coli* is an important indicator organism for detecting or assessing the magnitude of sewage pollution of a water body.

(ii) In a sense, *E. coli* is superior to Sodium chloride as a tracer in dispersion studies, because the range of allowable concentrations in experimental study is much larger. The membrane filter technique (MF), adopted in this work permits the measurements of concentrations as low as one cell per 100 ml, while there is no upper limit for the allowable concentration, due to the small difference in specific gravities of water and *E. coli*. This property ensures negligible change in the density of the carrier fluid, even at concentrations as high as millions of cells per ml.

In the field of study of dispersion of pollutants through porous media, the full coverage of the extensive multiplicity of relevent parameters is, well neigh, impossible in any single work of this nature, due to the common constraints. Despite this, it is hoped that this work could be a significant contribution, in adding to the limited techniques, at the disposal of the environmentalist, involved in the assessment of subsurface pollutant dispersion phenomena.

CHAPTER II

LITERATURE REVIEW

CONTENTS

2.1 GENERAL

Literature, on dispersion of pollutants through porous media, is abundant and, is from a wide range of sources, because of it's importance in several fields of activities. In the absence of true solutions to the real problems in dispersion, numerous approximations, suited to individual engineering applications, are being attempted. The basic techniques for modeling the dispersion phenomena may be classified as:

(i) Statistical
(ii) Analytical and
(iii) Numerical.

A proposed model is validated by experimental or field observations or some times with data generated by the stochastic disturbance of computed analytical values. An exhaustive coverage of the literature on dispersion is not attempted here because of the magnitude of available information. Instead, the review is confined, in general to the more recent and important works, as well as those of direct relevence to these studies.

2.2 STATISTICAL MODELS

One of the earliest statistical models for hydrodynamic dispersion is that of Scheidegger[68] (1954), in which the dispersion coefficient has been correlated to velocity, while molecular diffusion has been ignored.

De Josselin de Jong[18] (1958), established, with a statistical approach, that longitudinal dispersion was more than transverse dispersion. He derived that

$$C = \frac{\frac{C_o U}{\theta}}{4\pi \; t(D_L D_T)^{1/2}} \; \exp \left\{ - \frac{1}{4t} \left[\frac{(x - vt)^2}{D_L} + \frac{y^2}{D_T} \right] \right\} \qquad \ldots (2.1)$$

where,

C = Concentration at (x,y)

C_o = Concentration of instantaneous point injection

U = Volume of point injection

θ = Porosity

D_L, D_T = Longitudinal and lateral dispersion coefficients

t = Time

Saffman[67] (1959), presented a model similar to de Jong's, but including molecular diffusion.

Todorovic[79] (1975) gave a stochastic model to describe longitudinal dispersion of a set of tagged particles, released continuously in uniform flow through a homogeneous non-adsorbent porous medium. The model provided a unified treatment of both Lagrangian and Eulerian descriptions of dispersion.

Franklin Schwartz[21] (1977) has stated that the dispersivity of a heterogeneous medium can be estimated by using stochastic analysis, based on the statistical analysis of the mode of porous medium aggregation and the conductivity contrasts within the medium.

Lynn Gelhar et al.[50] (1979) analysed longitudinal dispersion in a stratified aquifer, by treating the variability of conductivity and concentration as a homogeneous stochastic process.

Leslie Smith[48] (1980) presented a stochastic analysis of macroscopic dispersion.

The statistical models, mentioned above, have been reasonably validated by experimental results, thereby establishing statistical analysis, as a useful tool in promoting the knowledge of dispersion phenomena.

2.3 ANALYTICAL MODELING

The analytical equations, predicting the dispersion of pollutants are mathematical solutions of the mass balance partial differential equation, known as the convective dispersive equation. For nonlinear adsorption or decay of the pollutant and for complicated initial and boundary conditions, the analytical solutions, if any, are based on some simplifying assumptions and approximations. At times, they are to be supplemented by numerical integrations, when closed form solutions are not possible.

Ogata[61] (1958) and Bear[35,36] (1961) solved the convective dispersion equation analytically. Ogata and Banks[62] (1961) gave the solution to one dimensional convective dispersive equation for a step function input of tracer. The solution is given by

$$\frac{C}{C_o} = \frac{1}{2}\left[\operatorname{erfc}\frac{(x-Ut)}{2\sqrt{Dt}} + \exp\left(\frac{Ux}{D}\right)\operatorname{erfc}\frac{(x+Ut)}{2\sqrt{Dt}}\right] \quad \ldots (2.2)$$

where,

C_o = Concentration of tracer at input

C = Concentration at distance x from input

t = Time after step function input

D = Dispersion coefficient

U = Pore Velocity

Harleman and Rumer[30,31] (1962, 1963) and Bachmat and Bear[7] (1964) derived the convective dispersive equation and showed that the dispersion coefficient at a point was related to the spatial variation of velocity and tracer concentration in a small volume, about that point, and the dispersion coefficient could vary in any direction with the velocity, to a power different from one. Bachmat and Bear[7] assumed a linear relationship between the velocity and dispersion coefficient in a general tensorial form, and derived the conservation equation of a substance as,

$$\frac{\partial C}{\partial t} + q\frac{\partial C}{\partial S} = (D_1 + D_m)\frac{\partial^2 C}{\partial S^2} + (D_2 + D_m)\frac{\partial^2 C}{\partial n^2}$$

$$+ \frac{D_m}{\Delta n} \cdot \frac{\partial C}{\partial S} \cdot \frac{\partial}{\partial S}(\Delta n)$$

$$+ \frac{D_m}{\Delta S} \cdot \frac{\partial C}{\partial n} \cdot \frac{\partial}{\partial n}(\Delta S) + s \qquad \ldots (2.3)$$

where,

C = Concentration of substance

q = Seepage velocity

D_1, D_2 = Longitudinal and lateral dispersion coefficients equal to $\alpha_1 q$ and $\alpha_2 q$ respectively.

α_1, α_2 = Intrinsic dispersivity coefficients

D_m = Molecular diffusion coefficient

s = Rate of gain of substance due to leaching or chemical reaction

t = Time

S, m = Coordinates along and perpendicular to streamlines respectively.

Hoopes and Harleman[40] (1967) modified eqn. 2.3, in terms of velocity potential ϕ and stream function ψ and for laminar flow, as

$$\frac{\partial C}{\partial t} + q^2\frac{\partial C}{\partial \phi} = q^2\frac{\partial}{\partial \phi}\left[(D_1 + D_m)\frac{\partial C}{\partial \phi}\right] + q^2\frac{\partial}{\partial \psi}\left[(D_2 + D_m)\frac{\partial C}{\partial \psi}\right] + s \qquad \ldots (2.4)$$

Using this equation they dealt with the problem of predicting the spatial and temporal distribution of a dissolved conservative substance, injected into steady flow between two wells, one of which recharged the dissolved substance into an infinite, horizontal, confined aquifer, while the other well pumped fresh water and the substance out of the aquifer. Approximate solutions were given and were verified by experimental results. They found that dispersion and diffusion were significant for the concentrations along the streamlines, while the convection of the pumping well dominated the local concentration distribution. Lateral dispersion was found to retard the break through at any point. Molecular diffusion was found to have negligible influence.

Shamir and Harleman[70] (1967) developed analytical solutions for layered porous media for axial dispersion and also for two dimensional dispersion with seepages parallel and perpendicular to the strata. Their solutions were verified experimentally. Wen-Hsiung Li and R.P. Canale[83] (1967) gave simple approximate equations of solute dispersion, for seepages with gentle convergence or divergence of streamlines, and verified those equations, numerically John Bruch Jr[41] (1970) conducted a series of experiments on a two dimensional laboratory model and verified analytical and numerical solutions. For the dispersive equation

$$\frac{\partial C_s}{\partial t} + v_s \frac{\partial C_s}{\partial y} = D_{11} \frac{\partial^2 C_s}{\partial x^2} + D_{22} \frac{\partial^2 C_s}{\partial y^2} \qquad \ldots (2.5)$$

with velocity v_s in the y direction. He assumed

$$\frac{D_{22}}{v} = 1.8\ R^{1.205} \quad \text{and} \quad \frac{D_{11}}{v} = 0.11\ R^{0.7}$$

where $R = v_s d_{50}/v$ and v = kinematic viscosity.

Eldor and Dagan[56] (1972) predicted, using an approximate analytical method, the two dimensional dispersion of a non-conservative pollutant and verified the solution with experimental and numerical values.

Bruce Hunt[13] (1973) obtained a solution for the steady state dispersion of a radioactive substance from a pit in uniform seepage. For a source of linear size 2B, he has shown that

$$C_{xy} = \frac{1}{2} e^{-\left(\frac{\lambda\sigma}{U_o}\right)x} \left[\mathrm{erf}\left(\frac{B-y}{2\sqrt{x}} \sqrt{\frac{U_o}{\sigma D_{yy}}}\right) + \mathrm{erf}\left(\frac{B+y}{2\sqrt{x}} \sqrt{\frac{U_o}{\sigma D_{yy}}}\right)\right] \qquad \dots (2.6)$$

where,

U_o = Gross seepage velocity

σ = Porosity

λ = decay factor (linear)

The maximum concentration occurs when $y = 0$ at any x and is given by

$$C_{x,o} = e^{-\left(\frac{\lambda\sigma}{U_o}\right)x}\ \mathrm{erf}\left[\frac{B}{2\sqrt{x}} \sqrt{\frac{U_o}{\sigma D_{yy}}}\right] \qquad \dots (2.6A)$$

Eqn.2.6A shows that longitudinal dispersion coefficient has insignificant influence on the steady state concentrations. Wolanski[20] (1973) generalized the two dimensional case of Bruce Hunt[13] to three dimensions and concluded that dispersion in a three dimensional case was drastically larger. Bruce Hunt[14] (1973) gave a general expression for the hydrodynamic dispersion tensor in a homogeneous, isotropic porous medium, assuming that the principal directions of the dispersion tensor are tangential and normal to the flow stream lines. He gave

$$D_{ij}(x) = D^2 \delta_{ij} + (D^1 - D^2) \frac{u_i u_j}{V^2} \qquad \ldots (2.7)$$

Dimensionless dispersion tensor

$$D^*_{ij} = \left(\frac{C_2 d}{L}\right)\left(\frac{V_o d}{D_d}\right)^{n_2 - 1} \left(\frac{V}{V_o}\right)^{n_2} \delta_{ij}$$

$$+\left(\frac{C_2 d}{L}\right)\left[\frac{C_1}{C_2}\left(\frac{V_o d}{D_d}\right)^{n_1 - 1} \left(\frac{V}{V_o}\right)^{n_1} - \left(\frac{V_o d}{D_d}\right)^{n_2 - 1} \left(\frac{V}{V_o}\right)^{n_2}\right] \frac{u_i u_j}{V^2} \qquad \ldots (2.8)$$

where,

D_{ij} = hydrodynamic dispersion tensor

n_1, n_2, and C_1, C_2 = experimental constants

D_d = Coefficient of molecular diffusivity

L = characteristic length

V = seepage vel. magnitude of fluid mixture

V_o = characteristic seepage velocity

δ_{ij} = kronecker delta

Vd/D_d = Peclet No.

This model (eqn. 2.8) is particularly useful for numerical solution of field problems from experimental piezometric data.

Marino[51,52] (1974) derived an analytical expression for axial dispersion with time dependent input concentration = $C_o(1 - e^{-\gamma t})$ and obtained the following equation

$$C_{x,t} = \frac{C_o}{2} \left\{ \text{erfc}\left(\frac{x-Ut}{2\sqrt{Dt}}\right) + \exp\frac{Ux}{D}\,\text{erfc}\left(\frac{x+Ut}{2\sqrt{Dt}}\right) - \exp(-\gamma t)\left[\exp\frac{x(U-\phi)}{2D}\,\text{erfc}\left(\frac{x-\phi t}{2\sqrt{Dt}}\right) + \exp\left(\frac{x(U+\phi)}{2D}\right)\text{erfc}\left(\frac{x+\phi t}{2\sqrt{Dt}}\right)\right]\right\} \quad \ldots (2.9)$$

in which

$\phi = (U^2 - 4D\gamma)^{1/2}$

U = pore velocity

D = dispersion coefficient

γ = decay factor.

Marino[58] (1974) derived an analytical solution, incorporating linear adsorption also, in extension of the above model.

Gupta and Greencorn[27] (1974) evaluated from experimental studies, the dispersion and nonlinear adsorption parameters for sand and clay mixtures in axial flows. Lindstorm[49] (1976) presented a mathematical model for the pulsed dispersion of tracer chemical concentration in a saturated sorbing porous medium with axial dispersion. Selim and Mansell[69] (1976) gave mathematical solutions for the differential equation governing the reactive solute transport in a finite soil column, for pulse and continuous inputs.

Thomas Blake and Garg[78] (1976) presented a species transport equation for porous media flow, based on the space averaging formulation. Hung Tao Shen[33] (1976) gave generalized analytical solutions for transient multidimensional dispersion of nonconservative substances in steady uniform seepage, with a plane boundary source, oriented normal to the flow, considering time dependent concentration, radioactive decay and linear adsorption. He modeled the convective dispersive equation as follows:

$$\frac{\partial}{\partial t}\left(C + \frac{1-n}{n} S\right) - \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j} - U_i C\right) + \lambda\left(C + \frac{1-n}{n} S\right) = 0 \qquad \ldots (2.10)$$

$i,j = 1,2,3 \ldots\ldots$

where

$S = KC$ = concentration of solute on solid phase

K = a constant

D_{ij} = the hydrodynamic dispersion coefficient tensor

λ = decay factor

n = porosity

C = Concentration of dispersing substance

U_i = seepage velocity in direction i.

His solutions are valid for convective dispersion in semi-infinite, homogeneous, isotropic, saturated porous medium. The solutions involve integrands, that need to be evaluated by a suitable numerical technique on a digital computer. Hence Michael Collins^{57} (1976) has commented that Shen's^{33} solutions are not closed form solutions in the real sense, and suggested an approximation method for evaluating the integrands in Shen's solutions, without resorting to numerical method. Collins^{57} method, though elegant, lacks in simplicity. Elprince and Day^{19} (1977) introduced an adjustable parameter, 'the effective solution volume' into the transport equation, to account for the negative adsorption of anions and also the stagnant volumes of soil solution, as follows:

$$\frac{C}{C_o} = \frac{1}{2} \left[\operatorname{erfc} \left(\frac{1 - P}{\sqrt{4DP/VL}} \right) + e^{VL/D} \operatorname{erfc} \left(\frac{1 + P}{\sqrt{4DP/VL}} \right) \right] \quad \ldots (2.11)$$

where,

V = pore velocity

L = Distance

P = No. of pore volumes

D = Dispersion coefficient.

Consequent to the introduction of the additional parameter, they found better correlation between predictions and observations of break throughs.

Wilson Miller[85] (1978) presented exact and approximate solutions (Vide Sec. 3.2) for a two dimensional dispersion plume in contaminated ground water in a uniform flow field. A graphical procedure, designed to ease visualization and evaluation of the contamination was described. The procedure was tested successfully, in a case of hexavalent chromium contamination of Long Island, New York.

Bruce Hunt[12] (1978), based on heat transfer analogies, listed out the solutions for instantaneous, continuous and steady state point sources of pollution in a uniform seepage field. For a continuous point source in a two-dimensional field

$$C_{x,y,t} = \frac{M_2 \exp\left(\frac{xV}{2D_{xx}}\right)}{4\pi\sigma \sqrt{D_{xx} \, D_{yy}}} \, W\left(\frac{R^2}{4D_{xx}t}, \frac{VR}{2D_{xx}}\right) \qquad \ldots (2.12)$$

where

$$M_2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} C_i(x,y,o) \, \sigma \, dx.dy \qquad \ldots (2.12A)$$

$$R = \left(x^2 + y^2 \frac{D_{xx}}{D_{yy}}\right)^{1/2}$$

where,

M_2 = Rate of pollutant mass input

σ = porosity

V = pore velocity

t = time

D_{xx} and D_{yy} = Dispersion coefficients

W(u,b) is known as leaky aquifer function. For convergence with larger values of arguments, as is often the case in dispersion studies, Bruce Hunt gave the following approximation

$$W(u,b) \simeq \sqrt{\pi/2b}\ \exp(-b)\ \{\ \mathrm{erfc}\ (a) + \sqrt{\frac{2}{\pi b}}\ a^2 \exp(-a^2) + \frac{1}{b}\Big[\ \frac{a \exp(-a^2)}{\sqrt{\pi}}\ (a^4 - \frac{3a^2}{2} - \frac{1}{4}) - \frac{1}{8}\ \mathrm{erfc}(a)\Big] + o(\frac{1}{b^{3/2}})\ \} \qquad \ldots (2.13)$$

where,

$$a = (\ \frac{2u}{b} - 1)\sqrt{\frac{b}{2}} \quad \text{for } b \gg 1$$

Bruce Hunt[12] (1978) has given analytical solutions, also for instantaneous point sources of pollution in one dimensional and two dimensional dispersion, as well as for a continuous point source pollution in one dimension, which is the same as Ogata's solution[61]. From these solutions he established the criteria for (i) the time required for the steady state to be attained (ii) the effect of a finite depth of aquifer as against the infinite depth, implied in the analytical solution (iii) the maximum concentration at any place for a given time or for any time at a give point, and (iv) the inaccuracy expected by treating a real finite size source as a hypothetical point source, given by

$$\frac{L^2}{t}\ (\ \frac{1}{D_{xx}} + \frac{1}{D_{yy}}\ ) \leqslant 0.48\ N \qquad \ldots (2.14)$$

where

N = percentage error

L = linear size of source

t = time

Phillips and Gelhar[43] (1978) gave an analytical-cum-numerical model for the convective transport to a deep pumping well, overlain by a zone of contaminated water. This model was demonstrated for three water supply wells on Long Island, New York. The model can also be applied to predict the decontamination curve, that would occur, after the pollutant source is eliminated. They found that local convection produced by the pumping well was more important than dispersive mixing. This finding is in conformity with the observation of Hoopes and Harleman[32].

Peatzold and Scott[65] (1978) discussed a method of finding the apparent dispersive coefficient of solutes in unsaturated soils, considering both the sorption and decay of the solute.

Gunter Hibsch and Andrzej Kreft[25] (1979), Basak and Murty[8] (1979) and Gupta, Batta and Pandey[26] (1980) suggested methods for the determination of aquifer transport parameters from observed transient concentrations of the solute in one and two dimensional dispersions.

Al-Niami and Rushton[2] (1979) gave analytical solutions for stratified porous media with seepages parallel or perpendicular to the stratification. They compared the solutions with the numerical schemes of Al Niami[1] (1977). Tang and Babu[76] (1979) derived an analytical solution for describing the convective-dispersion transport of a contaminant from an injection well, considering the velocity dependent dispersion coefficient, and the solution was compared with a numerical scheme.

Jean-Pierre Sauty[38] (1980) unified different solutions of one-dimensional, two-dimensional and radial dispersions, by transposing the solutions into dimensionless variables of concentration, time and Peclet no. A series of dimensionless curves was developed, enabling the direct determination of dispersivity and kinematic porosity from tracer test results.

Joe Nathan Lucas[39] (1980) gave a physical model of the transport of a radioactive salt through a semi-infinite column of porous medium. Shu Yuan Chu[72] (1980) derived a macroscopic solute transport equation for a homogeneous, saturated, porous medium. Budhisagar[15] (1982) gave approximate solutions to three-dimensional convection dispersion equation, under different boundary conditions in steady and unsaturated uniform seepage, with the pollutant source assumed to be an arbitrary function of time, and of a finite size in space. These approximate solutions have simplicity at the expense of accuracy and hence are useful for preliminary analyses of ground water pollution problems.

Anand Prakash[4] (1982) gave analytical models to simulate ground water contamination due to point, line, plane or parallele piped sources in confined or unconfined aquifers. For example for a vertical line source from $Z = Z_1$ to, $Z = Z_2$ at $x = 0$ and $y = y_o$ (origin)

$$C_{x,y,z} = \frac{C_o Q_o}{4U\,(Z_2 - Z_1)\sqrt{\pi x D_y^*}} \exp\left[\frac{-(y-y_o)^2}{\sqrt{4D_y^* x}} - \lambda^* x\right]$$

$$\times \left\{ \left[\sum_{m=o}^{\infty} \left[\operatorname{erf} \frac{Z-md-(-1)^m\ Z_1}{\sqrt{4D_z^*\ x}} - \operatorname{erf} \frac{Z-mD-(-1)^m Z_2}{\sqrt{4D_z^*\ x}} \right] \right] \right\} \qquad \ldots (2.15)$$

for parallel non flux boundaries confining the Water table above and below

C_o = concentration of contaminant

Q_o = discharge of contaminant

m = index no. for no. of images

U = seepage velocity in x direction

$D_y^* = D_y/U$; $D_z^* = D_z/U$; $\lambda^* = \frac{\lambda Rd}{U}$

λ = decay factor

R_d = retardation factor

D = aquifer thickness

The series in eqn. 2.15 is convergent m is chosen as per the degree of accuracy required.

Similar models have been given for a point source and a horizontal line source. The models were compared with solutions by the finite element method. These analytical models are expected to require lesser computer time and are also free from the convergence and stability problems, associated with the numerical techniques.

From the foregoing survey of analytical modeling, the limitations of the analytical solutions, particularly of those for nonconservative pollutant and complex initial and boundary conditions, can be generalized as follows:

(i) A homogeneous, isotropic porous medium, or such media in case of stratification, is necessary.

(ii) Non linearities of adsorption and decay can not be incorporated satisfactorily.

(iii) Some solutions will have integrands, that require numerical integration.

(iv) The involved simplifying assumptions are at the expense of accuracy.

(v) Tedious computation is involved.

(vi) Some solutions need supplementation or verification by numerical schemes. As such, the recent advances in analytical approaches have not substantially reduced the need for numerical modeling in dispersion studies.

2.4 NUMERICAL MODELING

The mass balance partial differential equation, of a solute in convective advective dispersion through a porous medium, is amendable to analytical solution only with restricted initial and boundary conditions. Since such restrictions are seldom realized in practice, the mass balance partial differential equation, usually named as the convective dispersive equation, has to be solved, more often, by suitable numerical techniques, the algorithms for which have to be developed for each case and have to be tested by comparison, with either known analytical solutions or experimental results.

Hoopes and Harleman[32] (1965) made extensive laboratory studies on a radial dispersion model and compared their results with numerical solutions. Shamir and Harleman[70] (1967) presented a numerical scheme, general enough to handle any problem of dispersion in a steady flow field, with any initial and boundary conditions.

Wen Hsiung Li[83] (1967) developed a numerical scheme for dispersion in a flow field, with gentle convergence and divergence of streamlines. Gary Guymon[22] (1970) developed a finite element solution of one dimensional diffusion-convection equation.

John Bruch Jr[41] (1970) obtained numerical solutions for two-dimensional dispersion in layered porous media and verified the solutions with experimental results. Guymon, Scott and Herrmann[28] (1970) gave a scheme for the general numerical solution of two-dimensional diffusion equation by the finite element method.

Redell and Sunada[66] (1970) gave numerical solution of dispersion in ground water aquifers, using the method of characteristics, which could reduce numerical dispersion. Gedeon Dagan[23] (1971) gave perturbation solutions for two-dimensional dispersion in non-uniform seepage. Lawson[47] (1971) suggested some improvements in the finite difference solutions of two-dimensional dispersion problems. Eldor and Dagan[56] (1972) compared their numerical solutions for the dispersion of a nonconservative pollutant in two-dimensional dispersion, with approximate analytical solutions.

Tagamets and Sternberg[75] (1974) gave a predictor-corrector finite difference scheme for the one-dimensional convection dispersion equation, subject to a non linear adsorption isotherm. Mou Sheng Wang and Ralph Ta-Shun Cheng[59] (1975) solved the convective dispersion equation numerically using isoparametric quadrilateral finite element method. William Gray and George Pinder[84] (1976) investigated various finite difference and finite element methods, for solving the one-dimensional convective - dispersive equation and found finite element methods to be superior to finite difference methods. Pickens and Lennox[42] (1976) solved the two-dimensional convective dispersive equation by finite element method on a Galerkin technique, using the conventional cartesian coordinate system and a transformed coordinate system, equivalent to the orthogonal curvilinear coordinate system of stream lines and normals to those lines. A sensivity analysis on dispersivity was performed.

Travis Nishi, John Bruch Jr. and Roland Lewis[80] (1976) employed the finite element method using isoparametric elements to solve hydrodynamic dispersion in seepage from a triangular channel, basing on the following mass balance equation

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial C}{\partial y} + D_{yx}\frac{\partial C}{\partial x}\right) \quad \ldots (2.16)$$

in which D_{xx}, D_{yy}, D_{xy} and D_{yx} were derived from Bear's[34] proposition for dispersion coefficients. When their solution was compared with the finite difference solution, they found the latter giving greater spread and movement of the pollutant, possibly due to numerical dispersion. Anand Prakash[3] (1976) used the finite element technique for the convective dispersion of a radioactive tracer through an adsorbing porous medium, in cylindrical polar system of coordinates. He, also, considered radioactive decay. His model was given by,

$$t = \frac{1}{\phi\sqrt{g}} \left[\sqrt{g} \, \frac{\phi}{h_i^2} \left[a_{ll} \, V C_{,i} + \frac{(a_l - a_{ll}) \, v_i v_j}{V h_j^2} \, C_{,j} + D_d T C_{,i} \right] \right]_{,i}$$

$$- \frac{V_i C_{,i}}{h_i^2} - \frac{1 - \phi}{\phi} F_t - \lambda \left(C + \frac{1 - \phi}{\phi} F \right) \qquad \ldots (2.17)$$

Where Alphabetic subscripts denote respective derivatives.

g = determinant of the metric tensor

h_i = scale of coordinate transformation

ϕ = porosity ; C = concentration of tracer

a_l, a_{ll} are longitudinal and lateral dispersivities

$,i$ denotes covariant derivative

V = Absolute velocity

D_d = Coefficient of molecular diffusion

T = tortuosity tensor treated as a scalar for an isotropic medium.

F = mass of tracer adsorbed per unit vol. of solid phase.

λ = radio active decay

v_i, v_j = components of the absolute velocity.

Genuchten and Pinder[53] (1977) simulated the two-dimensional contaminant transport with isoparametric Hermitian finite elements.

Murty and Scott[60] (1977) and Anjad Umari et al.[5] (1979) developed algorithms of the inverse problem, to determine longitudinal and lateral dispersivities, using transient concentration data from a two-dimensional aquifer.

Sheng H. Lin[71] (1977) solved numerically, the nonlinear partial differential equations of dispersion with simultaneous nonlinear adsorption and a time dependent exponential input. Phillips and Gelhar[43] (1978) developed a numerical model for the convective transport to a deep pumping well, overlain by a zone of contaminated water.

Benjamin Ross and Charles Koplik[9] (1979) solved the solute transport equation numerically, by approximating the water flow field by a network of stream tubes and using a Green's function solution within each stream tube. This method permitted greater computational efficiency and easier representation of small discontinuities. Guvanesan and Raymond Volker[82] (1981) gave a numerical scheme in finite element method, giving the nodes of the mesh, new positions in successive time intervals, which provided to allow for the moving water table. Pandey, Singh and Sinha[64] (1982) solved the one-dimensional convective-dispersive equation with nonlinear adsorption by an extrapolated Crank-Nicholson finite difference scheme.

The numerical models, listed above, have established the versatality of the numerical techniques in solving dispersion problems. The finite element method seems to yield better simulation, compared to the finite difference schemes. In spite of the advances made in numerical modeling the problems of convergenee, stability, numerical overshoot and numerical dispersion as well as the requirements of large computer times, are still a menace in the solution of practical problems of dispersion.

2.5 BACTERIAL DISPERSION

Studies on the dispersion of bacterial pollutants are extremely scanty and inconsistent. The earliest reports[10,16,44,73] on travel of bacteria through soils were essentially qualitative and with highly inconsistant observed distances and rates of travel. Task Group Report[77] (1957) stated that bacterial pollution travelled farthest in the direction of groundwater flow. Mathur, Chandra and Bhardwaj[54] (1968) found on a two-dimensional model, that, pollution travelled vertically downwards with no lateral dispersion, till intercepted by ground water table, where after the travel was vertical as well as horizontal. Mathur and Grewal[55] (1972) reported that bacteria showed a tendency of lateral dispersion after the bacterial break through.

Krone et al.[46] (1958) reported a logarithmic decrease in concentration of bacteria, with a sharp drop in concentration just below the input surface of the sand column of their study. Grewal[24] (1973), based on his studies of axial dispersion of E. coli has given the following conclusions.

(i) The breakthrough for bacteria is similar to that of a chemical tracer.

(ii) An organic mat formation, close to the place of pollutant input, results in a steep drop in concentration, and further downstream, Ogata's[61] analytical solution of the one-dimensional convective-dispersive equation is applicable.

(iii) The dispersion coefficients and times of travel for bacteria are considerably larger than for chemical tracers.

2.6 COMMENTS

From an overall survey of the literature, mentioned above, the following needs for further work are too apparent.

(i) Though a continuous pollutant input can be discretized to instantaneous mass injections, whose analytical solutions can be superposed in time, to obtain a breakthrough for the pollutant, subject to dispersion, little attempt has been made to exploit such a pulse technique, in spite of the simplicity of such a procedure.

(ii) The concentration decay, on the cessation of the pollutant inputs into an aquifer, has not attracted it's due attention, in spite of the practical need to predict the recovery of an aquifer from ceased pollutional inputs.

(iii) Bacterial dispersion has been poorly investigated, though pollution by pathogenic bacteria constitutes a major threat to ground water quality at several places.

Planning of the present studies has been inspired by the three needs mentioned above.

CHAPTER III

THEORY AND MODELING

CONTENTS

3.1 GENERAL

The available analytical solutions for two dimensional dispersion have been used in this work, in suitable forms, for a pulse technique and for a predictive model of an inverse break through. The ADIP numerical scheme has been modified to obtain simplicity, taking advantage of the facts that only axial concentrations are of interest in these studies.

3.2 ANALYTICAL SOLUTIONS[x]

For a dissolved substance subject to inherent decay and adsorption, the equation describing it's transport through a saturated porous medium with uniform steady flow in the x direction is given by

$$R_d \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - U \frac{\partial C}{\partial x} - \lambda R_d C \quad \ldots (3.1)$$

in which

C = concentration of substance in solution (mass of solute per unit volume of solution).

D_x = longitudinal dispersion coefficient

D_y , D_z = transverse dispersion coefficients

U = average pore velocity in the direction of flow along the x-axis.

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[x] All the analytical equations in Sec. 3.2 are from Ref.No. 85 after the needful changes in notation.

λ = inherent decay constant

x, y, z = cartesian coordinates

t = time

$R_d (\geq 1)$ = retardation factor, which slows the movement of the dissolved species due to adsorption.

For applied problems, in general, molecular diffusion can be ignored and the dispersion coefficients can be given, approximately, as

$$D_x = \alpha_x U \; ; \quad D_y = \alpha_y U \quad \text{and} \quad D_z = \alpha_z U$$

in which α values represent dispersivities in the respective directions. For laboratory scale problems α values can be of the order of the grain size of the medium.

Redefining the variables in equation 3.1 in terms of the retardation factor

$$\frac{\partial C}{\partial t} + U' \frac{\partial C}{\partial x} = D'_x \frac{\partial^2 C}{\partial x^2} + D'_y \frac{\partial^2 C}{\partial y^2} + D'_z \frac{\partial^2 C}{\partial z^2} - \lambda C \qquad \ldots (3.2)$$

in which $U' = \frac{U}{R_d}$; $D'_x = \frac{D_x}{R_d} = \alpha_x U'$; $D'_y = \frac{D_y}{R_d} = \alpha_y U'$;

$D'_z = \frac{D_z}{R_d} = \alpha_z U'$

After dropping the primes for convenience, the solution of equation 3.2 is given by

$$C_{x,y,t} = \frac{m}{4\pi n \;\; t (D_x D_y)^{1/2}} \exp \left[\frac{-(x - Ut)^2}{4 D_x t} - \frac{y^2}{4 D_y t} - \lambda t \right] \qquad \ldots (3.3)$$

for an infinite two dimensional porous medium in the x, y plane, with a mass per unit length, m (M/L) instantaneously injected along the z-axis, while

n = porosity of the medium.

For a constant injection rate along the z-axis the solution is given by

$$C_{x,y,t} = \frac{q' C_o \exp(\frac{x}{B})}{4\pi n(D_x \; D_y)^{1/2}} W(U_1, \frac{r}{B}) \qquad \ldots (3.4)$$

in which

q' = volumetric injection rate of the pollutant per unit length along the z-direction.

C_o = concentration of the injected waste (M/L^3)

$$B = \frac{2D_x}{U} \qquad \ldots (3.5)$$

$$\gamma = (1 + \frac{2B\lambda}{U}) \qquad \ldots (3.6)$$

$$U_1 = \frac{r^2}{4\gamma D_x t} \qquad \ldots (3.7)$$

$$r = [x^2 + \frac{D_x \; y^2}{D_y}]^{1/2} \qquad \ldots (3.8)$$

$$W(U_1, \frac{r}{B}) = \int_{U_1}^{\infty} \frac{1}{\theta} \exp - (\theta + \frac{r^2}{4B^2\theta}) \, d\theta \qquad \ldots (3.9)$$

Equation 3.4 describes the plume of pollution that develops down stream of the source. Further

$$W(U_1, \frac{r}{B}) \cong (\frac{\pi B}{2r})^{1/2} \exp(\frac{-r}{B}) \operatorname{erfc} [- \frac{\frac{r}{B} - 2U_1}{2U_1^{1/2}}] \qquad \ldots (3.10)$$

in which erfc = complementary error function = 1 - erf. This approximation is accurate, within 1 percent for $r/B > 10$ and within 10 percent for $r/B > 1$.

As time goes on the plume grows larger, until there is a balance between the rate at which pollution disperses and the rate of injection. For a steady state reached as $t \rightarrow \infty$ and $U_1 \rightarrow 0$, the concentration of the pollutant is given by

$$C_{x,y,\infty} = \frac{q'C_o \exp\left(\frac{x}{B}\right) K_o\left(\frac{r}{B}\right)}{2\pi n(D_x \; D_y)^{1/2}} \quad \ldots (3.11)$$

in which $K_o\left(\frac{r}{B}\right)$ = modified Bessel function of the second kind, which is approximated for large $r/B(> 1)$ by

$$K_o\left(\frac{r}{B}\right) \cong \left(\frac{2r}{\pi B}\right)^{-1/2} \exp\left(\frac{-r}{B}\right) \quad \ldots (3.12)$$

3.2.1 Concentrations Along the x-axis

For concentrations along the x-axis

$$y = 0$$

If $D_x = U\alpha_x$ and $D_y = U\alpha_y$ are assumed substitution of eqns. 3.5 to 3.10 in eqn. 3.4, the concentrations for $y = 0$ reduce to

$$C_{x,o,t} = \frac{q'C_o}{4nU\sqrt{\pi x \alpha_y}} \operatorname{erfc}\left[\frac{x - \gamma U t}{2\sqrt{\gamma U \alpha_x t}}\right] \quad \ldots (3.13)$$

and for steady state with $t = \infty$ and $\lambda = 0$, so that $\gamma = 1$,

$$C_{x,o,\infty} = \frac{q' C_o}{2nU\sqrt{\pi x \alpha_y}} \qquad \ldots. \ (3.14)$$

since erfc $(-\infty) = 2$

It may be recalled that U in eqns. 3.13 and 3.14 incorporates the retardation factor, R_d, and hence U is the apparent pore velocity but not the actual pore velocity, if adsorption is present.

3.2.2 Evaluation of α_y

Equation 3.14 may be rearranged as

$$\frac{C_{x,o,\infty}}{C_o} = \left(\frac{1}{2n\sqrt{\pi\alpha_y}}\right)\frac{q'}{U\sqrt{x}} \qquad \ldots \ (3.15)$$

A linear regression of experimental values of $\frac{C_{x,o,\infty}}{C_o}$ on $\frac{q'}{U\sqrt{x}}$ enables the computation of α_y from the slope of the regression line.

3.2.3 Evaluation of α_x

Equation 3.13 may be rearranged as

$$\text{erfc}^{-1}\left[\frac{C_{x,o,t}}{C_o}\left(\frac{4nU\sqrt{\pi x \alpha_y}}{q'}\right)\right] = \frac{1}{\sqrt{\alpha_x}}\left(\frac{x - \gamma U t}{2\sqrt{\gamma U t}}\right) \qquad \ldots \ (3.16)$$

A linear regression of the experimental values of the term on the left hand side of eqn. 3.16 on the values of $\left(\frac{x - \gamma Ut}{2\sqrt{\gamma Ut}}\right)$ permits the evaluation of α_x from the slope of the regression line.

3.3 PULSE TECHNIQUE

For an instantaneous point source of a pollutant mass, the concentrations of the pollutant are given by eqn. 3.3. For continuous but unsteady injection rates of a pollutant, correct analytical solutions are not available. However discretization in time, with pollutant masses of each duration treated as an instantaneous mass injection at the middle instant of the duration, permits the computation of concentrations at any point of interest due to individual discretized pollutant pulses. By superposing the concentrations due to the individual pulses, in time, the concentration at any point, due to continuous but unsteady injection rates of pollutant, can be obtained. The accuracy of the solution, by this pulse technique, increases with smaller time steps, entailing larger computation time. The time step size to achieve the desired degree of accuracy can be evolved from the comparison of the pulse technique solution with the analytical solution, for a case, where the latter is available.

For a discretized time step of Δt

$m = q'\Delta t C_o \rho$ where ρ = density. At a point of interest on the x-axis eqn. 3.3 reduces to

$$C_{x,o,t} = \frac{q'\Delta t C_o \rho}{4\pi n t (D_x D_y)^{1/2}} \exp\left[\frac{-(x - Ut)^2}{4 D_x t} - \lambda t \right] \quad \ldots(3.17)$$

3.4 INVERSE BREAK THROUGH (BY PULSE TECHNIQUE)

Inverse break through may be defined as the concentration decay with time, at any point of interest in the porous medium after a sudden cessation of pollutant injection, during a steady state. For a point on the x-axis, the steady state concentration is given by the eqn. 3.14. Let the inverse breakthrough at the point (X,0) be required. Let $\Delta x = \frac{X}{N}$ where N is an integer sufficiently large to ensure the required degree of accuracy of the solution. The value of N can be obtained by comparing the pulse technique solution with the analytical solution for the normal breakthrough curve at the point (X,0). In the model proposed here, the pollutant masses are considered as instantaneous, centralized in Δx, and simultaneous with the cessation of injection of the pollutant.

Each instantaneous mass is assumed as $q' \cdot \frac{\Delta x}{U} \cdot C_{x,o,\infty}$ where $C_{x,o,\infty}$ is the steady state concentration at the mid point of the corresponding Δx. The concentrations contributed by these individual pollutant pulses at (X,0) are superposed in time, to obtain the required inverse breakthrough. The procedure described above may be justified as follows. If lateral dispersion were totally absent, the pollutant pulse masses would have been equal to $q' \frac{\Delta x}{U} C_o$ during the steady state, and C_o would have been the steady state concentration at the mid point of Δx. Due to the presence of lateral dispersion, the steady state concentration at the mid point of $\triangle x$ is $C_{x,0,\infty}$, which is $< C_0$. The contribution of the axial (located on x-axis) masses at (X,0) is decreased by lateral dispersion while the laterally located masses can also contribute to the concentration at (X,0). As the loss from axial masses and the contribution from the lateral masses are of opposite effects and are of small magnitudes due to the low values of lateral dispersivity, they may be assumed to cancel each other and the effective pulse mass may be considered as equal to $[q' \frac{\triangle x}{U} C_{x,0,\infty}]$. The accuracy of solution is lesser at smaller values of t (time from the instant of cessation of pollutant injection) than for larger values. However the initial inaccuracy of the inverse break through thus obtained can be fairly circumvented, as the starting point ($C_{x,0,\infty}$) of the inverse break through curve is well defined. A smooth approximation of the inverse break through curve drawn from the correct starting point giving larger weightage to the predicted values of larger t, will be a fairly accurate model for the concentration decay.

3.5 NUMERICAL SOLUTION BY THE ADIP

The mass balance eqn. 3.1 has an analytical solution, eqns. 3.4 to 3.10, for a single case of initial and boundary conditions mentioned in Section 3.2. For any other initial or boundary conditions, numerical solutions are often feasible. In this work Peacemen and Rachford's Alternating Direction Implicit Procedure (ADIP), as explained by Shamir and Harleman[53], has been adopted with some modifications. ADIP is unconditionally stable. The method consists of dividing the time step into two halves and writing the 2-D dispersion eqn. 3.1 implicitly with respect to x derivatives and explicitly with respect to y derivatives, during the first half of the time step, and explicitly with respect to x derivatives and implicitly with respect to y derivatives, during the second half of the time step. Concentrations after half time step are computed to enable the solution during the second half. Otherwise half time concentrations have no physical significance[53] . The finite difference equivalents of eqn. 3.1 by the ADIP for a conservative pollutant are expressed as follows, using the central difference equivalent for the first space derivative.

$$\frac{E_{i,j} - B_{i,j}}{\Delta t/2} + U\left[\frac{E_{i+1,j} - E_{i-1,j}}{2\Delta x}\right] = D_x\left[\frac{E_{i-1,j} - 2E_{i,j} + E_{i+1,j}}{(\Delta x)^2}\right] + D_y\left[\frac{B_{i,j-1} - 2B_{i,j} + B_{i,j+1}}{(\Delta y)^2}\right] \quad \ldots (3.18)$$

for the first half of the time step, and for the second half of the time step

$$\frac{C_{i,j} - E_{i,j}}{\Delta t/2} + U \left[\frac{E_{i+1,j} - E_{i-1,j}}{2\Delta x} \right]$$

$$= D_x \left[\frac{E_{i-1,j} - 2E_{i,j} + E_{i+1,j}}{(\Delta x)^2} \right]$$

$$+ D_y \left[\frac{C_{i,j-1} - 2C_{i,j} + C_{i,j+1}}{(\Delta y)^2} \right] \quad \ldots (3.19)$$

Where Δx and Δy are step sizes in the x and y directions, Δt = time step, and $B_{i,j}$, $E_{i,j}$ and $C_{i,j}$ are concentrations of the pollutant at the previous time level at the middle of the time step and at the new time level, respectively, for each time step, at the space grid point $(i\Delta x,\ j\Delta y)$ Eqns. 3.18 and 3.19 can be rearranged as follows:

$$P\,E_{i-1,j} - Q\,E_{i,j} + R\,E_{i+1,j} = -SB_{i,j-1} + TB_{i,j} - SB_{i,j+1} \quad \ldots (3.20)$$

$$SC_{i,j-1} - VC_{i,j} + SC_{i,j+1} = -PE_{i-1,j} + WE_{i,j} - RE_{i+1,j} \quad \ldots (3.21)$$

Where

$P = D_x/(\Delta x)^2 + U/2\Delta x$

$Q = 2D_x/(\Delta x)^2 + 2/\Delta t$

$R = D_x/(\Delta x)^2 - U/2\Delta x$

$S = D_y/(\Delta y)^2$

$T = 2D_y/(\Delta y)^2 - 2/\Delta t$

$V = 2D_y/(\Delta y)^2 + 2/\Delta t$

$W = 2D_x/(\Delta x)^2 - 2/\Delta t$

The left hand sides of the iterative eqns. 3.20 and 3.21 form tridiagonal matrices, to be solved by a suitable TriDiagonal Matrix Algorithm (TDMA), since the right hand sides of the equations are determinate for the first and the second halves of the time step, successively.

3.5.1 Modifications to ADIP

The ADIP described above is modified in this work for simpler computation, taking advantage of the following two features in this work.

(i) Axial concentrations, alone, have been considered in these studies and

(ii) The ratio D_x/D_y is large enough to permit a few simplifying assumptions to be mentioned later.

From the symmetry of the 2-D pollutant plume about the x-axis (vide eqns. 3.4 and 3.8), it follows that

$$(\text{Concentration})_{i,j-1} = (\text{Concentration})_{i,j+1}$$

Further for a large value of D_x/D_y in a square grid with $\triangle x = \triangle y$, $S.(B \text{ or } E \text{ or } C)_{i,j \pm 1}$ is negligible, compared to the other terms in eqns. (3.20) and (3.21), which consequently reduce to

$$(P/T)E_{i-1} - (Q/T)E_i + (R/T)E_{i+1} = B_i \qquad \ldots (3.22)$$

and

$$C_i = (P/V)E_{i-1} - (W/V)E_i + (R/V)E_{i+1} \qquad \ldots (3.23)$$

after dropping the, now redundant, second suffix 'j'.

Equations (3.22) and (3.23) simplify the computation, due to the replacement by singly subscripted variables, and also due to the need to solve the tridiagonal matrix only once, instead of twice, for each time step. The solution of the tridiagonal matrix is not unique in eqn. 3.22 unless an additional boundary condition is specified. For this purpose a transmission boundary condition[37] at the exit (the last grid point) given by

$$(B \text{ or } E \text{ or } C)_{i+1} = 2 \cdot (B \text{ or } E \text{ or } C)_i - (B \text{ or } E \text{ or } C)_{i-1} \qquad \ldots (3.24)$$

is assumed. This modified ADIP for axial concentrations increases the ease of computation at the expense of accuracy (which decreases with decreasing values of Δy and D_x/D_y) and, hence, is applicable only in situations, where the benefit of easier computation outweighs the loss, of decreased, accuracy.

An [redacted] algorithm of the modified ADIP, suggested above, is given in Appendix II.

3.5.2 Modified ADIP for Predicting the Inverse Break Through

In the modified ADIP proposed in Section 3.5.1, the initialization of concentrations, at the commencement of the first time step during the computation of a normal break through, is based on the following conditions.

$B_i = 1.0$ for $i = 1$ and $t \geq 0$

$B_i = 0$ for $i > 1$ and $t = 0$.

For predicting the IBT at any axial point due to the sudden cessation of pollutant injection, during a steady state, the appropriate initial conditions will be as follows.

$B_i = 1.0$ for $i = 1$ and $t = 0$

$B_i = 0$ for $i = 1$ and $t > 0$

$B_i = C_{(i-1)\Delta x, o, \infty}$ for $i > 1$ and $t = 0$

where $C_{(i-1)\Delta x, o, \infty}$ is the steady state concentration at the axial point $[(i-1)\Delta x, 0]$, which can be obtained from eqn. 3.14. Further, at $t = 0$, B_i at $i = 1$ suddenly changes from 1.0 to 0. Hence it is more reasonable to assume $B_i = (1.0 + 0)/2 = 0.5$ at $i = 1$ and $t = 0$ for the numerical computations.

The ~~fortran IV~~ algorithm for the modified ADIP for predicting the IBT is given in Appendix III.

3.6 DISPERSION OF E.COLI

Dispersion of bacteria can differ from that of a non conservative chemical pollutant due to the following reasons.

(i) The exocellular biochemical activities of living organisms (in the presence of exogenous food) involve physical and chemical changes in their environment, which in turn can influence factors like permeability and adsorption characteristics within a porous medium. These changes in turn, can influence the dispersion pattern.

(ii) Unlike chemical species, bacteria can multiply under favourable conditions, sometimes at very high rates, with the population doubling period as low as 20 minutes. Death rate in bacteria can be analogous to the inherent decay of some chemicals and hence need not be considered as a special feature.

The first of the above two phenomena, does not permit theoretical modeling of bacterial dispersion, unless all the relevent parameters in the phenomenon have known functional relationships. The current level of human knowledge is grossly inadequate in this area and as such, purely empirical approaches and hypothetical analytical abstractions are inevitable in the near future. However a redeeming factor in this situation is that the major bulk of the exocellular metabolism is often confined to the immediate spatial vicinity of the pollutant input within the porous medium. A little further, the concentrations of bacteria and the magnitudes of biochemical activity decrease rapidly with distance, thereby permitting the application of analytical treatment, relevent to a non-conservative chemical pollutant. In this context it is relevent to note that even analytical solutions are applicable only beyond a minimum distance from the source. In view of these facts, the techniques of modeling the conservative pollutant have been extended to E. coli, with the only additional superposition of inherent decay and adsorption.

3.6.1 The following assumptions and their justifications are implied in the modeling of bacterial dispersion in this work.

(i) Permeability of the porous medium is unaffected during an experimental run, with bacterial pollutant.

An approximate estimate shows that with the level of concentrations of bacteria, adopted in these runs, 1% reduction in porosity due to adsorption of cells requires more than 100 hours of continuous run, while the actual runs have lasted for 5 or 6 hours only. Growth of E. coli results in an evolution of gases, causing the possibility of air binding, within the porous medium. This possibility is fairly eliminated in these studies by taking washed, nutrient free bacterial suspension.

(ii) Adsorption of bacteria on particle surfaces of the porous medium follows a linear equilibrium adsorption isotherm.

This assumption permits the incorporation of a retardation factor to enable the usage of dispersion equations, as for a conservative pollutant[85].

Linear equilibrium adsorption isotherm implies the abundance of adsorption sites with respect to the adsorbed species. This condition is well satisfied in these studies, as each particle, of size 0.055 cm, (= d_{50} of the porous medium used), is potentially capable of adsorbing around 1 million cells in a single layer on 50% of it's surface area, while in contrast, the cell concentrations employed in the experimental runs are extremely low, in these studies.

(iii) For the runs, whose results are used for the evaluation of α_y, the bacterial death rates have been neglected. Zero death rate is experimentally impossible to ensure. Death upto 5% in the input pollutant has been neglected in the above mentioned runs, which reflects on the accuracy of the evaluated α_y.

(iv) For the evaluation of apparent α_x for <u>E.coli</u> it is assumed that the ratio α_y/α_x is the same for conservative and non-conservative pollutants.

The assumption is based on the findings of Murthy and Scott[9], who have reported that α_x/α_y is generally constant for a particular material in the aquifer and this ratio can be considered a basic property of the aquifer.

CHAPTER - IV

EXPERIMENTAL PROGRAM

CONTENTS

4.1 EXPERIMENTAL SET UP

The experimental facility (vide Fig.4.1 and 4.2) consists of a box, made of 0.6 cm thick perspex sheets, with inner dimensions of 77.5 cm length, 80 cm depth and 5 cm width. With flow parallel to the length of the box, the inlet zone, of 10 cm length, and out let zone, of 7.5 cm length, were filled with gravel of 0.5 to 2.0 cm size, and were partitioned from the experimental zone by vertical perforated perspex sheets lined with plastic mesh with 0.03 cm square openings. The lid of the box could be clamped air tight, with synthetic sponge packing underneath, to prevent short circuiting, in case of a slight settlement of the porous medium.

Tappings, of 0.03 cm internal diameter, were provided on one large face of the box, and were spaced at 20 cm horizontally and 15 cm, vertically. Two additional tappings were added 5 cm above the last two tappings of the middle row. The tapping tubes extended 2.5 cm into the box and their inlets were screened with plastic mesh. Pollutant was injected through either of the end tappings of the middle row. Porous tubes, lined with plastic mesh and of size 5 cm long and 1 cm in dia, inside the box at the injection tappings, ensured uniform line injection over the 5 cm width of the model. The box was suitably supported by steel frame work. All the tappings, through which

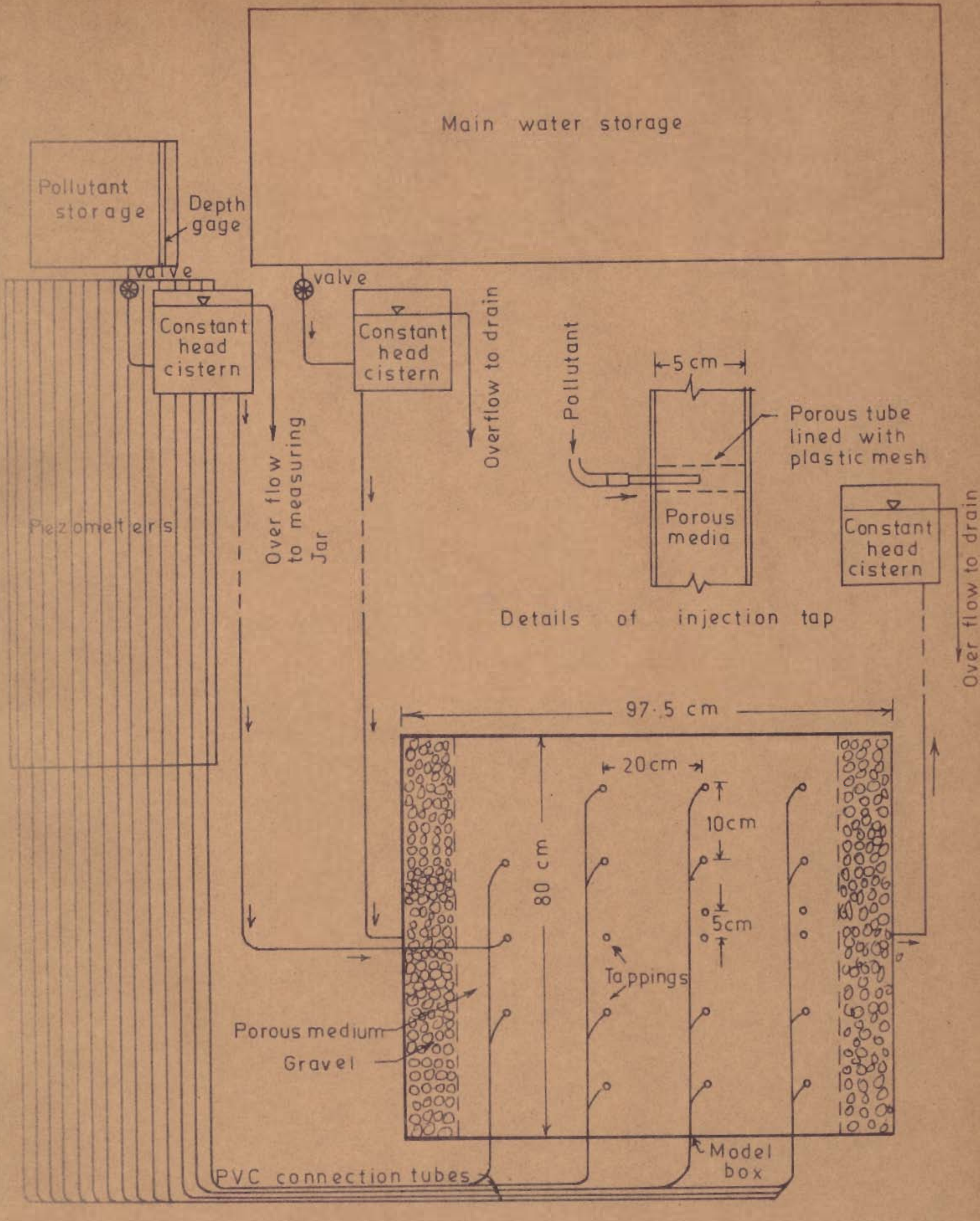

FIG.4·1-SCHEMATIC DIAGRAM OF EXPERIMENTAL SET-UP

FIG. 4.2. EXPERIMENTAL MODEL BOX.

samples were not being drawn, were connected through 0.03 cm dia P.V.C. tubes to piezometers mounted on a vertical graduated plane board. Steady flow rates of the main flow and the injected pollutants were maintained with separate storage tanks and constant head cisterns. The outlet of the model was connected to another constant head cistern of adjustable height. The flow rates were controlled by screw clamps on the supply pipes, as well as by the heights of the constant head cisterns.

The model box was uniformly packed with clean sand, as the porous medium. The sand, used, had the following characteristics.

Porosity 0.46 ; Specific gravity 2.567
d_{50} 0.055 cm; d_{10} 0.045 cm
d_{60} 0.058 cm; Uniformity Coefficient 1.29

As the diurnal temperature range in the laboratory was as large as 15° C, a reflux condenser was attached in the path of the pollutant flow to ensure equalization of temperatures between the main flow and the pollutant, so as to avoid the possibility of thermal convections in the porous medium during the injection of pollutant.

4.2 COLLECTION OF SAMPLES

With Sodium chloride solution as the pollutant, the samples were collected in clean 50 ml glass beakers. After removing the PVC cap of the tapping, the stagnant fluid was let to waste for about 5 seconds. About 40 ml of sample was collected each time; the duration of collection was approximately 20 seconds. With E. coli suspension as the pollutant, the samples were collected by the same procedure, but in sterile test tubes in volumes of 10 ml each, and were immediately plugged with sterile cotton. The processing of the samples was done within one hour after collection.

4.3 MEASUREMENTS

4.3.1 Main Flow Rate

After attaining a steady state of flow, as indicated by the piezometric levels, the discharge of the main flow was measured at the outlet by noting the duration of collection of a measured volume of water. Tap water stored in a tank, constituted the main flow.

4.3.2 Pollutant Flow Rate

The pollutant flow rate was measured by noting the rate of depletion in the pollutant storage tank. In the case of Sodium chloride the concentration of the effluent from the model box, during the steady state, was also measured for additional confirmation.

4.3.3 Concentrations of Sodium Chloride Samples

Concentrations of Sodium chloride samples were estimated from the measurements of electrical conductivity of the solution, using a 'WISS-TECHN-WERKSTÄTTEN-TYPE LBR" conductivity bridge. The concentrations were obtained from a calibration curve prepared for each run of the experiment. Temperature corrections for conductivities were applied whenever necessary, assuming 2 percent increase in conductivity per 1°C rise in temperature. The range of temperature variations of the samples during any run was less than 5°C.

4.3.4 Concentrations of Bacterial Samples

Concentrations of E.coli were estimated by the standard membrane fitter (MF) technique[6] . The media used for the growth of bacteria was 'HI-MEDIA" M-coliform broth base (Dehydrated) M 1103, having the following composition.

	gm/litre
Polypeptone peptone	10.00
Thiotone peptone	5.00
Trypticase peptone	5.00
Yeast extract	1.50
Lactose	12.50
Sodium chloride	5.00
Potassium phosphate	5.75
Sodium lauryl sulfate	0.05
Sodium Desoxycholate	0.10
Sodium Sulfite	2.10
Basic Fuchsin	1.05

pH 7.2 ±

As per the specifications indicated, 48 gm of dry media was added to one litre of distilled water and heated to boiling. The solution was autoclaved at 121° C for 15 minutes and stored under sterile conditions.

4.4 PREPARATION OF POLLUTANTS

4.4.1 Sodium Chloride Solution

1% Sodium chloride solution (tap water) was used as stock solution. For preparing different dilutions for obtaining the calibration curve, the same tap water was used.

4.4.2 E. Coli Suspension

Raw sewage was innoculated into sterile McConkey broth and was incubated at 35° C for 24 hours. The growth, thus obtained, was streaked on a sterile EMB agar[6] plate and was again incubated at 35° C for 24 hours. E. coli (Var. I) colony was selectively picked up and was streaked on sterile agar slants, which were incubated at 35° C for 48 hours. The slants were then stored in a refrigerator. The bacterial culture was confirmed, as E. coli Var. I, by the standard IMVIC reactions[6] To prepare the bacterial suspension, the culture from the stored agar slants was innoculated into sterile, 6 percent, peptone water, buffered to a pH of 7.2 and was incubated at 35° C for 18 hours. The suspension of bacteria, thus obtained was filtered and washed with sterile distilled water, using the membrane filter assembly. The filter paper with the washed cells was transferred to a 2 litre glass bottle, containing sterile distilled water. The distilled water, used for bacterial suspensions, washing of cells and serial dilutions, was autoclaved and buffered to a pH of 7.0. The initial concentration of the suspension was estimated by the membrane filter technique (MF)[6]. To prepare the suspension for the experimental run, the stock suspension was diluted with chlorine free tap water and left for one hour for acclimatisation. Chlorine in tap water was neutralized with Sodium thiosulfate, for the main flow water as well as the bacterial pollutant water. Where, rapid death rate was wanted for the experimental run, chlorinated tap water was employed.

4.5 PROCEDURAL DETAILS (EXPERIMENTAL)

4.5.1 Prior to each experimental run, flow through the model was allowed for about 30 minutes to ensure the removal of the pollutants of the previous run remaining in the porous medium and also for obtaining uniformity of temperature of the porous medium and the main flow.

4.5.2 Prior to each run with the bacterial pollutant, chlorinated water followed by water, treated with Sodium thiosulfate, was run through the model to remove the bacteria remaining in the porous medium after the previous run. Blank samples from the tappings were collected prior to the injection of the bacterial pollutant to confirm the absence of coliform bacteria in the main flow and the porous medium.

4.5.3 The main flow direction in the model box was being reversed for different runs to avoid a possible vertical stratification of the porous medium.

4.5.4 Equal piezometric levels at tappings in each vertical row, confirmed uniform, horizontal seepage velocity.

4.5.5 At the end of all experimental runs, the expected qualitative shape of the 2 dimensional pollution plume was, visually, confirmed, by injecting a coloured pollutant (1 percent Potassium permanganate solution).

4.6 PROCEDURAL DETAILS-COMPUTATIONAL

In the experimental facility (vide Sec. 4.1), the porous medium used has a porosity = n = 0.46.

Gross area of flow = 80x5 = 400 cm^2

Thickness of porous medium = 5 cm

Hence $q' = q/5$ where q is the rate of injection (ml/sec) of the pollutant into the model.

$U = Q/(400 \times 0.46)$ where Q is mainflow in ml/sec.

ρ = Density of fluid = 1 gm/ml. and

$D_x = \alpha_x.U$ and $D_y = \alpha_y.U$ are assumed.

4.6.1 Evaluation of α_x and α_y

Substituting the numerical values given in Sec. 4.6, Eqn. 3.15 reduces to

$$\frac{C_{x,o,\infty}}{C_o} = \frac{22.56}{\sqrt{\alpha_y}} \cdot \frac{q}{Q\sqrt{x}} \qquad \dots (4.1)$$

and eqn. 3.16 reduces to

$$F = \frac{1}{\sqrt{\alpha_x}} \left[\frac{x - Ut}{2\sqrt{Ut}} \right] \qquad \dots (4.2)$$

where

$$F = \text{erfc}^{-1} \left[\frac{C_{x,o,t}}{C_o} \cdot \frac{Q\sqrt{x\alpha_y}}{11.28q} \right] \qquad \dots (4.3)$$

x and t are to be measured in cm and sec. respectively. α_y and α_x are evaluated from eqns. 4.1 to 4.3 along the lines suggested in Sec. 3.2.2 and 3.2.3 respectively.

4.6.2 Pulse Technique

Substituting the numerical values given in Sec. 4.6, eqn. 3.17 reduces to

$$C_{x,o,t} = \frac{q C_o \Delta t}{28.9\ Ut\ \sqrt{\alpha_x \alpha_y}} \exp\left[- \frac{(x - Ut)^2}{4\alpha_x Ut} - \lambda t\right] \qquad \ldots (4.4)$$

where $\lambda = 0$ for sodium chloride

and $\quad = $ linear death rate constant for <u>E. coli</u>

Pulse technique calculations have been based on eqn. 4.4 on the lines suggested in Sec. 3.3. Where C_o and q are variable, the values, corresponding to the time of commencement of the pulse, are taken.

In the computations of IBT $\Delta t = \Delta x/U$. The value of Δx has been varied, increasing with the distance from (X,0), the point of interest, upto a maximumvalue after which Δx has been kept constant. This has improved the accuracy as against a constant Δx for all pulses.

4.6.3 Numerical Solutions

Fortran IV programs of the Algorithms in Appendix II and Appendix III have been run on IBM 1130 at Andhra University, Waltair, feeding the relevent data. The space and time step sizes have been constant and arbitrary and of the same order, as employed in the pulse technique solutions of the same problems. No attempt has been made to optimize the time and space steps to improve the convergence.

CHAPTER V

ANALYSIS OF DATA

CONSERVATIVE POLLUTANT

CONTENTS

5.1 EVALUATION OF α_y

The steady state concentrations ofthe pollutant at selected axial distances, and the computed values of the functional parameters of eqn. 4.1 are shown in Table 5.1. These are selectively values that have persisted for a long duration of observation of steady state.

Linear regression between the functional parameters of eqn. 4.1 has yielded a slope = 0.145 (Vide Fig. 5.1) from which $\alpha_y = 0.024$ cm.

The small scatter of points (Vide Fig. 5.1) about the regression line could be the result of all the approximations inherent in eqns. 4.1, in addition to the experimental limitations.

5.2 EVALUATION OF α_x

The transient concentrations of the pollutant at selected axial distances have been given along with the functional parameters of eqn. 4.2, in Table 5.2.

A linear regression between the functional parameters of eqn. 4.2 has yielded a slope = 1.667 (Vide Fig. 5.2) from which the evaluated $\alpha_x = 0.36$ cm.

From Fig. 5.2, it is evident that the scatter of the experimental results is larger than in Fig. 5.1, of steady state values. This larger scatter arises from the following factors.

TABLE -5.1

COMPUTATIONS FOR THE EVALUATION OF α_y

Run No.	Q ml/sec	q ml/sec	C_o % by wt.	x cm	$C_{x,o,\infty}$ % by wt	$\frac{C_{x,o,\infty}}{C_o}$	$\frac{q \times 10^3}{Q\sqrt{x}}$
5	56.70	0.608	0.1	20	0.033	0.33	2.398
6	77.2	0.480	0.1	20	0.020	0.20	1.390
	77.2	0.480	0.1	40	0.014	0.14	0.983
7	75.55	0.404	0.1	20	0.019	0.19	1.196
	75.55	0.404	0.1	40	0.013	0.13	0.846
	64.40	0.440	0.1	20	0.023	0.23	1.528
	64.40	0.440	0.1	40	0.016	0.16	1.080
	45.30	0.398	0.1	20	0.030	0.30	1.965
	45.30	0.398	0.1	40	0.021	0.21	1.389
	20.95	0.299	0.1	20	0.045	0.45	3.191
	20.95	0.299	0.1	40	0.037	0.37	2.257
8	58.80	0.407	0.05	20	0.011	0.22	1.548
11	22.80	0.453	0.1	40	0.048	0.48	3.141
	22.80	0.453	0.1	60	0.038	0.38	2.565

TABLE -5.2

COMPUTATIONS FOR THE EVALUATION OF α_x

Run No.	Q ml/sec	q ml/sec	C_o % by wt	x cm	t sec	$C_{x,o,t}$ % by wt	F^x	$\frac{x - Ut}{2\sqrt{Ut}}$
1	35.7	0.582	1.0	20	120	26.00	0.018	-0.340
				20	240	30.00	-0.116	-1.946
				20	305	30.00	-0.116	-2.546
				40	205	2.50	1.062	-0.018
2	40.0	2.460	1.0	40	197	0.50	1.900	-0.216
3	43.3	0.838	1.0	20	35	6.10	0.920	2.048
				20	95	24.00	0.214	-0.251
				20	165	29.00	0.070	-1.513
				40	190	3.60	0.990	-0.355
				40	300	5.60	0.811	-1.823
				60	320	0.35	1.650	-0.885
4	42.0	0.183	0.1	20	35	0.25	0.656	2.124
				60	390	0.40	0.019	-1.539
5	56.7	0.608	0.1	20	120	2.10	0.155	-1.395
				20	215	2.30	-0.288	-2.840
				40	180	0.80	0.323	-1.037
6	77.2	0.480	0.1	20	35	0.30	0.738	0.702
				20	120	2.00	-1.264	-2.129
				40	180	1.35	-1.118	-2.031
				60	205	0.25	0.561	-1.388
8	58.8	0.407	0.05	20	30	0.40	0.265	1.681
				20	72	0.80	-0.390	-0.314
				20	165	1.10	-1.388	-2.254
				40	50	0.50	-0.229	3.004
				60	128	0.20	0.356	1.492

Contd....

TABLE -5.2 (contd.)

Run No.	Q ml/sec	q ml/sec	C_o % by wt.	x cm	t sec	$C_{x,o,t}$ x10^2 % by wt.	F[x]	$\frac{x - Ut}{2\sqrt{Ut}}$
9	59.2	1.112	0.1	20	35	0.20	1.302	1.300
				20	93	1.70	0.417	-0.909
10	65.0	0.445	0.1	20	25	0.07	1.329	1.879
				20	87	0.04	1.483	-0.968
				40	54	0.03	1.497	3.441
				40	120	0.05	1.288	-0.184
				60	160	0.05	1.222	0.231
11	22.80	0.453	0.1	40	320	2.30	-0.001	0.232
				40	480	4.50	-1.510	-1.262
				40	750	4.63	-3.300	-2.745

[x] Vide eqn. 4.3.

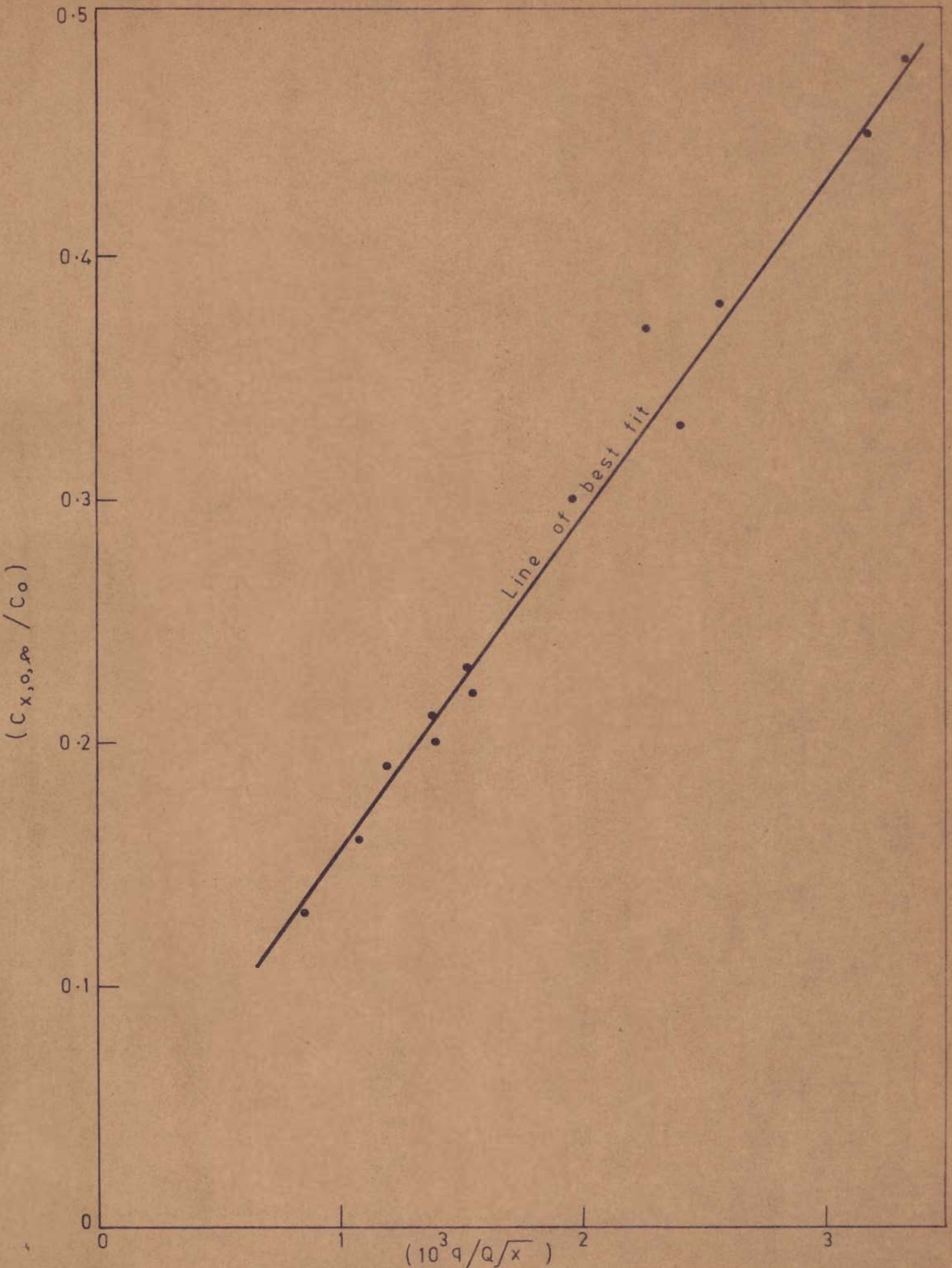

FIG. 5·1 - EVALUATION OF α_y

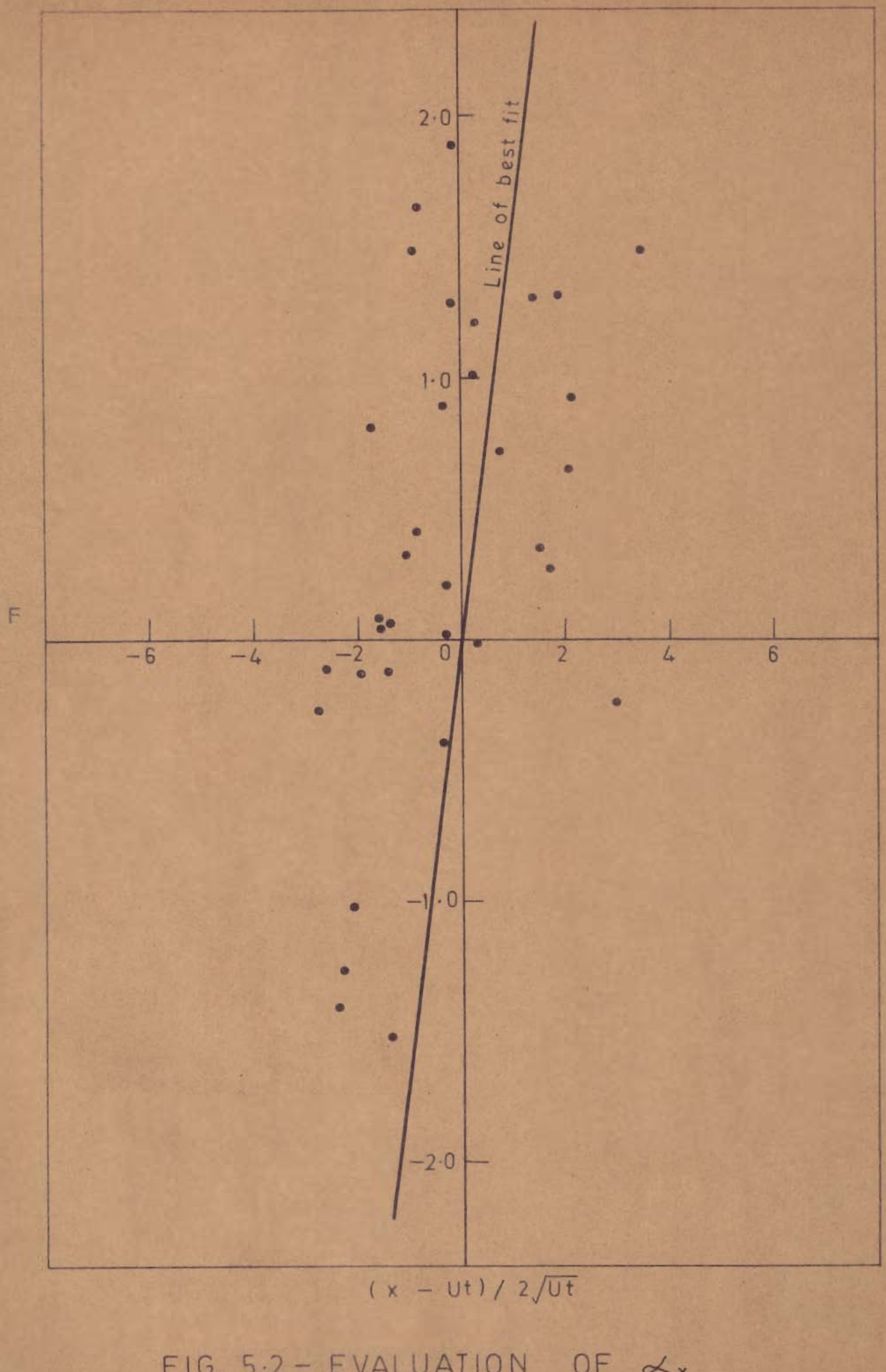

FIG. 5·2 – EVALUATION OF α_x

(i) Limitation of the experimental technique adopted can introduce some error. The duration of collection of the sample extending over 10 to 20 sec is a substantial part of the time base of the break through curve, particularly for the lower x values. Hence the measured concentration of the sample is some average for a duration, and the instant to which it is exactly related is not located accurately. In the procedure adopted here, the middle of the duration of collection is chosen, arbitrarily. In-situ electronic probing for the pollutant concentration monitoring is a superior method, but the choice of the method in this work is governed by the need to compare with the dispersion of E. coli, for which in-situ monitoring is ruled out. Hence, for better comparability, similar sampling procedures have been adopted for both the pollutants.

(ii) In addition to the experimental limitation mentioned above, the functional relationships defined by eqns. 4.2 and 4.3 are such, that $\partial F/\partial C_{x,o,t}$ is much larger for smaller values of $C_{x,o,t}$. Hence small inevitable experimental errors in the measurement of earlier concentrations of the break through get amplified in the result of α_x.

(iii) The error caused by treating a finite sized source as a point source decreases with increasing t and x values. This error was checked treating the size of the source as equal to q/U and was found to be within ±5% for time

$t = \frac{2x}{U}$, using Hunt's criteria[12]. But the same degree of accuracy can not be expected at low values of 't'. On this count also, the observed transient values depart from the theoretical values.

In spite of the above three limitations, the method, adopted, is justified since linear regression is theoretically established and the departures of experimental results are two sided and can balance about the regression line, with a sufficiently large number of observations.

The ratio of α_x/α_y in this study works out to 15, which compares favourably with the earlier reports of the following investigators[60].

De Josseline de Jong (1958)	6 to 10
Bear (1961)	7 to 22.7 (Mean 17.7)
Blackwell (1962)	24

5.3 BREAK THROUGH CURVES

Using the values of α_y and α_x evaluated in secs. 5.1 and 5.2 the break throughs have been computed for the parameters of Run 11 (Vide Table I.1 in Appendix I) by the different models explained in Secs. 3.2, 3.3 and 3.5. The results of these computations have been graphically presented in Fig. 5.3.

The analytical breakthrough has been computed from eqn. 3.13. The concentrations of each pulse are computed

TABLE -5.3

BREAKTHROUGH BY PULSE TECHNIQUE

Data: $U = 0.1239$ cm/sec ; $Q = 22.8$ ml/sec

$q = 0.453$ ml/sec; $\Delta t = 20$ sec ;

$\alpha_x = 0.36$ cm ; $\alpha_y = 0.024$ Cm (Ref Run 11)
Table I.1 App. I.

t sec.	t for pulse sec.	$C_{x,o,t}$ from eqn. 4.4 %. by wt.	$\sum C_{x,o,t}$ %. by wt.
190	180	0	0
210	200	0	0
230	220	0.0002	0.0002
250	240	0.0010	0.0012
270	260	0.0028	0.0040
290	280	0.0055	0.0095
310	300	0.0078	0.0173
330	320	0.0085	0.0258
350	340	0.0074	0.0332
370	360	0.0054	0.0386
390	380	0.0034	0.0420
410	400	0.0019	0.0439
430	420	0.0009	0.0448
450	440	0.0004	0.0452
470	460	0.0002	0.0454
490	480	0.0001	0.0455
510	500	0	0.0455

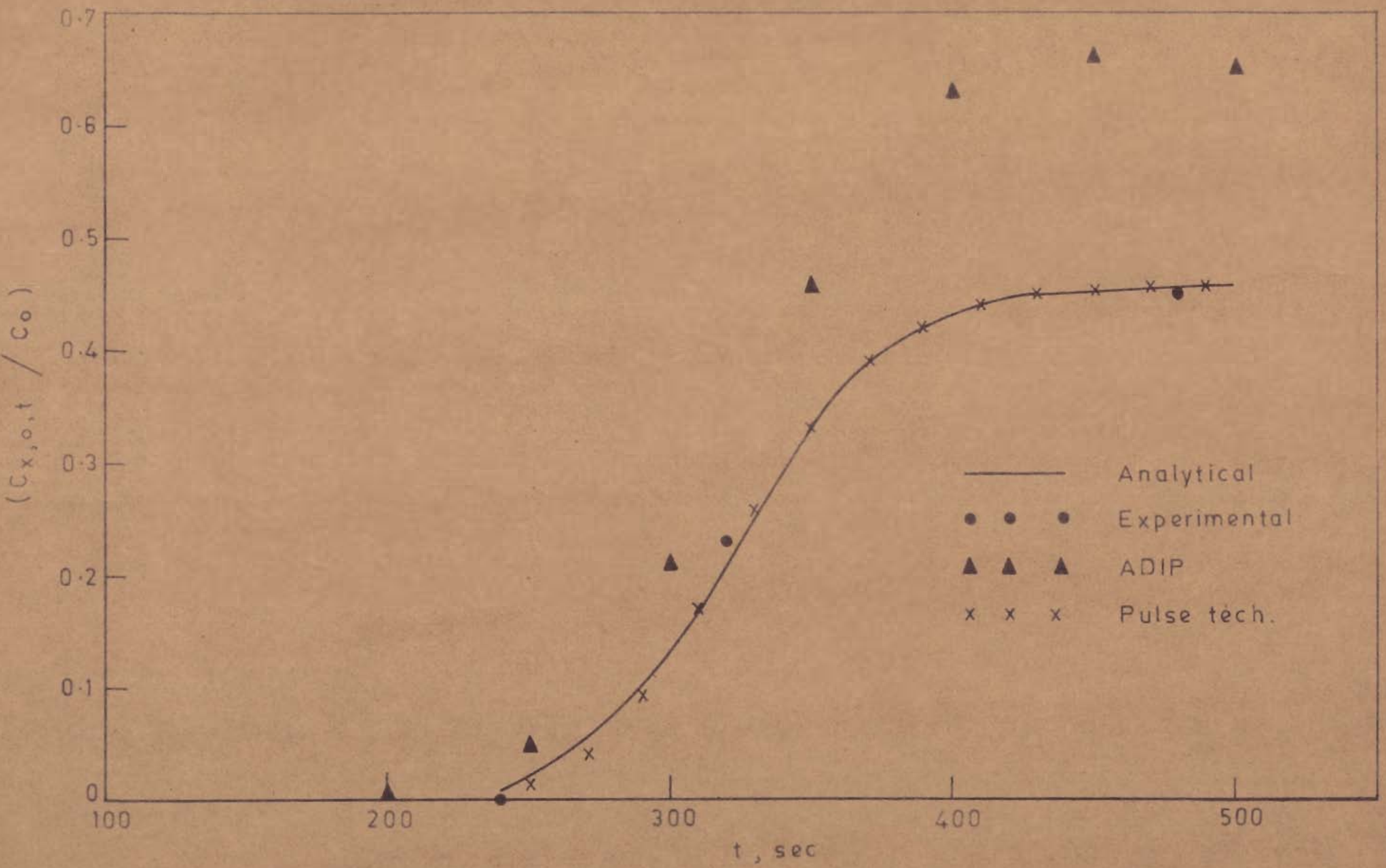

FIG. 5·3 – BREAK THROUGHS (NaCl) – RUN 11 from eqn. 4.4, in the pulse technique, whose results are shown in Table 5.3. For obtaining the numerical solution, a Fortran IV program based on the algorithm given in Appendix II has been run on IBM 1130 in Andhra University Waltair. Time step Δt = 20 sec and Space steps $\Delta x = \Delta y$ = 2 cm have been used.

From Fig. 5.3, it is seen that the analytical and pulse technique solutions are in fair conformity. The experimental values also agree fairly, but are too few in number. This could not be helped due to the limited scope of getting transient data from the experimental technique adopted. The numerical solution by the modified ADIP is fairly stable but, the convergence is not good with the step sizes adopted. In fact the step sizes should be small enough to define the shape and size of the transient interface, between the injected fluid and the main flow. Otherwise, with a strict point source assumption, the ADIP algorithm gives plume concentrations, independent of the rate of injection of the pollutant, which is untenable.

The computation of the transient interface has to be done by the procedure given by Jacob Bear[34], assuming immiscible fluids.

However, the time base of the numerical break through is in fair synchronization with that of the analytical solution (Vide Fig. 5.3).

Computations of the interface and optimization of the grid density and time steps, to also incorporate the physical size of the pollutant source as a function of time, can improve the convergence, but this has not been attempted, since the pulse technique has been much simpler and more satisfactory and hence, has been favoured for subsequent computations in these studies.

The preceding observations and discussions in this section validate, to a fair degree of accuracy, the following concepts implied in the models and computations, involved.

(i) The procedures of evaluation of α_x and α_y adopted in this work yield dependable values.

(ii) The pulse technique solutions with step sizes large enough to permit hand calculations are fairly accurate when compared with analytical solutions for pollutant breakthroughs, in 2-dimensional dispersion through porous media flow.

(iii) The pulse technique approach is simpler and more accurate than numerical technique, for the set of initial and boundary conditions considered in this section.

5.4 INVERSE BREAKTHROUGH CURVES

The experimental observations for inverse break through curves have been shown in Table I-2 of Appendix I.

5.4.1 IBT by Pulse Technique

The IBT values have been computed according to the model explained in Sec. 3.4. Detailed computations for one run are shown in Tables 5.4 and 5.5, while the summary of all IBT computations are presented in Table 5.6 and Fig. 5.6. A graphical comparison of the values obtained by pulse technique with the experimental results is shown in Figs. 5.4, 5.5 and 5.6. The pulse technique values shown in Table 5.6 have been read for the specific values of t, from smooth curves drawn through values computed by pulse technique.

From Figs. 5.4, 5.5 and 5.6, it is evident that the solution proposed by the pulse technique model for the IBT, is fairly satisfactory. The model presumes that the concentration contributions, at the point of interest, from axial pollutant masses alone are significant for computing IBT and also that the axial masses are defined by the steady state concentrations prior to the cessation of the injection of the pollutant. The latter part of the above presumption is closer to the fact, if lateral spread of the pollutant is limited, which is the case nearer to the point of injection. This can be visually seen in Fig. 5.7, presenting the analytical concentration profiles at different axial distances, during the steady state for Run No. 12. As the pollutant pulses, at longer distances from the point of interest, are in greater conformity with the model premises, the trailing end of the IBT is expected to be more accurate. This expectation is confirmed by the observations (Vide Figs. 5.4 and 5.5). In the earlier part of the IBT, the error inherent in the premises of the model can be circumvented to a large extent since the starting point of the IBT (i.e. $C/C_{x,o,\infty} = 1$ at $t = 0$) is definite and a smooth curve, through the computed pulse technique values, can be drawn from the correct starting point, giving greater weightage to the points at the trailing end.

From Fig. 5.6, higher accuracy of the predictions is apparent, when $C/C_{x,o,\infty}$ is closer to 1.0 and 0.0, thereby reinforcing the concepts discussed above. Larger discrepencies with $C/C_{x,o,\infty}$ around 0.5, arise also from another source, namely, the inadequacy of the experimental technique to monitor the rapidly changing concentrations, characteristic of IBT around $C/C_{x,o,\infty} \simeq 0.5$ state. Thus the benefit of doubt, may perhaps be credited to the credence of the proposed model, wherein a maximum discrepency around $C/C_{x,o,\infty} \simeq 0.5$ state is apparent.

5.4.2 IBT by Modified ADIP

A fortran IV version of the algorithm given in Appendix III has been run on IBM 1130 at Andhra University Waltair, The data has been relevent to Run No. 12 (Vide Table I.2-Appendix I). The outputs have been obtained at both $X = 20$ cm and $X = 40$ cm. The IBT curves thus obtained are given in Figs. 5.4 and 5.5, along with the experimental and pulse technique values. The step sizes for time and space in the numerical program have been chosen arbitrarily as $\Delta t = 20$ sec and $\Delta x = \Delta y = 2$ cm. The numerical solutions yielded consistently higher values as in the case of breakthrough curves also (Vide Fig. 5.3). However, the synchronization of the time base and the convergence towards the trailing end are on the merit side, for the proposed numerical model. No further attempt has been made to optimize the step sizes for obtaining better convergence, as the choice has been in favour of the pulse technique, for the rest of this work, for reasons, already mentioned in Sec. 5.3.

The reasonable degree of concurrence, of the IBT model with the experimental observations, establishes the following,

(i) The longitudinal and lateral dispersivities evaluated from normal breakthrough data are applicable to IBT as well.

(ii) A simple pulse technique enables the prediction of IBT with a reasonable degree of accuracy.

(iii) Axial concentration profile, during a steady state pollution, solely governs the IBT at an axial location.

(iv) ADIP is more complex with no assurance of better accuracy compared to the pulse technique, for the model considered in this section.

TABLE -5.4

INVERSE BREAK THROUGH COMPUTATIONS BY PULSE TECHNIQUE AT THE POINT (20,0)

(Ref. Run No. 12 in Table I-2 App. I)

Pulse No.	Δx cm	$\Sigma \Delta x$ cm	x cm	X cm	$C_{x,o,\infty}$ % by wt.	$M \times 10^5$ gm
1	0.1	0.1	0.05	19.95	0.0465	2.44
2	0.2	0.3	0.20	19.80	0.0467	4.91
3	0.3	0.6	0.45	19.55	0.0470	7.41
4	0.4	1.0	0.80	19.20	0.0474	9.96
5	0.6	1.6	1.30	18.70	0.0480	15.13
6	0.9	2.5	2.05	17.95	0.0490	23.17
7	1.5	4.0	3.25	16.75	0.0508	40.04
8	2.0	6.0	5.00	15.00	0.0537	56.44
9	2.0	8.0	7.00	13.00	0.0576	60.54
10	2.0	10.0	9.00	11.00	0.0627	65.90
11	2.0	12.0	11.00	9.00	0.0693	72.83
12	2.0	14.0	13.00	7.00	0.0785	82.50
13	2.0	16.0	15.00	5.00	0.0929	97.63
14	2.0	18.0	17.00	3.00	0.1000	105.10
15	2.0	20.0	19.00	1.00	0.1000	105.10

Δx = Thickness of slice along x-axis.

x = Distance from the point (20,0)

X = 20-x

$C_{x,o,\infty}$ = Steady state concentration by eqn. 4.1

M = Pollutant mass of the pulse, per 1 cm in z direction and is given by

Δt = 30 sec

$$M = \frac{q}{5} \frac{\Delta x}{U} \cdot C_{x,o,\infty}$$

(5M) replaces ($q C_o \Delta t$) in eqn. 4.4.

TABLE - 5.5.

SAMPLE CALCULATIONS OF CONCENTRATIONS FROM DIFFERENT PULSES AT (20,0) [Using eqn 4.4]
$\alpha_y = 0.024$ cm ; $\alpha_x = 0.36$ cm ; Units for concentrations % by wt. x 10^3.

Pulse[x] / t sec	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Total	$\frac{C}{C_{20,0,\infty}}$
30	0.1	0.3	0.7	1.4	3.5	9.0	22.1	18.0	2.2	0.1	0	0				57.4	1.28
60	0	0	0	0.1	0.2	0.7	3.2	11.5	16.6	10.7	3.1	0.4	0	0	0	46.5	1.03
90				0	0	0.1	0.3	1.7	5.8	11.2	12.7	8.5	3.5	0.7	0.1	44.6	0.99
120						0	0	0.2	1.0	3.3	7.4	11.3	11.9	7.6	3.0	45.7	1.01
150								0	0.1	0.6	2.0	5.0	9.4	11.6	9.6	38.3	0.85
180									0	0.1	0.4	1.3	3.6	6.8	9.2	21.4	0.48
210										0	0.1	0.2	0.9	2.3	4.5	8.0	0.18
240											0	0	0.2	0.6	1.4	2.2	0.05
270													0	0.1	0.3	0.4	0.01
300														0	0.1	0.1	0

[x] Ref. Table 5.4.

TABLE -5.6

INVERSE BREAK THROUGH VALUES (Also Vide Fig. 5.6)

Run No.	X cm	t sec	$C/C_{x,o,\infty}$	
			Obtained by[x] Pulse tech. model	Experimental
12	20	30	1.000	1.022
12	20	70	1.000	0.967
12	20	155	0.790	0.900
12	20	220	0.130	0.144
12	40	50	0.970	1.027
12	40	88	0.940	0.972
12	40	173	0.850	0.797
12	40	240	0.720	0.554
12	40	340	0.450	0.446
13	20	40	0.939	1.000
13	20	100	0.170	0.232
13	20	190	0.000	0.007
13	40	60	0.655	0.431
13	40	135	0.397	0.328
13	40	215	0.017	0.017

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[x] From interpolated smooth curve.

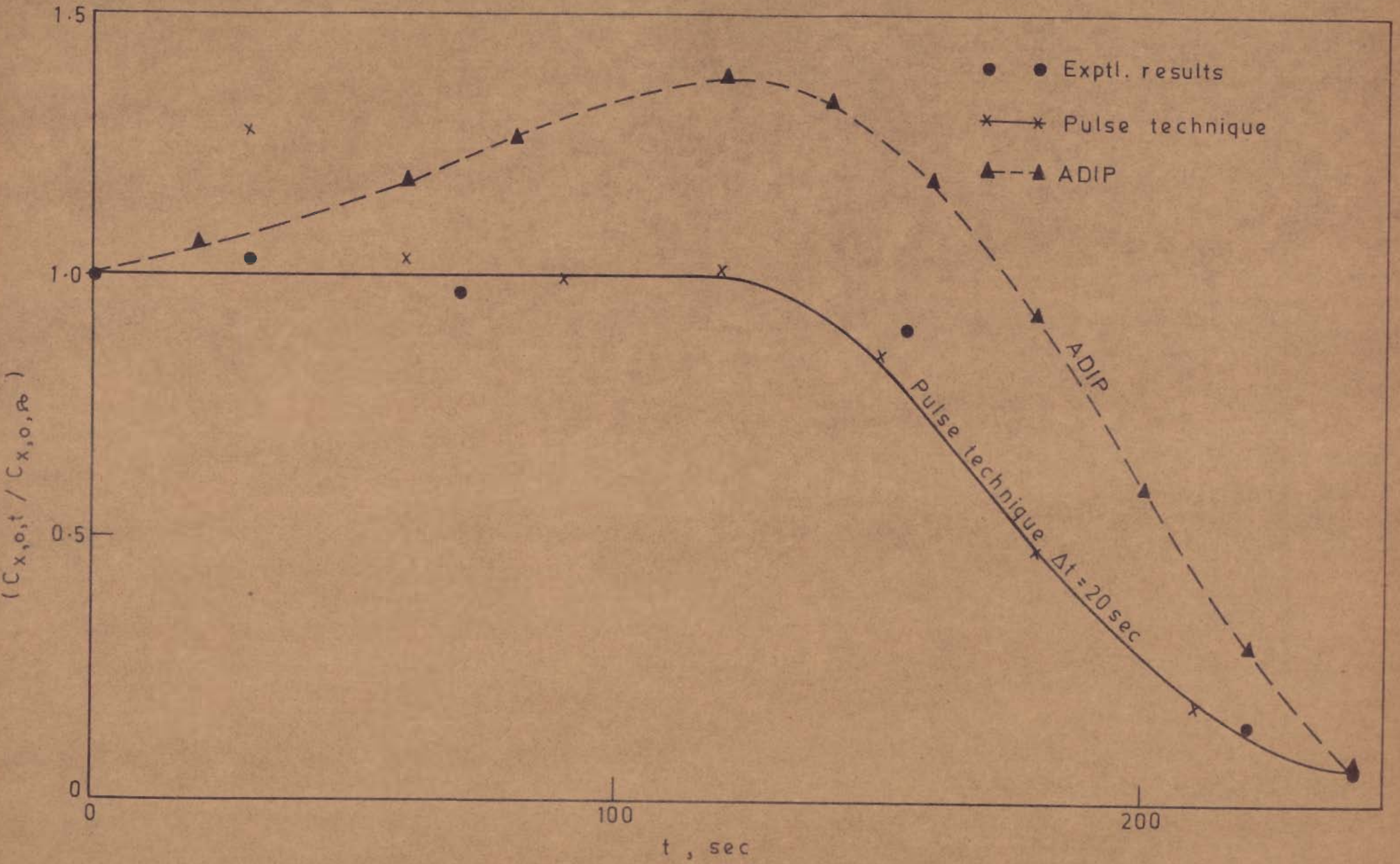

FIG. 5·4 – I B T CURVES FOR RUN 12 (x = 20 cm)

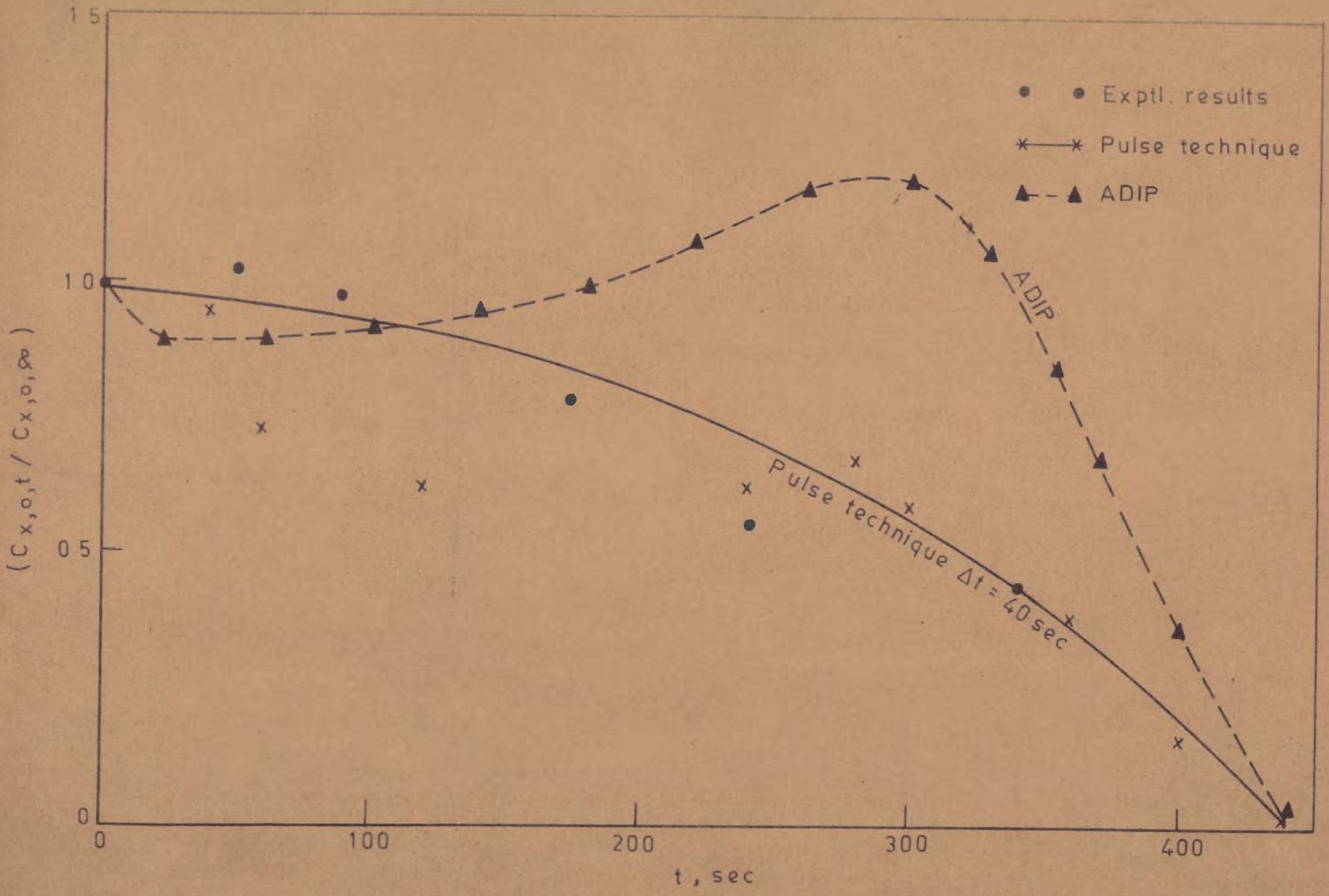

FIG. 5.5 – I B T CURVES FOR RUN 12 (x = 40 cm)

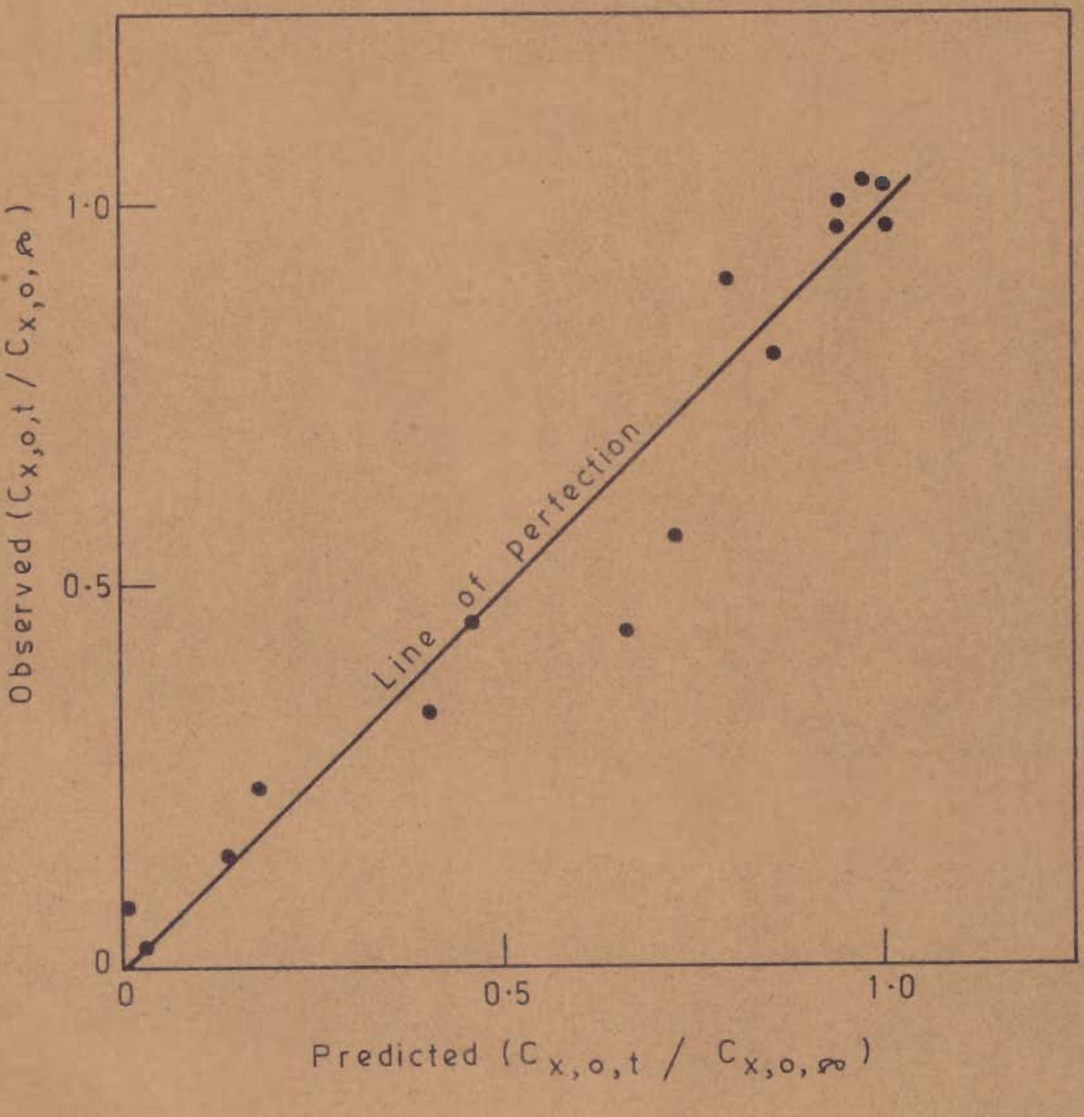

FIG. 5·6 – I B T CONCENTRATIONS (RUNS 12 & 13)

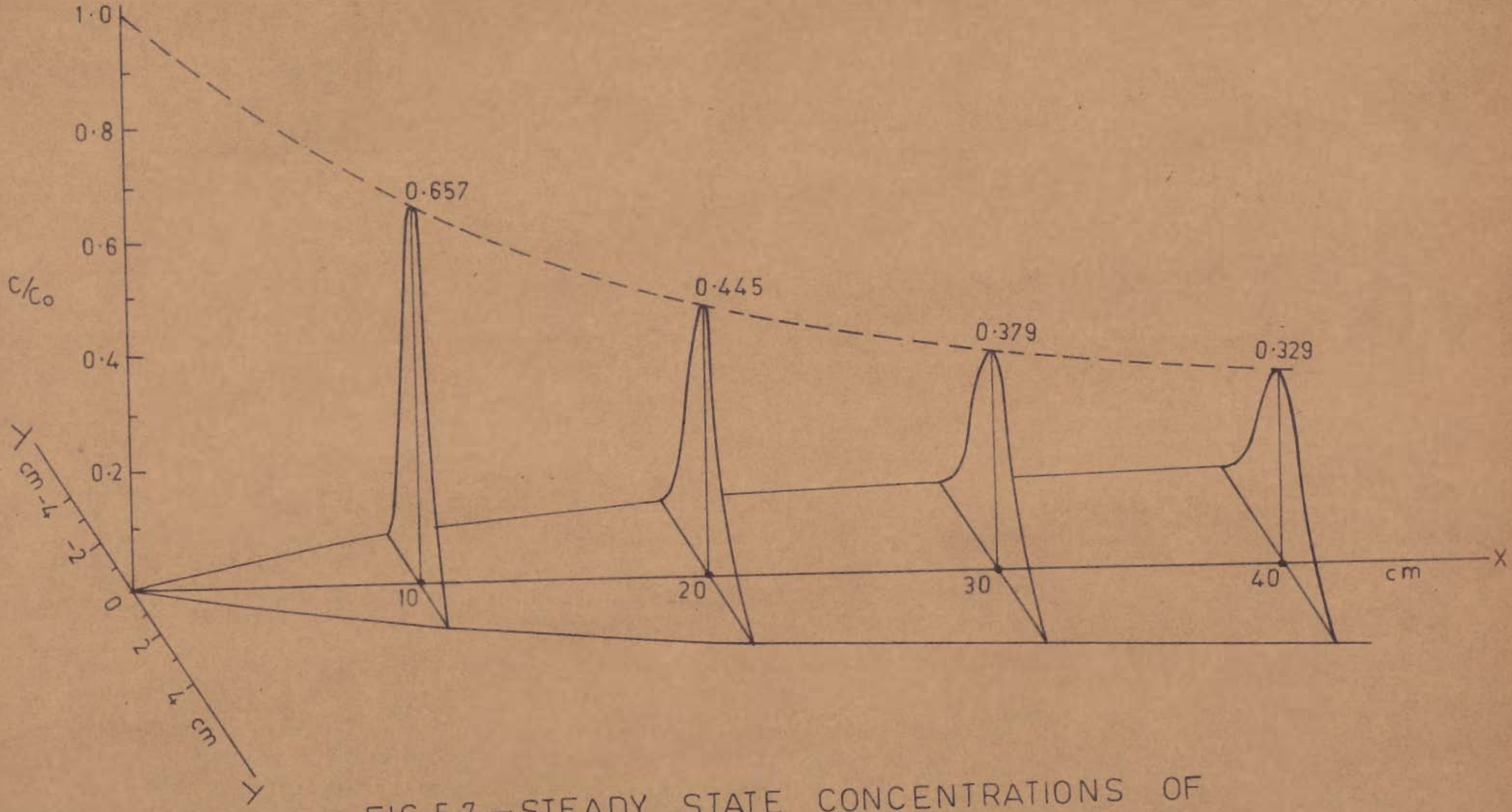

FIG.5·7 – STEADY STATE CONCENTRATIONS OF POLLUTANT IN 2-D DISPERSION (RUN 12)

CHAPTER VI

ANALYSIS OF DATA

NON CONSERVATIVE POLLUTANT

CONTENTS

6.1 EVALUATION OF APPARENT α_y

The steady state concentrations of E. coli at selected axial distances from the injection point, and the computed functional parameters of eqn. 4.1 have been shown in Table 6.1. A linear regression between the functional parameters of eqn. 4.1 has yielded a slope = 0.0146 (Vide Fig. 6.1), from which the value of the apparent α_y = 2.385 cm (Vide eqn. 4.1).

From Fig. 6.1, it is seen that the scatter of experimental results about the regression line is wider, than in the case of the conservative pollutant. The following reasons for the wider scatter are plausible.

(i) Though the death rate in the pollutant feed has been negligible during the runs, considered for steady state concentrations, the death rate of a higher magnitude within the porous medium can not be ruled out, as mechanical injury to the delicate cells during advection among the soil grains can be fatal to the cells. This hypothesis is substantiated by the observed concentrations being lower than expected, in cases of larger x and Q, with larger potential for injury. However, the data is inadequate to prove this contention.

(ii) The laboratory techniques for measuring bacterial concentrations have inherent limitations, that reflect on

TABLE -6.1

EVALUATION OF APPARENT α_y

Run[x] No.	q ml/sec	C_o nos/ml	Q ml/sec	x cm	$C_{x,o,\infty}$ nos/ml	$\frac{C_{x,o,\infty}}{C_o}$	$\frac{q}{Q\sqrt{x}} \times 10^3$
1	1.656	3.5	48.68	20	0.80	0.229	7.607
	1.656	3.5	48.68	40	0.14	0.040	5.379
2	1.074	235	48.05	20	20.00	0.085	4.998
3	0.379	170	29.33	60	2.00	0.012	1.668
4	0.639	500	62.80	40	8.00	0.016	1.609
	0.639	500	62.80	60	5.00	0.010	1.314
5	0.469	400	46.00	20	9.00	0.023	2.280
	0.469	400	46.00	40	8.00	0.020	1.612
	0.469	400	46.00	60	5.00	0.013	1.316
6	0.504	83	35.10	20	5.00	0.060	3.211
8[xx]	0.382	425	23.43	20	25.00	0.059	2.132
	0.382	425	23.43	60	11.00	0.026	3.211

[x] Vide Table I-3 and I-5 Appendix I.

[xx] Approximate steady state values neglecting input variations.

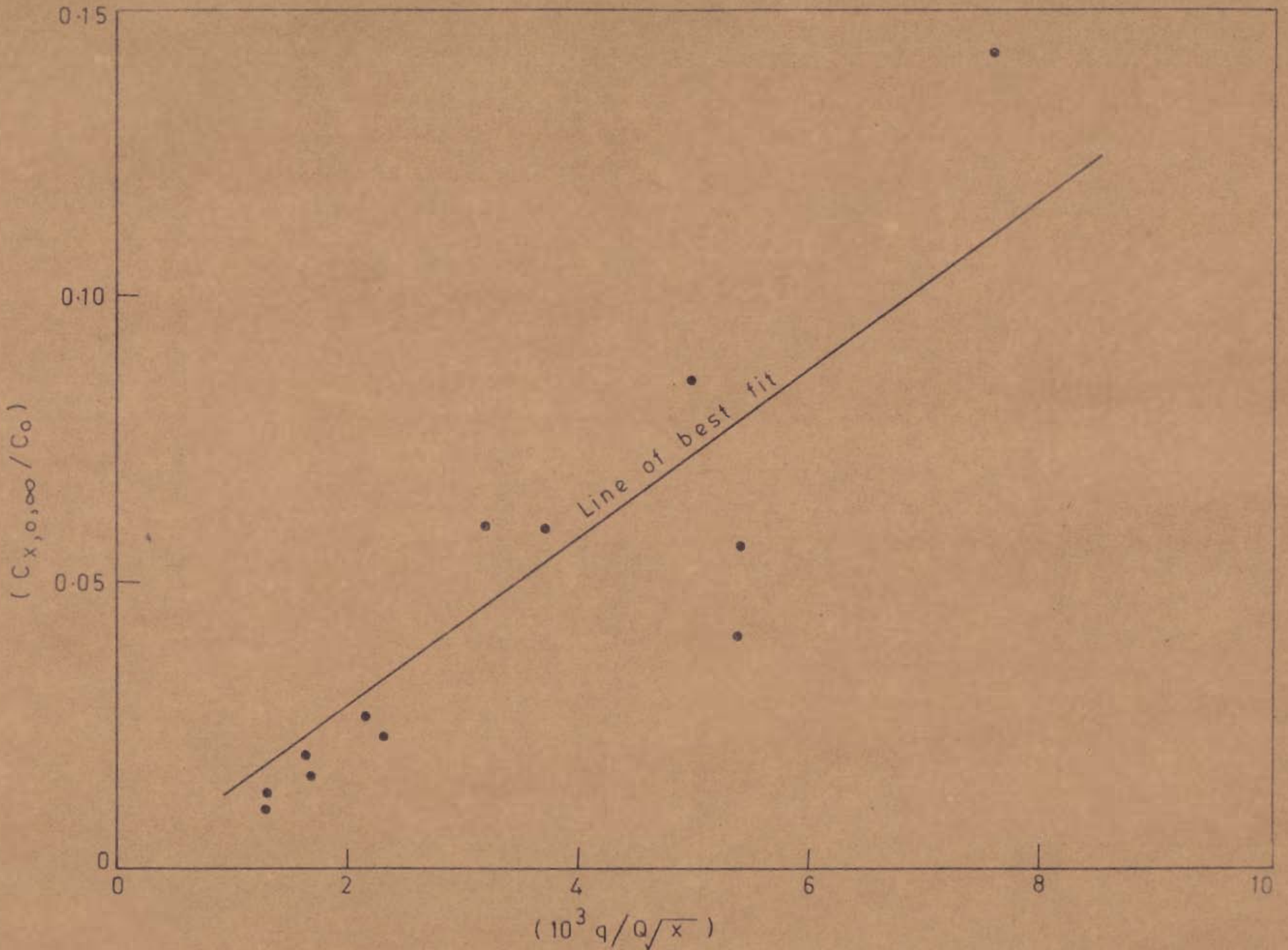

FIG. 6·1 – EVALUATION OF APPARENT α_y (E. Coli) the relative accuracy, in contrast to the measurement of chemical concentrations.

(iii) Inconsistent clustering of E. coli can influence the count, causing some error.

In spite of the limitations cited above, as well as the limitations inherent in modeling the dispersion of bacteria (Vide Sec. 4.4), the correlation coefficient between the functional parameters of eqn. 4.1 has worked out to 0.92, which is satisfactory.

Considering all the factors, mentioned above, the conformity, of the steady state concentrations of E. coli with eqn. 4.1, is fairly acceptable.

Equation 4.1 implies an average pore velocity of the pollutant, equal to that of the carrier fluid. The macroscopic averaging of the microscopic variations of the individual fluid particle velocities, holds good for a conservative pollutant as well, but in the case of a non-conservative pollutant, the physical significance of average velocity is ambiguous. For example, some E. coli cells may be retained on the soil particle surfaces, by adsorptive forces till their death, while on the other hand some other cells may be carried away by the fluid particles of the largest velocity. Earlier works, dealing with dispersion of pollutants in the presence of linear adsorption, have suggested a retardation factor R_d[85,65,33], so that U can be replaced by U/R_d in the analysis. However, this is not a satisfactory theoretical answer to the case of adsorption of E. coli and it's influence on their dispersion.

In this study R_d has not been evaluated and the pore velocity as implied in eqn. 4.1 is that of the carrier fluid only, and hence the influence of adsorption gets incorporated into the value of apparent α_y. Thus, α_y ceases to be a function of the pore geometry alone, as it happens to be in the case of a conservative pollutant. The utility, of the concept of the apparent α_y for bacteria, has been examined in this study and the results are not disappointing as can be seen in the sections to follow. This concept of apparent dispersivity, delinked with the actual average velocity of the pollutant species, is very convenient as the average velocity of a non-conservative pollutant is a vague concept and cumbersome to evaluate, even if it were to be defined, arbitrarily, as the velocity of the centre of gravity of the pollutant flux for an instantaneous mass injection, which coincides with the pore velocity in the case of a conservative pollutant.

6.2 EVALUATION OF APPARENT α_x

The procedure followed (Vide Sec. 4.2), in the case of the conservative pollutant, for the evaluation of α_x

requires the availability of sufficiently large data, for reasons discussed in Sec. 5.2. In the case of bacterial pollutant, large data, of transient concentrations with steady inputs, is extremely difficult, for the following reasons.

(i) The concentration of the input pollutant is subject to an inevitable natural death rate, and some decay of the input concentration with time, is unavoidable.

(ii) Equilibrium adsorption of bacteria by the porous medium can be attained only after some time, often overlapping the transient phase.

(iii) Death of bacteria, by injury and by shock of the new environment can occur soon after the injection into the porous medium.

(iv) Clogging in the immediate vicinity[46] of the injection point in the porous medium, reduces the injection rate, unless the injection head increases in tune, which is extremely difficult to attain in an experiment.Under these conditions, the only way, for experimental evaluation of α_x, is to collect large data, monitoring all the relevent parameters and obtain α_x by [illegible] inverse methods as suggested by Anjad[5], Murty and Scott[60], using the analytical equations, with a suitable optimization technique. This procedure is cumbersome and is not attempted here.

Because of these limitations, the apparent α_x for E. coli has been obtained indirectly from the (α_x/α_y) ratio as mentioned in Sec. 3.6.1 - (iv).

Based on this, the apparent α_x for E. coli

$= \alpha_x/\alpha_y$ for Sodium chloride x α_y for E. coli.

$= 15 \times 2.385 = 35.775$ cm.

However this method of evaluating the apparent α_x is subject to some error as the concept of 'apparent dispersivity' employed in this work, is not a function of the property of the porous medium alone. In this connection, it is partly relieving to note that errors in α_x have decreasing impact with increasing time, till the errors become insignificant, in the estimation of steady state concentrations (Vide eqn. 3.14). In the only available earlier report on axial dispersion of E. coli through porous media, Grewal[24] has reported longitudinal dispersion coefficients for different bacterial velocities. The values of α_x computed from his findings range between 4.36 to 13.13 cm for sands with d_{50} from 0.0395 cm to 0.0695 cm. Thus α_x evaluated in this study, is about 4 times larger, than the average value of Grewal. This discrepency may be the result of the following differences between the two studies.

Grewal's[24] study	Present study
i) Experimental model was one dimensional.	Two dimensional
ii) Sampling was by suction with needle and syringe.	Collection trhough tapping.
iii) High concentrations of <u>E. coli</u> were run with reported mat formation between injection and samplings.	Only low concentrations were employed.
iv) Pollutant solution was not devoid of nutrients, enabling multiplication of cells within the porous medium.	Multiplication was ruled out by employing washed cells in nutrient free water.
v) Velocity of pollutant was the estimated velocity of the centre of gravity of the pollutant flux.	Equal to the average pore velocity.
vi) α_x was computed directly from experimental results.	Evaluated indirectly from α_x/α_y ratio of a conservative pollutant.

The approximate ratios of the time bases for break throughs and the dispersivities for conservative pollutant and bacterial pollutant, observed in this study, are of the same order as reported by Grewal[24].

6.3 BREAKTHROUGH CURVES (STEADY INPUT)

With the apparent values of α_y and α_x for E. coli, the breakthroughs have been computed by analytical and pulse technique methods, following the same procedures as for the conservative pollutant. The results for Run 7 are shown in Table 6.2 and a graphical plot of the same is shown in Fig. 6.2. From this figure it is apparent that the pulse technique solution for the breakthrough of E. coli for run no. 7 agrees fairly with the analytical solution. The experimental values, only two in number are comparitively low, as expected, since qC_0 is treated as a constant in the analytical and pulse technique solutions while it has been decreased with time during the run. Variation in the input magnitudes, with time, has been considered in the following section, for the same run.

6.4 BREAK THROUGH CURVES (UNSTEADY INPUT)

6.4.1 Unsteady Injection of Pollutant Without Death Rate

Experimental results of break through at a selected axial distance, due to an unsteady pollutant injection neglecting death rate of E. coli, have been shown in Table I-4 Appendix I. The break through for this run, has been computed by the pulse technique explained in Sec. 4.3, the results of which, are shown in Table 6.3 and Fig. 6.4.

From this figure, the concurrence of the trend of the experimental values, with the pulse technique solution is

TABLE -6.2

BREAKTHROUGHS FOR E. COLI

(Vide Table I-4 Appendix I)

Data : $Q = 37.76$ ml/sec
$q = 0.304$ ml/sec (approx) $C_o = 8000$ no /ml
$x = 40$ cm ; $U = 0.205$ cm/sec
$\alpha_y = 2.39$ cm; $\alpha_x = 35.78$ cm
Δt for pulse technique = 100 sec.

t sec	$C_{x,o,t}/C_{40,0,\infty}$	
	Analytical	Pulse technique
100	0.305	0.327
200	0.508	0.523
300	0.627	0.640
400	0.708	0.718
500	0.767	0.772
600	0.812	0.811
700	0.846	0.840
800	0.874	0.862
1000	0.914	0.893
2000	0.985	0.940

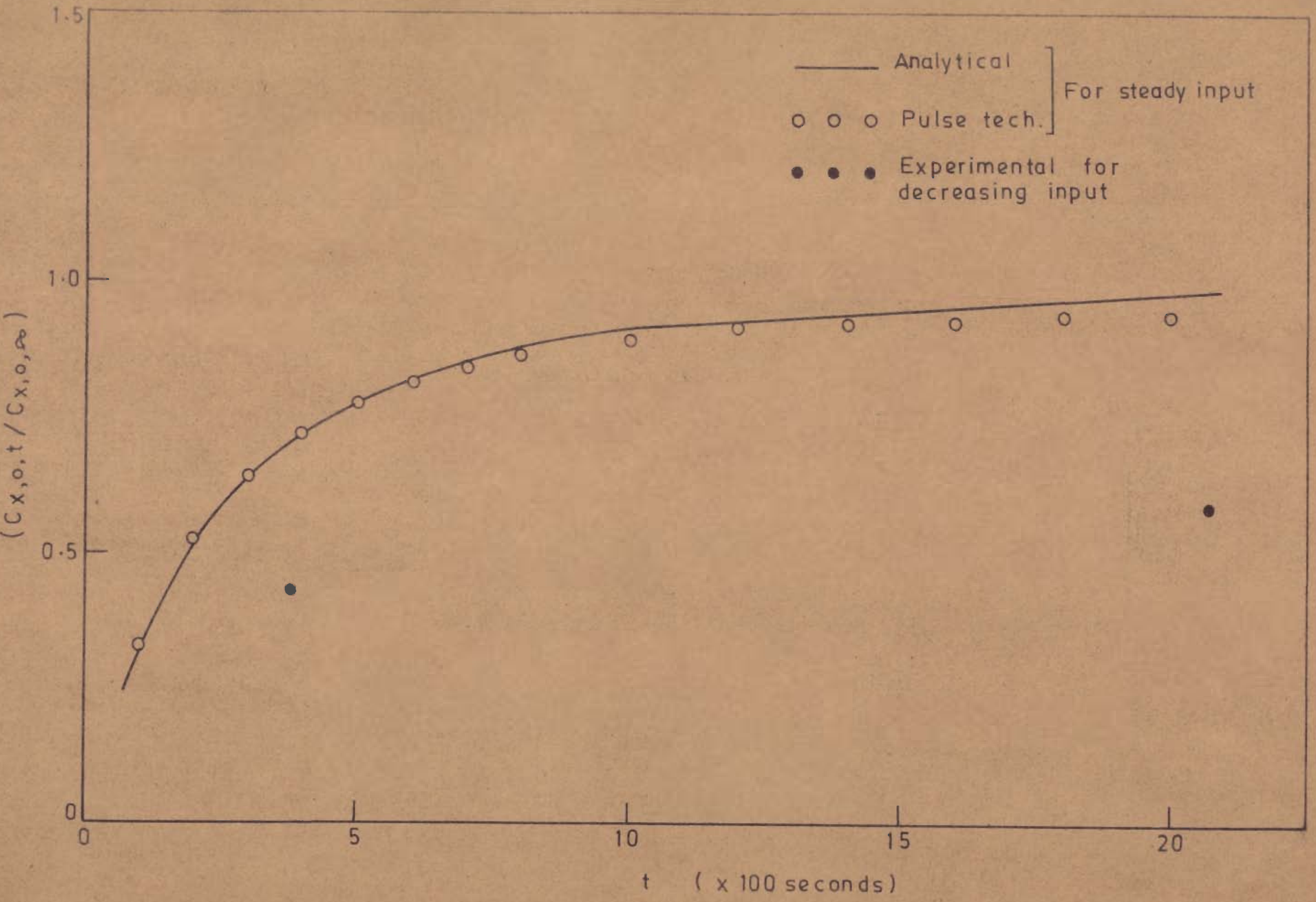

FIG. 6·2 — BACTERIAL BREAK THROUGHS (RUN 8)

TABLE -6.3

COMPUTATION OF BREAKTHROUGH FOR UNSTEADY INPUT NEGLECTING DEATH RATE

(Vide TABLE I-4 Appendix I)

Data : C_o = 8000 no/ml

$U = 0.205$ cm/sec ; $x = 40$ cm

$\alpha_y = 2.39$ cm ; $\alpha_x = 15\,\alpha_y$

$\Delta t = 5$ min. ; q-vs-t as in Fig. 6.3

t min	$C_{x,o,t}$ no/ml by pulse tech.
7.5	58.2
17.5	86.3
27.5	87.5
37.5	85.5
47.5	83.3
67.5	80.0
87.5	78.1
107.5	76.2
127.5	74.7
157.5	72.6
187.5	70.7
222.5	68.7
262.5	67.0
307.5	65.0
387.5	62.7

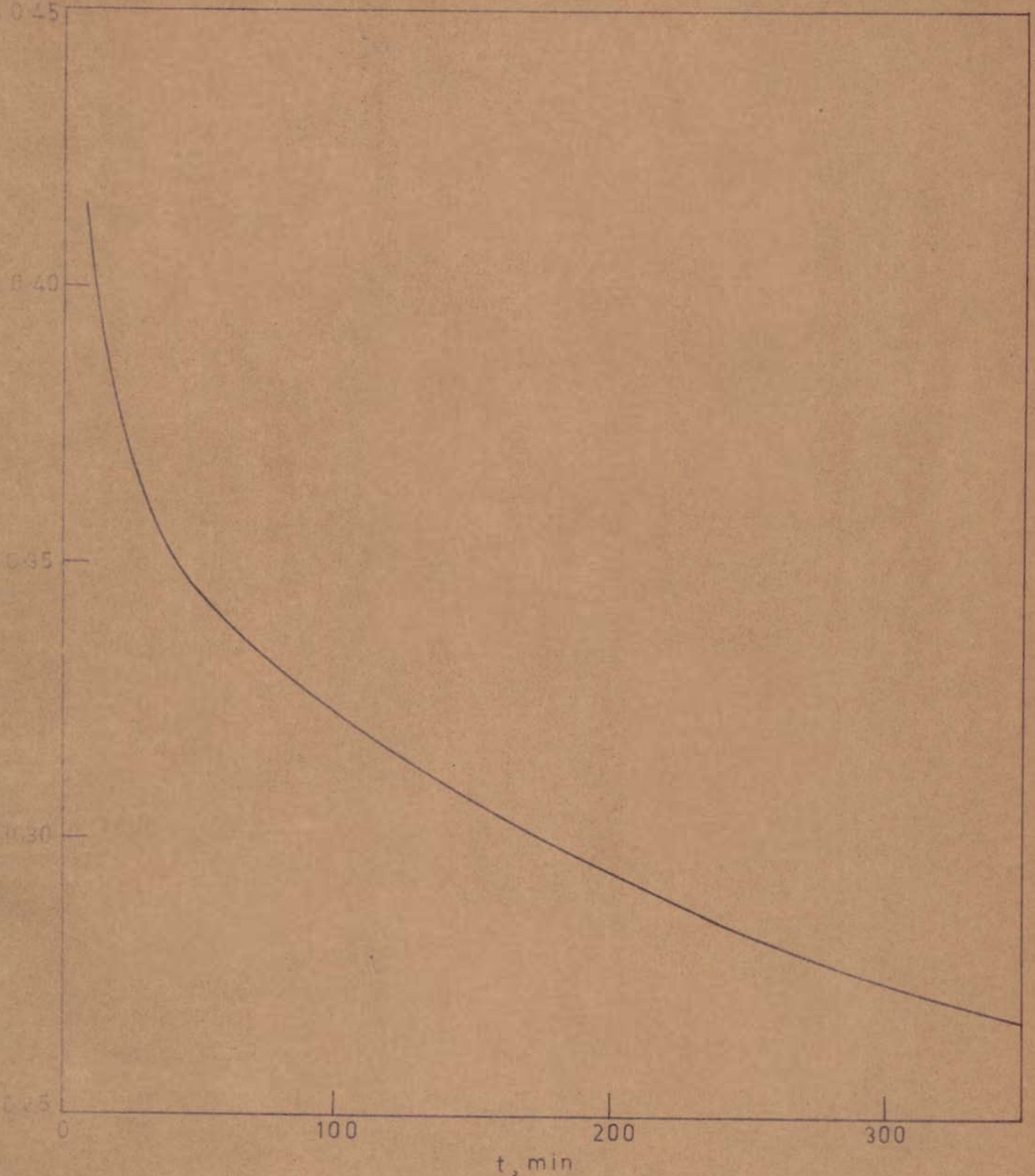

FIG. 6.3 - POLLUTANT INJECTION RATE VS TIME (RUN-7)

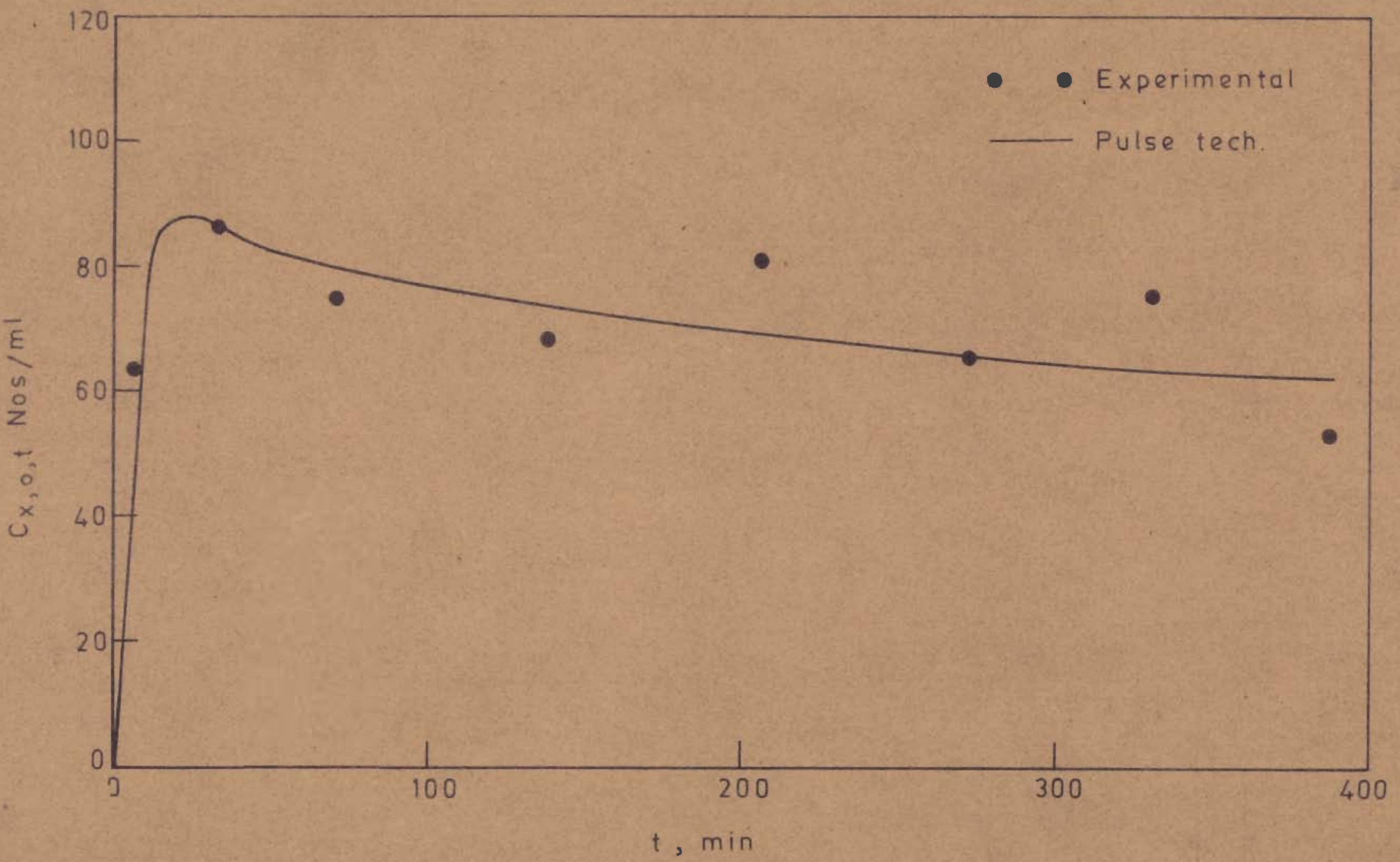

FIG. 6·4 – BACTERIAL BREAK THROUGH (UNSTEADY INPUT-RUN 7) apparent in spite of the scatter of the experimental values. The scatter may be attributed to (i) the experimental limitations in the enumeration of bacteria, (ii) the limitations in the concepts of apparent α_x and apparent α_y as discussed in Sec. 6.2, (iii) the limitations in modeling the bacterial dispersion as discussed in Sec. 3.

6.4.2 Unsteady Injection of Pollutant with Death Rate

The natural death rate of E. coli is too small (of the order of 20% per day) to monitor in an experimental run of a few hours duration. Hence the water used in the experiment was chlorinated in Run No. 8 (Vide Table I-5, Appendix I), to induce a higher death rate. Computed break through, using the pulse technique, (Vide Sec. 4.3) is shown in Table 6.4 and Fig. 6.6.

From this figure it is seen that, the general trend of the experimental results conforms with the pulse technique solution. The apparent discrepencies between the experimental and pulse technique break through (Vide Fig. 6.6) is not unexpected for the following reason.

The death rate of E. coli has been taken as a constant to conform to the linear death rate requirement in eqn. 4.4. In practice, a retarded death rate, with λ decreasing with time is more common. A higher λ in the initial phase of the break through will increase the slope of the curve because

TABLE -6.4

COMPUTATION OF BREAKTHROUGH FOR UNSTEADY INPUT WITH DEATH RATE

(Vide TABLE I-5 Appendix I)

Linear death rate is assumed according to $(C_o)_t = (C_o)_o x\ e^{-\lambda t}$

Evaluated results $(C_o)_o$ = 880 no /ml

λ = 0.0059/min

t = time in min.

Data : U = 7.56 cm/min ; α_y = 2.39 cm

$\alpha_x = 15\ \alpha_y$; x = 40 cm

Δt = 1.0 min q_t-vs-t as in Fig. 6.5.

t min	$C_{x,o,t}$ no /ml (By pulse tech.)
5	17.4
10	24.2
20	28.5
30	28.8
40	25.8
50	23.0
80	17.6
100	15.5
120	13.6
140	11.9
180	9.3

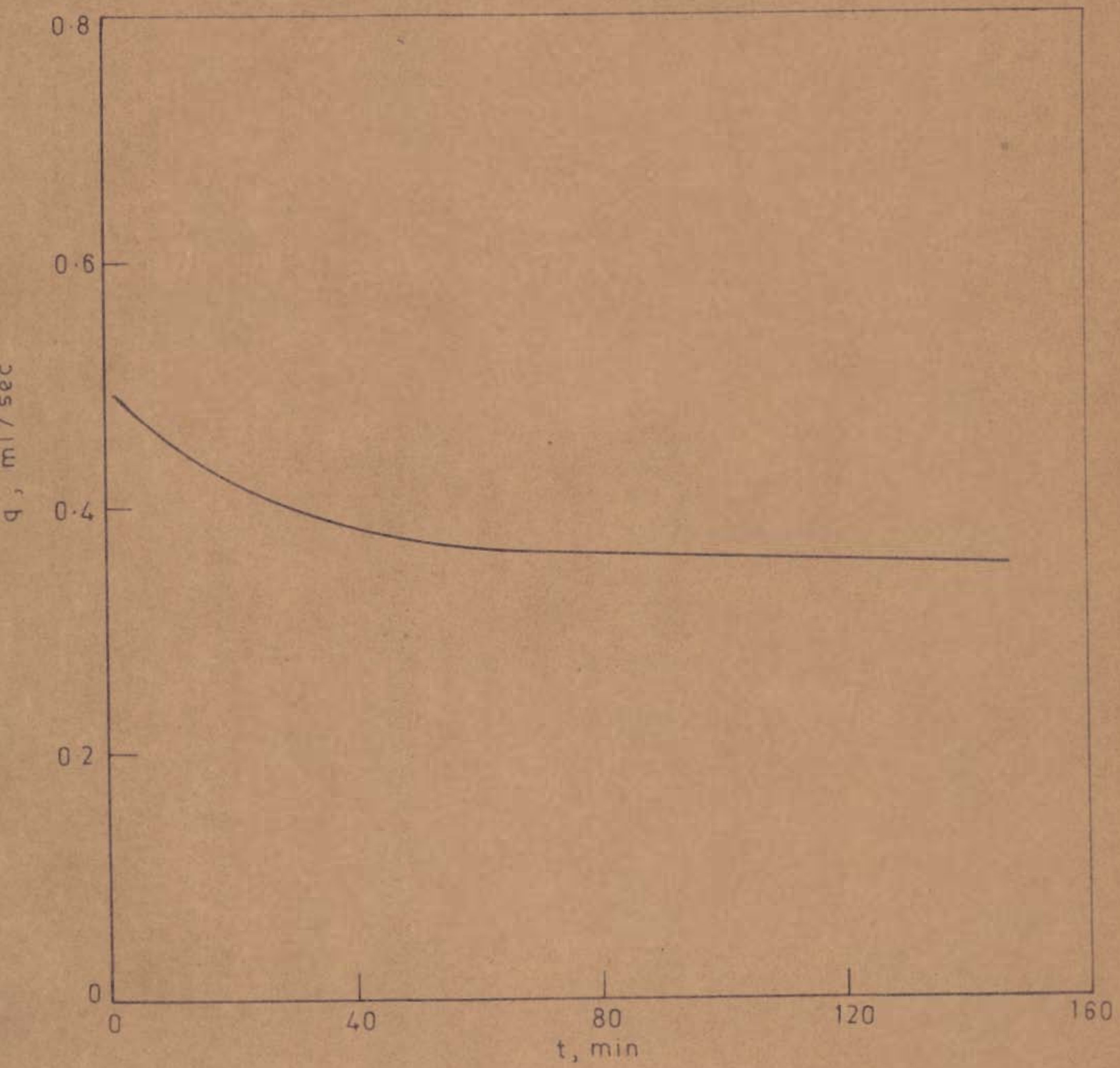

FIG. 6·5–POLLUTANT INJECTION RATE VS TIME (RUN-8)

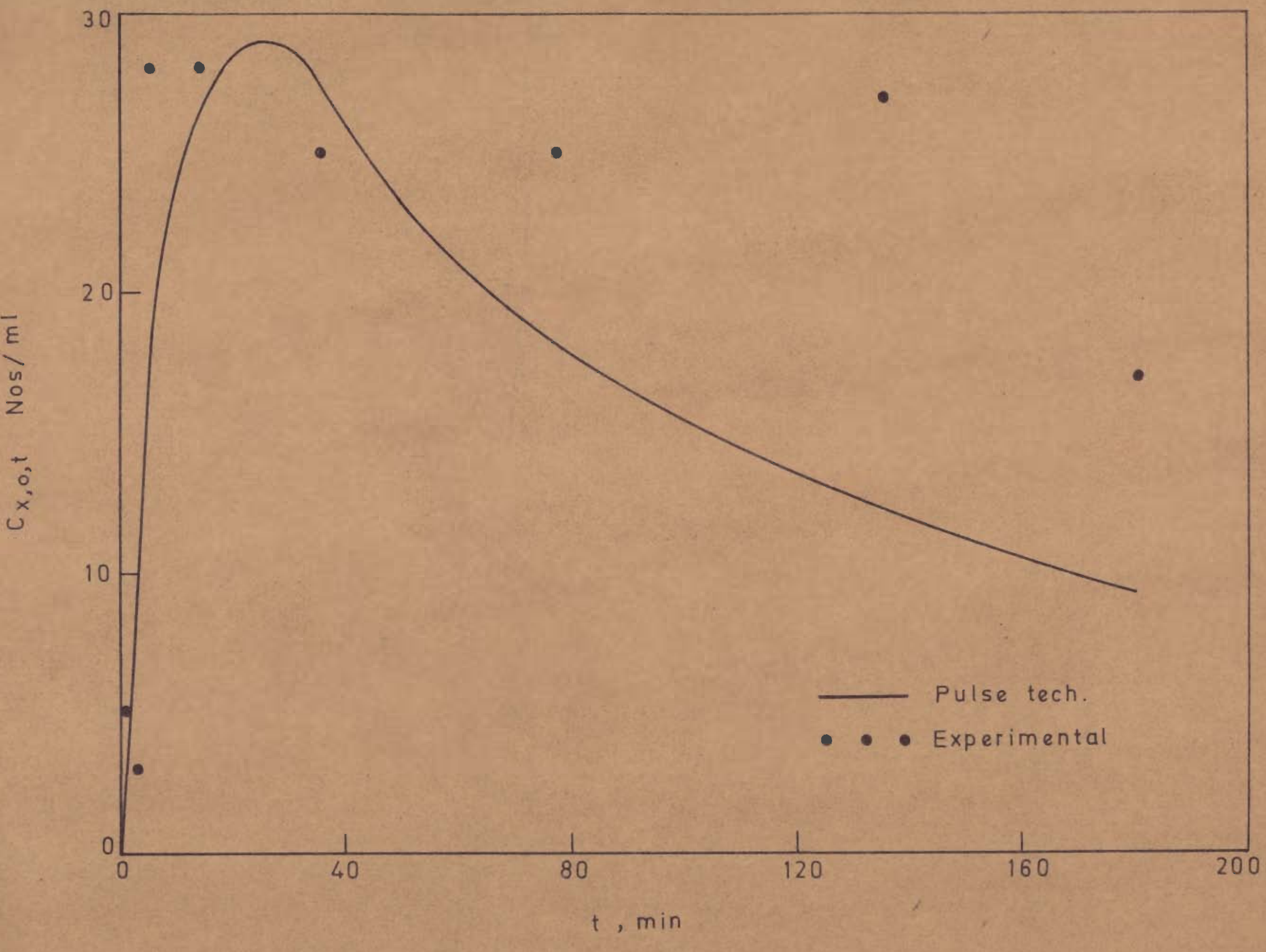

FIG. 6·6 – BACTERIAL BREAK THROUGH (UNSTEADY INPUT RUN 8) of a higher $(C_o)_o$ value while, a lower λ in the latter part of the break through will decrease the slope of the curve, as can be seen from eqn. 4.4. Thus the discrepency arising out of the assumption of a linear death rate for E. coli can explain the discrepency between the observed and pulse technique values in Fig. 6.6.

In view of these considerations, the pulse technique solution may be considered to be reasonably validated. ~~The~~

The acceptable degree of conformity of the pulse technique break throughs for unsteady, bacterial pollutant inputs, with the experimental values (Vide Secs. 6.4.1 and 6.4.2) validate, to a high degree of probability, the following concepts implied in the modelling and computational methods followed in this section.

(i) The concept of an apparent dispersivity, delinked from the actual 'average velocity' of the pollutant species, for a non-conservative pollutant.

(ii) Applicability of the analytical solutions, intended for non conservative chemical pollutants, to bacterial pollutants as well.

(iii) α_x/α_y being treated as a constant for a given medium, even for bacterial pollutants.

(iv) Workability of the simple pulse technique for complex pollutant input conditions along with adsorption in

2-dimensional dispersion through porous media flows, for which the corresponding analytical and numerical methods are much more complex with no assurance of better accuracies.

(v) Linear adsorption model for bacteria at low concentrations, advected through porous media. and

(vi) Permeability of a porous medium remaining unaffected by the dispersion of low concentrations of bacteria without ambient nutrition [With alterations in permeability U will change during a run, affecting the results. The consistency of permeability during a run is also evidenced by experimental observations (Vide Table I-3, 4 and 5 Appendix I)]

CHAPTER VII

SUMMARY AND CONCLUSIONS

CONTENTS

7.1 CONSERVATIVE POLLUTANT

Based on the results and discussions presented in Chapter V, it may be summarized and concluded as follows, with respect to the conservative pollutant studied in this work, namely Sodium chloride.

7.1.1 Summary

(i) Lateral and longitudinal dispersivities of a homogeneous, isotropic porous medium have been evaluated from experimental results on a two-dimensional laboratory model, for a saturated and uniform seepage condition.

(ii) Using the evaluated dispersivities, break throughs have been computed by

a) analytical solutions

b) pulse technique

and c) (modified ADIP) numerical algorithm

and they have been compared with experimental results.

(iii) A theoretical model for the inverse break through (IBT), at an axial point has been proposed.

(iv) The IBT model has been worked out by

a) (modified ADIP) numerical algorithm

and b) pulse technique

and the solutions have been compared with experimental results.

7.1.2 Conclusions

(i) The evaluated α_y (lateral dispersivity) and α_x (longitudinal dispersivity) are 0.024 cm and 0.36 cm respectively while the ratio α_x/α_y is 15, for the porous medium in the study. (d_{50} = 0.055 cm, U.C = 1.3 and porosity = 0.46).

(ii) For a concentration break through at an axial distance, the pulse technique solution converges with the analytical solution efficiently, with even reasonably large pulse sizes, that enable computation, without a digital computer.

(iii) The modified ADIP algorithm given in Appendix II is simpler and saves computer time if, axial concentrations alone are required. Though a stable, solution is expected, the algorithm requires the optimization of grid density for satisfactory convergence.

(iv) Pulse technique is simpler and more accurate than modified ADIP for obtaining break throughs, with the initial and boundary conditions considered in this study.

(v) The IBT model proposed in this study predicts the concentration decay, at an axial point on the sudden cessation of the pollutant input during a steady state, with a reasonable degree of accuracy.

(vi) The modified ADIP algorithm for the IBT model, given in Appendix III, gives a solution that is stable but needs the optimization of the time and space steps for satisfactory convergence.

(v) Pulse technique is simpler and more accurate than modified ADIP for predicting the IBT at an axial location.

7.2 NON CONSERVATIVE POLLUTANT

The summary and conclusions following from the results and discussions in Chapter VI, with respect to a non conservative pollutant, namely *E. coli* are given below.

7.2.1 Summary

(i) The apparent longitudinal and lateral dispersivities of a homogeneous, isotropic porous medium have been evaluated from experimental results on a two dimensional laboratory model, for saturated and uniform seepage condition.

(ii) Using the evaluated apparent dispersivities, break throughs have been computed by

a) analytical solutions and

b) pulse technique

and have been compared with experimental results.

(iii) Pulse technique solutions for the break throughs have been obtained with

a) variable input, with bacterial death rate neglected,

and b) variable input, with also a linear bacterial death rate and they have been compared with experimental results.

7.2.2 Direct Conclusions

(i) The evaluated apparent lateral dispersivity, α_y is 2.385 cm and with (α_x/α_y), assumed to be the same as for a conservative pollutant, the apparent longitudinal dispersivity $\alpha_x = 35.775$ cm for the porous medium in the study ($d_{50} = 0.055$ cm, U.C. = 1.3 and Porosity = 0.46.)

(ii) With the evaluated apparent α_x and α_y the pulse technique break through converges with the analytical solution efficiently, even with reasonably large pulse sizes, that enable computation without a digital computer.

(iii) The pulse technique solution compares favourably with the experimental results in the following cases.

a) Pollutant injection rate changes with time and death rate of bacteria is negligible.

and b) Pollutant injection rate changes with time and a linear death rate of bacteria is considered.

7.2.3 Indirect Conclusions

The conclusions, given below, follow indirectly from this study.

(i) Bacterial pollutants, at low concentrations are amenable to the theoretical treatment relevent to non-conservative chemical pollutants.

(ii) The apparent dispersivity values, delinked from the actual velocity of the centre of gravity of the pollutant flux, enable reasonably accurate predictions of pollution plumes.

(iii) The dispersivities and the time base for the break through are considerably larger for bacteria than for the conservative pollutant.

(iv) α_x/α_y ratio for a given porous medium can be taken as equal for conservative and non-conservative pollutants.

(v) Linear-adsorption-rate assumption is fairly valid for bacterial pollutants, at low concentrations.

(vi) Linear death rate of bacteria can be assumed with reasonable accuracy, though (non-linear) decreasing death rate appears to be better for predicting the dispersion of bacteria.

(vii) At low concentrations, nutrient-free-bacterial pollutants have no significant influence on the permeability of the porous medium, during their advection by seepage.

CHAPTER VIII

SUGGESTIONS FOR FURTHER STUDY

SUGGESTIONS FOR FURTHER STUDY

Based on the experience of this study the following suggestions have been listed out, for any further work in this area of investigation.

(1) Numerical algorithms have to be developed to evaluate the dispersivities from observed data with unsteady pollutant inputs and non-linearities in the functional relationships of the parameters, for non-conservative pollutants.

(2) Numerical algorithms are to be developed for solutions, incorporating the complex initial and boundary conditions, often encountered in field problems. For example, the expanding interface, at the point of injection during the transient phase, has to be included in the algorithm.

(3) Effects of density and viscosity changes, degree of saturation, nonuniformity of seepage flow, heterogenity and anisotropy of the porous medium and thermal convections within the porous medium are to be investigated in relation to the dispersion phenomena.

(4) Dispersion patterns for the common ground water pollutants, like pesticides, fertilizers, detergents, toxins, radioactive wastes, B.O.D., pathogenic virus, bacteria and cysts and spores, associated with human ill health, are to be investigated.

(5) Mat formation and clogging in the immediate vicinity of the pollutant injection area, needs to be investigated for effective theoretical modeling.

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APPENDIX I

SUMMARY OF EXPERIMENTAL DATA FOR SODIUM CHLORIDE AND *E. COLI* POLLUTANTS

TABLE I-1

EXPERIMENTAL RESULTS OF BREAKTHROUGHS FOR SODIUM CHLORIDE

Run No.	C_o % by wt.	q ml/sec	Q ml/sec	x cm	t sec	$C_{x,o,t}$ % by wt.	K cm/sec	T °C
1	1.0	0.582	35.70	20	60	0.000	0.59	18
	1.0	0.582	35.70	20	120	0.260	0.59	18
	1.0	0.582	35.70	20	240	0.300	0.59	18
	1.0	0.582	35.70	20	305	0.300	0.59	18
	1.0	0.582	35.70	40	205	0.025	0.59	18
2	1.0	2.460	40.00	40	110	0.000	0.55	16
	1.0	2.460	40.00	40	197	0.005	0.55	16
3	1.0	0.838	43.33	20	35	0.061	0.58	24
	1.0	0.838	43.33	20	95	0.240	0.58	24
	1.0	0.838	43.33	20	165	0.290	0.58	24
	1.0	0.838	43.33	40	190	0.036	0.58	24
	1.0	0.838	43.33	40	300	0.056	0.58	24
	1.0	0.838	43.33	60	320	0.004	0.58	24
4	0.1	0.183	42.00	20	35	0.003	0.59	24
	0.1	0.183	42.00	60	240	0.000	0.59	24
	0.1	0.183	42.00	60	390	0.004	0.59	24
5	0.1	0.608	56.70	20	30	0.000	0.60	24
	0.1	0.608	56.70	20	120	0.021	0.60	24
	0.1	0.608	56.70	20	215	0.023	0.60	24
	0.1	0.608	56.70	20	3000	0.033	0.60	24
	0.1	0.608	56.70	40	60	0.000	0.60	24
	0.1	0.608	56.70	40	180	0.008	0.60	24

Continued...

TABLE I-1 (contd.)

Run No.	C_o % by wt.	q ml/sec	Q ml/sec	x cm	t sec	$C_{x,o,t}$ % by wt.	K cm/sec	T °C
6	0.1	0.480	77.20	20	35	0.003	0.61	27
	0.1	0.480	77.20	20	120	0.020	0.61	27
	0.1	0.480	77.20	20	246	0.020	0.61	27
	0.1	0.480	77.20	40	180	0.014	0.61	27
	0.1	0.480	77.20	40	360	0.014	0.61	27
	0.1	0.480	77.20	60	90	0.000	0.61	27
	0.1	0.480	77.20	60	205	0.003	0.61	27
7	0.1	0.404	75.55	20	1200	0.019	0.61	27
	0.1	0.404	75.55	40	1230	0.013	0.61	27
	0.1	0.440	64.40	20	1200	0.023	0.60	27
	0.1	0.440	64.40	40	1230	0.016	0.60	27
	0.1	0.398	45.30	20	1200	0.030	0.60	27
	0.1	0.398	45.30	40	1230	0.021	0.60	27
	0.1	0.299	20.95	20	1200	0.045	0.60	27
	0.1	0.299	20.95	40	1230	0.037	0.60	27
8	0.05	0.407	58.80	20	30	0.004	0.53	26
	0.05	0.407	58.80	20	72	0.008	0.53	26
	0.05	0.407	58.80	20	165	0.011	0.53	26
	0.05	0.407	58.80	40	50	0.005	0.53	26
	0.05	0.407	58.80	60	128	0.002	0.53	26
9	0.1	1.112	59.20	20	35	0.002	0.45	15
	0.1	1.112	59.20	20	93	0.017	0.45	15
10	0.1	0.445	65.00	20	25	0.0007	0.59	33
	0.1	0.445	65.00	20	87	0.0004	0.59	33
	0.1	0.445	65.00	40	54	0.0003	0.59	33
	0.1	0.445	65.00	40	120	0.0005	0.59	33
	0.1	0.445	65.00	60	160	0.0005	0.59	33

Contd....

TABLE I-1 (Contd.)

Run No.	C_o % by wt.	q ml/sec	Q ml/sec	x cm	t sec	$C_{x,o,t}$ % by wt.	K cm/sec	T °C
11	0.1	0.453	22.80[x]	40	60	0.0007	0.36	29
	0.1	0.453	22.80	40	120	0.0007	0.36	29
	0.1	0.453	22.80	40	320	0.023	0.36	29
	0.1	0.453	22.80	40	480	0.045	0.36	29
	0.1	0.453	22.80	40	750	0.046	0.36	29
	0.1	0.453	22.80	40	900	0.048	0.36	29
	0.1	0.453	22.80	60	1200	0.038	0.36	29

[x] 0.1% by wt. Sucrose Solution.

TABLE I-2

EXPERIMENTAL RESULTS OF INVERSE BREAKTHROUGHS FOR SODIUM CHLORIDE

Run No.	Steady State			X cm	t sec	$C_{x,o,t}$ % by wt.
	C_o % by wt.	q ml/sec	Q ml/sec			
12	0.1	0.299	20.65	20	0	0.045
				20	30	0.046
				20	70	0.044
				20	155	0.041
				20	220	0.007
				20	330	0.000
				40	0	0.037
				40	50	0.038
				40	88	0.036
				40	173	0.030
				40	240	0.021
				40	340	0.017
13	1.0	0.546	43.33	20	0	0.410
				20	40	0.410
				20	100	0.095
				20	190	0.003
				40	0	0.290
				40	60	0.125
				40	135	0.095
				40	215	0.005

TABLE I-3

EXPERIMENTAL RESULTS OF BREAK THROUGHS FOR *E. COLI*

Run No.	q ml/sec	Q ml/sec	C_o no/ml	x cm	t mnts	$C_{x,o,t}$ no/ml	K cm/sec
1	1.656	48.68	3.5	20	1.0	0.80	0.70
				20	3.0	0.80	0.70
				20	5.0	0.50	0.70
				20	10.0	0.80	0.70
				20	25.0	0.63	0.70
				40	25.5	0.14	0.70
2	1.074	48.05	235	20	1.0	0.00	0.66
				20	2.1	20.00	0.66
				20	5.7	9.00	0.66
				20	10.3	20.00	0.66
				20	30.0	20.00	0.66
2A	0.706	48.05	235	20	50.0	16.00	0.66
3	0.379	29.33	170	60	220.0	2.00	0.67
4	0.639	62.80	500	40	38.8	8.00	0.71
				60	39.0	5.00	0.71
5	0.469	46.00	400	20	14.8	9.00	0.42
				40	399.0	8.00	0.34
				60	460.0	5.00	0.32
6	0.504	35.10	83	20	10.3	5.00	0.39

TABLE I-4

RUN No. 7

EXPERIMENTAL RESULTS OF BREAKTHROUGH (UNSTEADY INPUT) FOR *E. COLI* (DEATH RATE $\simeq 0$)

Q = 37.76 ml/sec

q = as shown in Fig. 6.3

C_o = 8000 no/ml (Assumed Constant)

x = 40 cm ; y = 0 cm

Ambient temperature 30° C

t min	$C_{x,o,t}$ no/ml	K cm/sec
6.4	64	0.35
34.5	86	0.35
70.3	75	0.35
139	68	0.35
206	86	0.35
270	66	0.35
330	76	0.35
387	53	0.35

TABLE I-5

RUN No. 8

EXPERIMENTAL RESULTS OF BREAKTHROUGH (UNSTEADY INPUT) FOR E. COLI (DEATH RATE $\neq$ 0)

Q = 23.43 ml/sec

q = as shown in Fig. 6.5

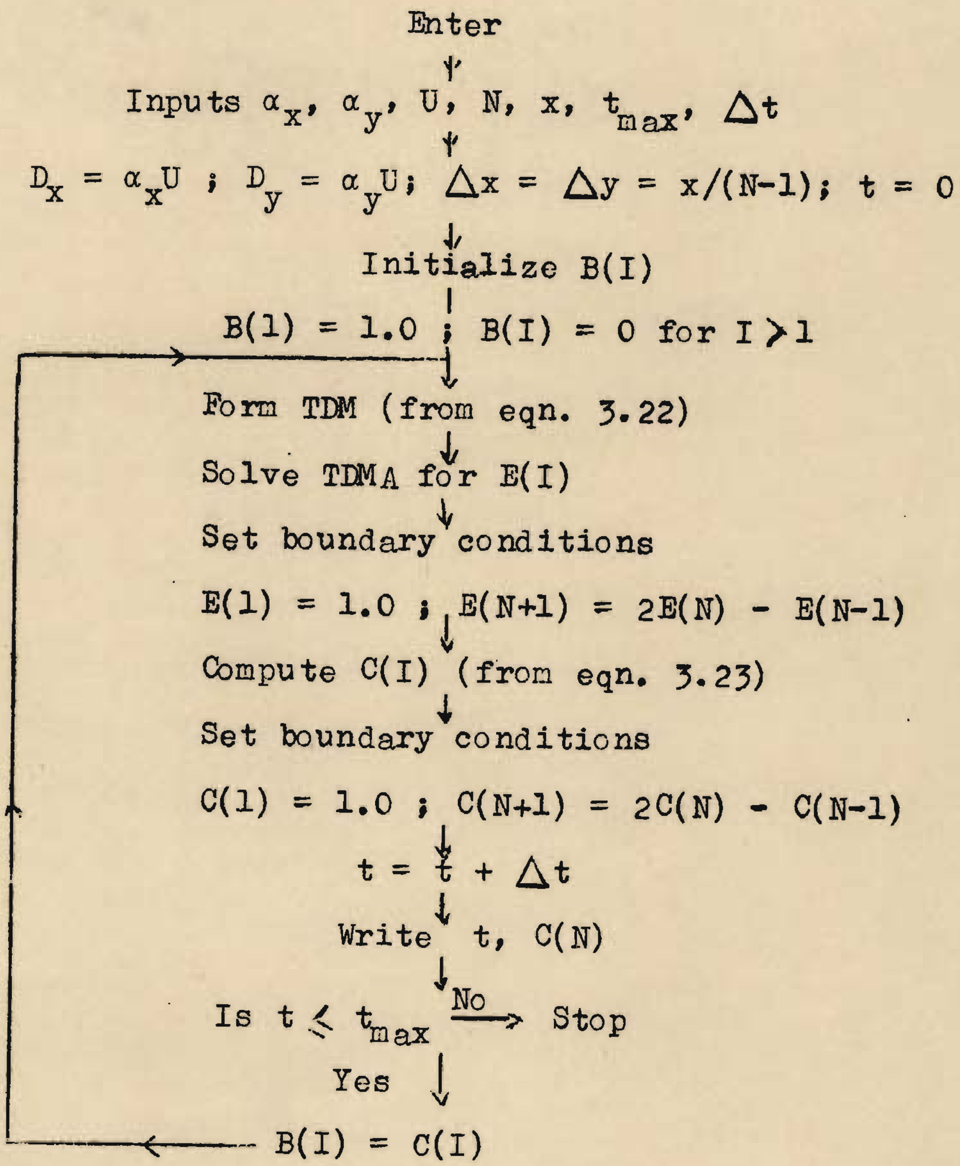
x = 40 cm ; y = 0 cm

Ambient temperature 30° C

t min	$(C_o)_t$	$C_{x,o,t}$ no/ml	K cm/sec
1.0	-	5	0.33
3.0	-	3	0.33
5.0	-	28	0.33
10.8	-	28	0.33
35.4	-	25	0.33
77.0	-	25	0.33
80.0	550	-	0.33
135.0	-	27	0.33
180.0	-	17	0.33
300.0	150	-	0.33

APPENDIX II

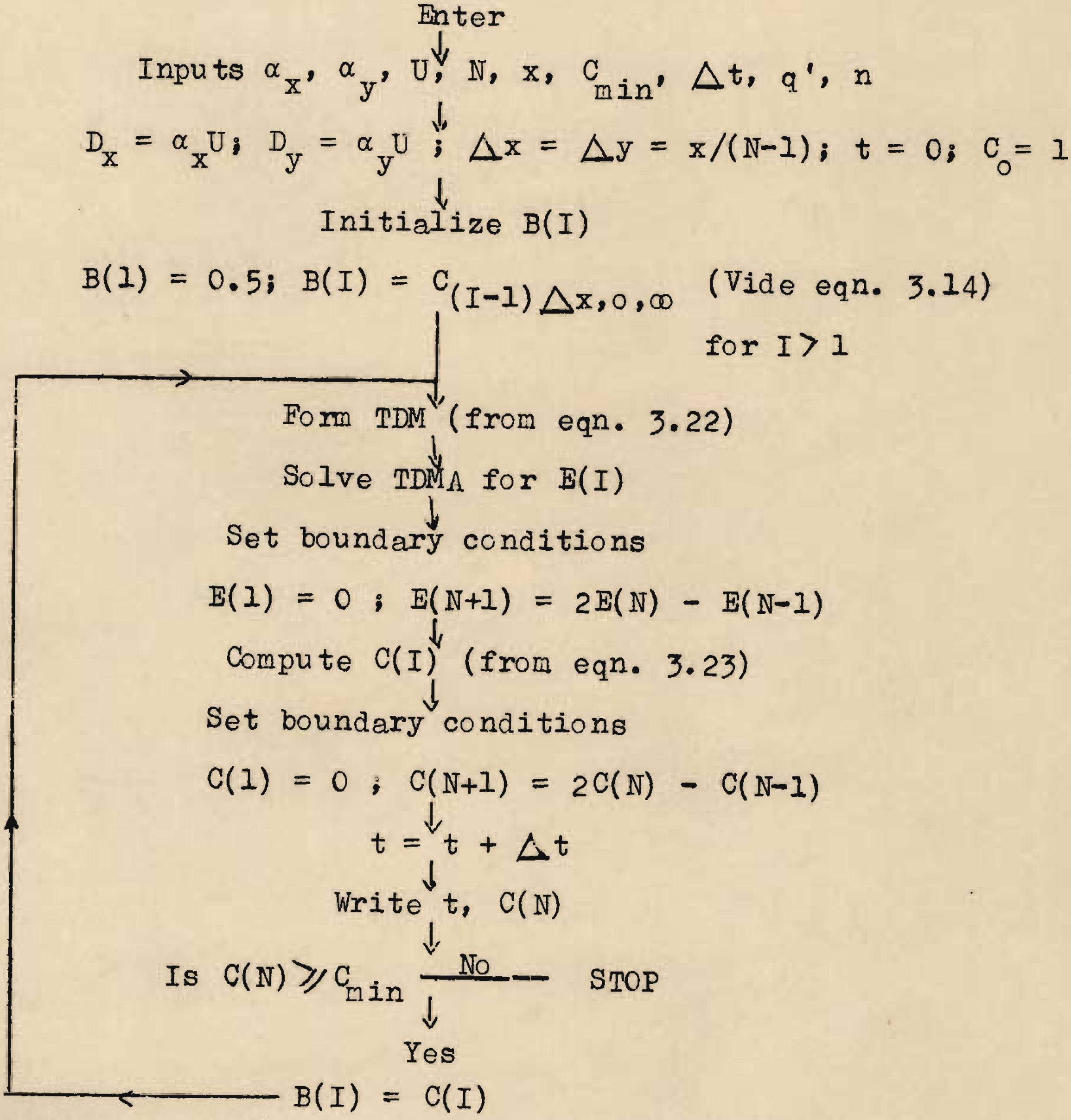
ALGORITHM FOR BREAK THROUGH AT AXIAL DISTANCE BY MODIFIED ADIP



Alternatively, $C(N)_{max.}$ may be set for termination.

APPENDIX III

ALGORITHM FOR IBT AT AXIAL DISTANCE BY MODIFIED ADIP



Alternatively, t_{max} may be set for termination.