A STUDY OF A NON-LINEAR DIFFUSION EQUATION

A Thesis

by

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TABLE OF CONTENTS

		Page
LIST OF FIGURES		iv
SUMMARY		v
ACKNOWLEDGMENTS		vii
CHAPTER I	INTRODUCTION	1
CHAPTER II	PHYSICAL BACKGROUND AND FORMULATION OF PROBLEM	4
§ 1	On the Nature of Phosphate Uptake by Plants	4
§ 2	Experimental Work and Formulation of the Problem	6
§ 3	Two Mathematical Models	8
§ 4	The Boundary Condition at $r = a$	11
CHAPTER III	FINITE DIFFERENCE REPRESENTATIONS OF THE PROBLEM	15
§ 1	Description of Finite Difference Schemes	15
§ 2	Detailed Discussion of Implicit Difference Schemes	16
§ 3	On Implicit Difference Representations of Problem	19
CHAPTER IV	THE NUMERICAL TREATMENT OF THE PROBLEM	22
§ 1	Detailed Description of Selected Difference Schemes	22
§ 2	The Starting Procedure	26
§ 3	An Improved Asymptotic Approximation	31
§ 4	A Further Note on Numerical Procedures	34
CHAPTER V	AN ALTERNATIVE PROBLEM	35
§ 1	The Numerical Procedure	35
§ 2	Summary of Results	37
CHAPTER VI	FURTHER DEVELOPMENTS OF THE PROBLEM	43
§ 1	An Asymptotic Approximation for Large Times	43
§ 2	Conclusions	47

Page

APPENDIX I SUMMARY OF RELEVANT EXPERIMENTAL WORK 49

§ 1 Measurement and Calculation of Diffusion Coefficient 49

§ 2 The Experiment for the first Model 50

§ 3 The Experiment for the second Model 52

APPENDIX II ANALYTICAL AND ASYMPTOTIC SOLUTIONS OF THE LINEAR DIFFUSION EQUATION 54

§ 1 Solutions of Linear Diffusion Equations by Laplace Transforms 54

§ 2 An Asymptotic Solution of the Non-linear Diffusion Problem 57

APPENDIX III USEFUL MODIFICATIONS OF THE METHOD OF GAUSSIAN ELIMINATION 59

§ 1 Matrices of Tridiagonal Form 59

§ 2 Matrices with Five Diagonals of Non-zero Elements 61

BIBLIOGRAPHY 63

LIST OF FIGURES

		Page
Fig. 1	Diffusion Coefficient - Concentration Relationship	9
Fig. 2	Comparison of Asymptotic Estimate and Computed Values. No special starting procedure.	28
Fig. 3	Comparison of Asymptotic Estimate and Computed Values. Initial data : V(s, 0·0005) .	29
Fig. 4	Computed Phosphorus Depletions at 150 p.p.m. (for alternative problem)	39
Fig. 5	Computed Phosphorus Depletions at 600 p.p.m. (for alternative problem)	40
Fig. 6	Computed Phosphorus Uptake - Root Hair Dimensions (for alternative problem)	41
Fig. 7	Computed Phosphorus Uptake - Main Root Dimensions (for alternative problem)	42

SUMMARY

The absorption mechanism by which a plant removes ions from the soil can often be represented by a non-linear radial diffusion equation , in which the diffusion coefficient is dependent on concentration and the boundary condition applied at the absorbing surface is initially discontinuous . In the study of this equation numerical solutions are obtained using an IBM 1620 digital computer by setting up suitable implicit finite difference schemes . The initial discontinuity of the solution gives rise to difficulties in starting the computational procedure and an attempt is made to overcome these difficulties by utilizing suitable asymptotic approximations . An asymptotic approximation not only makes it possible to begin the numerical solution at a finite time , where the boundary condition is continuous , but provides a means of checking the numerical results and furthermore suggests a means of solving the problem without using finite differences . However , the simplest and most easily applied asymptotic approximation is useful only in a very small time range . Other asymptotic solutions are also developed and discussed , but it is found that their application would involve extensive computations .

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To the best of my knowledge and belief this thesis contains no material which has been accepted for the award of another degree at any University and contains no material previously published or written by another person , except where due reference is made in the text of the thesis .

1/8/63

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CHAPTER I

Introduction

This thesis comprises the numerical study of a non-linear diffusion equation which arises as a model for the absorption mechanism by which plants in the soil-plant system absorb substances from the soil.

The mathematical problem consists in utilizing suitable numerical and analytical techniques for solving a non-linear parabolic partial differential equation of the form

$$\frac{\partial C}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\, D \frac{\partial C}{\partial r} \right] ,$$

$$0 < a \leq r < \infty \;, \quad t > 0 \;,$$

subject to the initial condition

$$\text{(i)} \quad C(r,0) = C_0 \;, \text{ (constant)} \;, \quad a \leq r < \infty \;, \qquad (1\cdot1)$$

and the boundary conditions

$$\text{(ii)} \quad \frac{\partial C}{\partial r} = h' C \;, \quad r = a \;, \quad t > 0 \;,$$

$$\text{(iii)} \quad C(r,t) \rightarrow C_0 \quad \text{as } r \rightarrow \infty \;,$$

where the diffusion coefficient D is related to the concentration $C(r,t)$ by the law

$$D = \alpha C^2 \;,$$

and a , h' , and α are positive constants.

Numerical solutions of (1·1) are obtained by setting up suitable implicit difference schemes , viz., a modified backward difference scheme (based on two time levels) or a modified Crank-Nicolson scheme (based on three time levels) , over a truncated spatial range

$$a \leq r \leq a^* < \infty \;,$$

where a^* denotes a 'sufficiently large' distance from $r = a$, an additional boundary condition being prescribed at $r = a^*$.

The fact that the boundary condition (1·1)(ii) is actually discontinuous at $t = 0$ leads to some difficulty in obtaining good numerical results at small times and therefore demands special consideration. For small values of the parameter $a h'$ it is found that, for small times, useful solution values (i.e. two or three figure accuracy) can be obtained from a straightforward asymptotic approximation, thus making it possible to begin the solution of the difference equations at some $t = t_0 > 0$ and also providing a check on the numerical work. However, for large values of ah', such accuracy can unfortunately only be achieved for extremely small times. Hence this asymptotic approximation is almost useless as a check on the numerical solution at or near the boundary.

More useful, though more complicated, asymptotic approximations based on estimating the non-linear terms are also obtained, but these too are best applied to the case of small values of ah' and a limited time range. In addition it is shown how an approximate solution valid for large times might be obtained, but in both cases full scale numerical work and proofs of convergence of the proposed iteration scheme have not been attempted. The study of the problem for large values of ah' also requires further attention.

Apart from the main problem (1·1) other interesting diffusion problems obtained by employing a somewhat different boundary condition at $r = a$ are also discussed, but only the case of exponential decay of concentration at $r = a$ is treated in fair detail.

Computations have been performed using experimental results and data supplied by Mr. D.G.Lewis and Dr.J.P.Quirk , Waite Agricultural Research Institute , Adelaide , in order to assist them in analysing mathematically the part played by diffusion in the uptake of phosphorus from soil by a wheat plant. Some details of the experiments leading directly to the formulation of the model have been included in Appendix I , but complete details of the diffusion coefficient measurements and the plant experiments are to be found in a thesis by Lewis [22], (1963) . The numerical results sought are the phosphate mass uptake versus time relationships at several levels of added phosphorus concentration for both main root and root hair dimensions. Hence the relative effectiveness of main roots and root hairs may be evaluated ; also some evidence can be gained to support a theory to account for the mass of phosphorus transferred from the soil at the various stages of the growth of the plant.

For these purposes it would really be necessary to continue the numerical solutions for times up to 120 hours - a task which involves only considerable amounts of computing but presents no new mathematical problem. On the other hand successful asymptotic approximations taking due account of the non-linear terms would probably eliminate the need for finite difference methods here, and it is felt that further research should be directed along these lines . Except for the case of exponential decay of concentration at the boundary , the numerical solutions in this thesis are over a physically small time range only , because computations have been carried out mainly for their mathematical interest.

CHAPTER II

Physical Background and Formulation of Problem

§ 1: On the Nature of Phosphate Uptake by Plants:

In considering diffusion and ionic transport as an explanation for the uptake of substances by a plant in the, soil-plant system, it is well to note that these effects occur on two scales.

(a) Microscopically :

Such phenomena pertain to the field of the plant physiologist, whose concern is the movement of substances across the cell membrane. Here free diffusion under a concentration gradient is controlled by the permeability of the cell membrane. Another kind of ionic transfer across the cell membrane is caused by an electrochemical potential difference between the inside and the outside of the membrane. Sometimes, a non-osmotic active transport working against both concentration and electric gradients causes internal concentrations greater than the external. Cytoplasmic particles, e.g. mitochondria, also play an important role in absorption mechanisms.

(b) Macroscopically :

To account for the relatively large amounts of phosphorus removed from the soil, there must necessarily be ionic transport from the neighbouring soil. There may be :

(1) diffusion of ions along a concentration gradient,

(2) transport of ions by mass flow of water.

Both these processes occur together, but studies have shown that water and ions are not necessarily absorbed through the same region of the root, and the degree to which water and ion absorption are linked is still undetermined.

The effects considered in this work are macroscopic , and the assumption is made that the main root (or root hair) acts as a cylindrical sink in an infinite unstirred medium and diffusion is radial at all times.

It is generally believed that plants absorb phosphorus largely through the medium of the soil solution and not by contact feeding or contact exchange. The surface area of soil particles in contact with the absorbing region of a root is thought to be too small to permit absorption by contact exchange to an appreciable extent. However, at the microscopic level, colloidal clay particles present a sufficiently large surface for cation exchange in close proximity to the root surface. Jenny (1951)[13] estimated that 1 $m.m.^2$ of root surface can make contact with 10^8 clay particles each carrying 6000 to 7000 exchangeable monovalent cations (K^+ ions , for example), but the absorption of phosphate anions by contact feeding , according to Dean and Rubins (1945)[8] , occurs to a relatively minor degree.

Many studies , e.g. Overstreet and Dean (1951)[26] , have been conducted wherein the phosphate content of the soil solution , as removed by different procedures, has been determined, and the conclusion is that even many productive soils contain less than 0·1 parts per million of phosphorus in solution , which is inadequate for maintaining good growth in culture solutions. These low solution concentrations have led many workers to believe that plants cannot absorb enough phosphorus from this source alone to sustain normal growth.

However Tidmore (1930)[32] showed by experiments with flowing culture solutions that even rapidly growing plants can absorb adequate amounts of phosphorus from media containing as little as 0·5 p.p.m. of phosphorus in solution. This implies that soluble soil phosphorus must continually be renewed in order to supply the growing plant with its phosphorus requirements. Overstreet and Dean also conducted greenhouse experiments to illustrate this turnover concept :

Plants were grown in soils of average fertility , the water content of which was maintained at a level sufficiently high to keep the concentration of phosphorus in the soil solution at 1 p.p.m. The total solution at any instant contained approximately 400 μgms of soluble phosphorus , and forty-day-old plants contained a total of 0·2 grams of phosphorus per plant . Hence the amount absorbed per plant per day was 5000 μgms , implying a twelvefold turnover of phosphorus fron an insoluble to a soluble and absorbable state.

These results form a basis for introducing the mathematical models which are considered in this thesis.

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§ 2: Experimental Work and Formulation of the Problem :

Cylindrical coordinates (r,θ,z) are used with no dependence on θ and z . For this simplified model root the total uptake is simply the sum of the individual uptakes of the main roots and root hairs considered separately. Examination and measurement of actual roots [22] give average diameters of 0·3 to 0·5 m.m. for main roots and 0·01 m.m. for root hairs, and , per millimetre of active main root , there is an average of fifty root hairs each of average length about 1 m.m. The regions of soil from which phosphorus is absorbed can never be mutually independent , because the root hairs are attached to the active part of the main root . Nevertheless we propose this hypothetical root as the most tractable representation of the physical situation .

Let us denote

$C = C(r,t) =$ concentration of absorbable phosphorus ,

(C is measured as grams of phosphorus per gram of soil) ,

$D =$ diffusion coefficient (m.m.^{2} / hour) ,

$a =$ main root (or root hair) radius (m.m.) .

Then the diffusion equation for cylindrical coordinates [5] is

$$\frac{\partial C}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r D \frac{\partial C}{\partial r} \right] ,$$

$$a \leqslant r < \infty , \quad t \geqslant 0 , \qquad (2\cdot1)$$

subject to

(i) $C(r,0) = C_0$, $a \leqslant r < \infty$,

(ii) a suitable boundary condition at $r = a$,

(iii) $C(r,t) \to C_0$ as $r \to \infty$.

The condition (2·1)(i) is the initial condition of constant concentration of phosphorus throughout the soil and (2·1)(ii) is the boundary condition at $r = a$, which is treated in detail in § 4 . In addition to these conditions we know that

$$0 \leqslant C(r,t) \leqslant C_0 , \text{ for all } a \leqslant r < \infty , \; t \geqslant 0 .$$

We assume that the concentration of phosphorus within the root is always zero , which implies immediate transfer of phosphorus to the plant above the ground , viz.,

$$C(r,t) = 0 , \qquad (2\cdot2)$$

$$\text{for all } 0 \leqslant r < a , \; t \geqslant 0 .$$

We also expect that , as $t \to \infty$, $C(a,t) \to 0$, and $C(r,t)$ (in $a < r < \infty$) tends asymptotically to some value (different for each r) .

The simplest case where D is constant gives rise to the linear diffusion equation which is useful in obtaining asymptotic approximations of the non-linear problem. Of greatest interest here is the case

$$D = \alpha C^2 , \qquad (2\cdot3)$$

where α is a constant. This law is obtained from the results of the diffusion experiment described in Appendix I , § 2 .

---

§ 3 : Two Mathematical Models :

First Model :

Let $C = C(r,t)$ = concentration of absorbable phosphorus , as defined in § 2 ,

a = root radius (m.m.) ,

$D = \alpha C^2$,

where α is a constant. It is important to note that the 'absorbable' phosphorus includes the phosphorus in the soil solution and also that amount of phosphorus in the soil which can be desorbed into the soil solution.

In view of the existing difficulties in obtaining accurate measurements of D at the low phosphate levels (vide Appendix 1 ,§2) , it was decided that a 'first order' estimate of the law

$$D = \alpha C^M ,$$

where α and M are constants to be determined from the table of values of D for corresponding values of C , would be adequate. Hence we obtain

$$D = \alpha C^2 ,$$

where

$$\alpha = 2560 \quad (mm^2\ 3/hour) .$$

DIFFUSION COEFFICIENT — CONCENTRATION RELATIONSHIP

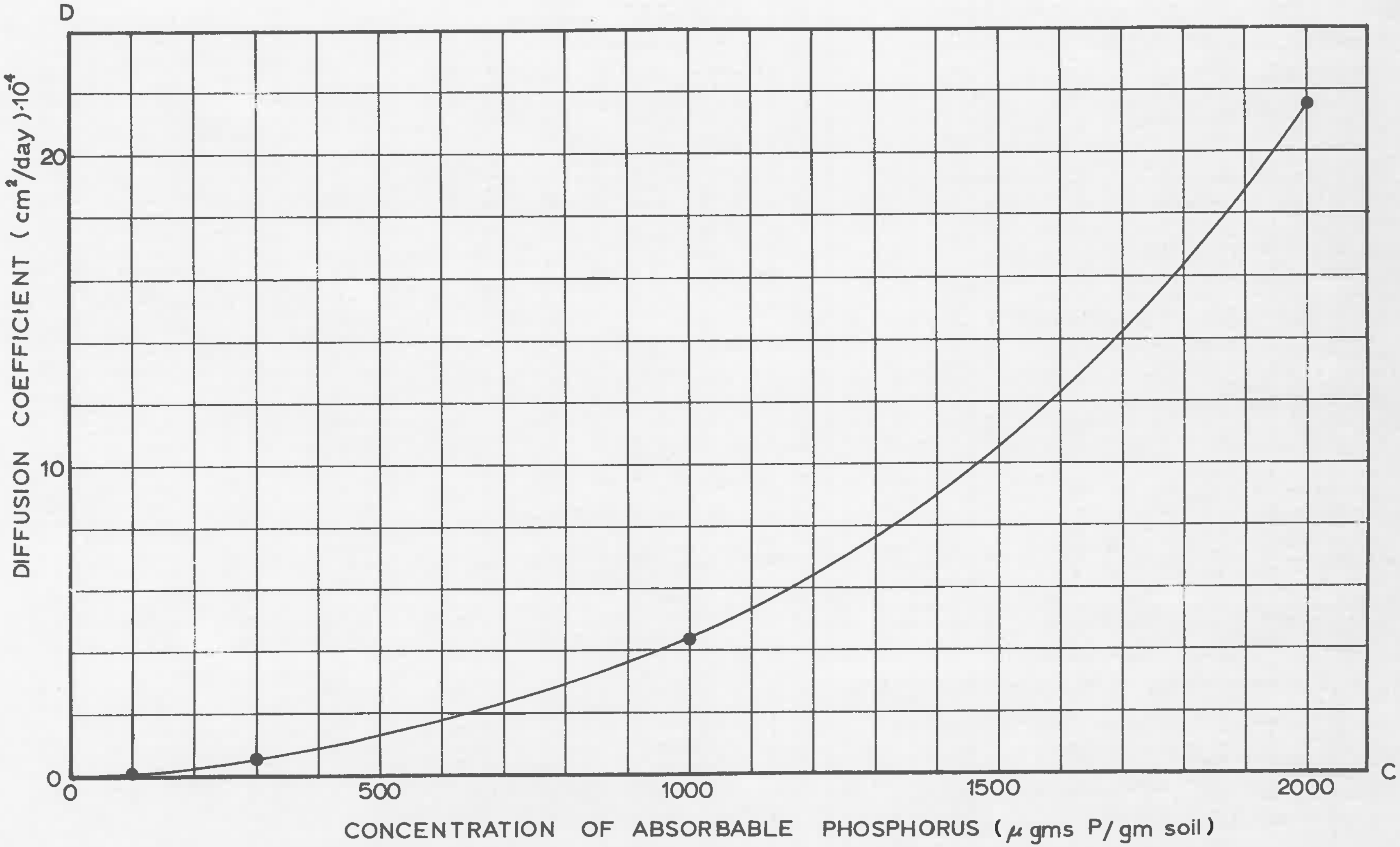


Fig. 1

Second Model :

The assumption is made that the phosphate absorbed by the main root (or root hair) is absorbed from the soil solution and that phosphorus is continually being desorbed from the solid phase - an idea discussed at some length by Crank [5] . The balance between the 'absorbable' phosphorus concentration , denoted by C in the first model and now denoted by C_1 , and the soil solution concentration , denoted by C can be related by a law of the form

$$C_1 = A C^N , \qquad (2\cdot4)$$

where A and N are constants to be determined experimentally . This type of relation has been considered by Olsen et alia [25] who actually use the one dimensional plane diffusion equation with constant diffusion coefficient to represent radial phosphate diffusion to plant roots.

However the radial diffusion equation for this model is

$$\frac{\partial C_1}{\partial t} = k \left[\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right] , \qquad (2\cdot5)$$

$$a \leqslant r < \infty , \quad t \geqslant 0 ,$$

subject to

(i) $C(r,0) = C_0 \;, \quad a \leqslant r < \infty$,

(ii) a suitable boundary condition at $r = a$,

(iii) $C(r,t) \rightarrow C_0$ as $r \rightarrow \infty$,

where k is constant being a solution diffusion coefficient.

If for the first model the law

$$D = \alpha C^M ,$$

where α and M are constants , is assumed to be valid for eq.(2·1) , then by simple substitution and comparison of coefficients the conditions that (2·1) and (2·5) be identical are readily obtained.

These are

$$(1) \quad N = \frac{1}{M+1} \, , \qquad (2) \quad \alpha = \frac{k}{N A^{1/N}} \, . \qquad (2\cdot6)$$

The determination of the constants A and N in eq.(2·4) and experimental results are given in Appendix 1 , §3 . The values obtained are

$$N = 0\cdot330 \, ,$$

$$A = 0\cdot0394 \, ;$$

so eq.(2·4) becomes

$$C_1 = 0\cdot0394 \, C^{0\cdot330} \, . \qquad (2\cdot7)$$

In the case $N = \frac{1}{3}$ the two models become identical if

$$\alpha = \frac{3 \, k}{A^3} \, . \qquad (2\cdot8)$$

Taking

$$k = 1\cdot0 \quad (\text{m.m.}^2 / \text{hour}) \, , [22] \, ,$$

$$A = 0\cdot0394 \, ,$$

the predicted value of α using (2·8) is

$$\alpha = 49000 \, ,$$

which is considerably higher than expected , but it is anticipated that improved experimental techniques would lead to a much closer agreement.

---

§ 4 : <u>The Boundary Condition at $r = a$</u> :

Let $U = U(t)$ denote the mass uptake of phosphorus per m.m. of main root (or root hair) length , and let ρ = density of soil . In this case $\rho = 1\cdot6 \times 10^{-3}$ gms / m.m.^{3} . Then U is given by

$$U = 2 \pi \rho \int_a^\infty (C_e - C_1) \, r \, dr \, , \qquad (2\cdot9)$$

where C_1 = concentration of absorbable phosphorus as defined in § 3 ; and the rate of mass uptake is

$$\frac{dU}{dt} = 2\pi\rho \int_{\infty}^{a} \frac{\partial C_1}{\partial t} r\, dr \quad . \qquad (2\cdot10)$$

For the first model , using eq.(2·1) and condition (2·3) in eq.(2·10) , we obtain one expression for the rate of uptake , viz.,

$$\frac{dU}{dt} = 2\pi\rho\alpha a \left[C_1^2 \frac{\partial C_1}{\partial r}\right]_{r=a} \quad . \qquad (2\cdot11)$$

And for the second model , using eq.(2·5) in eq.(2·10) , we obtain a second expression for the rate of uptake , viz.,

$$\frac{dU}{dt} = 2\pi\rho a k \left[\frac{\partial C}{\partial r}\right]_{r=a} \quad . \qquad (2\cdot12)$$

If in eq.(2·4) $N = \frac{1}{3}$, then (2·11) and (2·12) become identical when condition (2·8) is satisfied.

Now we may select one of two boundary conditions commonly used to describe the diffusion of substances into plant roots - vide Crank [5] . One reasonable assumption is that the rate of uptake $\frac{dU}{dt}$ is proportional to the difference in concentration between the inside and the outside of the root surface - and we note the two possibilities , viz.,

(1) to assume $\frac{dU}{dt}$ proportional to the difference in solution concentrations , i.e. (assuming the equivalence of the two models) ,

$$\frac{\partial C_1}{\partial r} = h' C_1 \quad , \quad r = a \, , \quad t > 0 \, , \qquad (2\cdot13a)$$

or

$$\frac{\partial C}{\partial r} = h\, C \quad , \quad r = a \, , \quad t > 0 \, , \qquad (2\cdot13b)$$

(i.e. linear boundary conditions) , where h and h' are constants associated with the permeability of the main root (or root hair) membrane , and the concentration inside the root is assumed to be zero.

These conditions imply that as $C(a,t) \to 0$, $[\frac{\partial C}{\partial r}]_{r=a} \to 0$.

(2) to assume $\frac{dU}{dt}$ proportional to the difference in concentrations of absorbable phosphorus , i.e.

$$\alpha C_1^2 \frac{\partial C_1}{\partial r} = h'' C_1 \quad , \quad r = a , t > 0 , \qquad (2\cdot14)$$

(i.e. a non-linear boundary condition) , where h" is also a constant depending on the permeability of the root membrane. This condition implies that as $C(a,t) \to 0$, $[\frac{\partial C}{\partial r}]_{r=a} \to \infty$.

A second reasonable assumption is that the rate of uptake $\frac{dU}{dt}$ is constant at $r = a$, i.e.

$$\alpha C_1^2 \frac{\partial C_1}{\partial r} = q \; , \; r = a , \; t > 0 , \qquad (2\cdot15a)$$

where q is a constant ; or equivalently

$$\frac{\partial C}{\partial r} = q_1 \; , \; r = a , \; t > 0 , \qquad (2\cdot15b)$$

where q_1 is a constant.

It can readily be seen that each of the boundary conditions (2·13a) , (2·13b) , (2·14) , (2·15a) and (2·15b) is discontinuous at $t = 0$, since it follows from (2·1)(i) that

$$[\frac{\partial C}{\partial r}]_{t=0} = 0 \; , \; r = a .$$

Just this type of boundary condition presents a definite problem to the finite difference methods which are commonly used to obtain numerical solutions of parabolic partial differential equations.

We shall now accept the hypothesis that phosphate absorption occurs largely from the soil solution and , in view of the expected equivalence of the first and second models , we shall work with eq.(2·1).

Substituting (2·3) into (2·1) we obtain

$$\frac{1}{\alpha}\ \frac{\partial C}{\partial t} \quad = \frac{C^2}{r}\frac{\partial C}{\partial r} \quad + \quad 2C\,[\frac{\partial C}{\partial r}]^2 \quad + \quad C^2\,\frac{\partial^2 C}{\partial r^2} \quad , \qquad (2\cdot16)$$

$$a \leq r < \infty , \quad t \geq 0 .$$

Eq.(2·16) is then rewritten in terms of $u = \frac{C_o - C}{C_o}$. This is a step of vital importance for obtaining accurate numerical results , because only then can the maximum number of significant figures be retained throughout the computation. We also write $s = \frac{r}{a}$; hence we obtain the diffusion equation for $u(s,t)$, viz.,

$$\frac{a^2}{\alpha\ C_o^2}\ \frac{\partial u}{\partial t} \quad = \quad \frac{(1-u)^2}{s}\frac{\partial u}{\partial s} - 2(1-u)(\frac{\partial u}{\partial s})^2 + (1-u)^2\,\frac{\partial^2 u}{\partial s^2} ,$$

$$1 \leq s < \infty , \quad t \geq 0 ,$$

subject to

$$\text{(i)}\quad u(s,0) = 0 , \quad 1 \leq s < \infty , \qquad (2\cdot17)$$

$$\text{(ii)}\quad \frac{\partial u}{\partial s} = -ah'(1-u) , \quad s = 1 , \quad t > 0 .$$

$$\text{(iii)}\quad u(s,t) \rightarrow 0 \quad \text{as} \quad s \rightarrow \infty .$$

Actually we require a numerical solution of this problem for $0 < t \leq T$, where T is finite and chosen according to practical requirements .

CHAPTER III

Finite Difference Representations of the Problem

§1: Description of Finite Difference Schemes :

Let us write

$$u(R_i , t) = \theta_i ,$$
$$u(R_i , t + \tfrac{1}{2}\delta t) = \Phi_i ,$$
$$u(R_i , t + \delta t) = \phi_i ,$$

and consider our diffusion equation in the form

$$\frac{\partial^2 u}{\partial R^2} = F(R, t, u, \frac{\partial u}{\partial R}, \frac{\partial u}{\partial t}) . \qquad (3\cdot1)$$

Then the forward difference scheme for eq.(3·1) is

$$\frac{\theta_{i+1} - 2\theta_i + \theta_{i-1}}{(\delta R)^2} = F \{ R_i, t, \theta_i, \frac{\theta_{i+1} - \theta_{i-1}}{2(\delta R)} , \frac{\phi_i - \theta_i}{\delta t} \} . \qquad (3\cdot2)$$

The appropriate backward difference scheme is

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\delta R)^2} = F \{ R_i , t , \phi_i , \frac{\phi_{i+1} - \phi_{i-1}}{2(\delta R)} , \frac{\phi_i - \theta_i}{\delta t} \} . \qquad (3\cdot3)$$

A modified backward difference scheme for (3·1) is

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\delta R)^2} = F \{ R_i , t , \theta_i , \frac{\theta_{i+1} - \theta_{i-1}}{2(\delta R)}, \frac{\phi_i - \theta_i}{\delta t} \} , \qquad (3\cdot4)$$

and the Crank-Nicolson scheme for (3·1) is

$$\frac{1}{2(\delta R)^2} [\phi_{i+1} - 2\phi_i + \phi_{i-1} + \theta_{i+1} - 2\theta_i + \theta_{i-1}]$$

$$= F \{ R_i , t, \Phi_i , \frac{\phi_{i+1} - \phi_{i-1} + \theta_{i+1} - \theta_{i-1}}{4(\delta R)} , \frac{\phi_i - \theta_i}{\delta t} \} . \qquad (3\cdot5)$$

Other difference schemes have been obtained by adopting different weights to those used in eq.(3·5) .

Furthermore, a system of non-linear simultaneous differential equations of the form

$$\frac{d\phi_i}{dt} = G_i \left\{ R_i , t, \phi_i , \frac{\phi_{i+1} - \phi_{i-1}}{2(\delta R)}, \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\delta R)^2} \right\} ,$$

can be obtained from (3·1) by replacing only the derivatives $\frac{\partial u}{\partial R}$ and $\frac{\partial^2 u}{\partial R^2}$ by their finite difference equivalents.

The above difference schemes are all commonly used to obtain numerical solutions of parabolic differential equations , and error estimates , conditions of stability and proofs of convergence to the correct solution are given by John [16] , Rose [30] , Lees [20] ,[21] , and other authors. The usual procedure is to examine the convergence of the solution of the difference equations as δR and δt tend to zero in such a way that $\frac{\delta t}{(\delta R)^2}$ remains constant. John [16] has found the criteria which determine the convergence of explicit difference schemes (of which (3·2) is an example) for linear and quasilinear parabolic equations. The scheme (3·2) is correct to $O[(\delta R)^2 + \delta t]$, but its chief disadvantage is that its solution does not converge for all values of $\frac{\delta t}{(\delta R)^2}$, and an excessively small time step (compared with the implicit schemes) must be used to achieve good numerical results. Consequently we turn our attention to implicit schemes.

---

§ 2 : Detailed Discussion of Implicit Difference Schemes :

In all implicit difference schemes it is necessary to solve a system of simultaneous algebraic equations at each time step . When this system is non-linear , as in the backward difference method (3·3) or in the Crank-Nicolson scheme (3·5) , an iterative procedure must be used. The backward difference method and the modified backward difference method

(3·4) both give a truncation error of order $[(\delta R)^2 + \delta t]$, whereas the Crank-Nicolson scheme gives a truncation error of order $[(\delta R)^2 + (\delta t)^2]$; however the modified scheme (3·4) has the advantage that the difference equations can be solved by inverting a tridiagonal matrix at each time step. In our particular case there is a possible modification of the Crank-Nicolson method which 'linearizes' the $(\frac{\partial u}{\partial R})^2$ term , and the difference equations can again be solved by inverting a tridiagonal matrix. However the Crank-Nicolson scheme requires a knowledge of function values at two time levels , and , as only function values at t = 0 are known initially , it will still be necessary to use the modified backward difference scheme to start the solution .

Consider the general non-linear parabolic differential equation

$$\frac{\partial^2 u}{\partial R^2} = F\left(R, t, u, \frac{\partial u}{\partial R}, \frac{\partial u}{\partial t}\right) ,$$

$$0 < R < 1 , \quad 0 < t \leq T ,$$

subject to the initial condition

$$\text{(i)} \quad u(R,0) = 0 , \quad 0 < R \leq 1 , \tag{3·6}$$

and boundary conditions

$$\text{(ii)} \quad \frac{\partial u}{\partial R} + Hu = H , \quad R = 1 , \; t > 0 ,$$

$$\text{(iii)} \quad u(0,t) = g(t) , \quad t \geq 0 ,$$

where H is a constant and g(t) is a known function.

Consider also a family of rectangular lattices with mesh $(\delta R , \delta t)$, and let β be a 'weighting' parameter such that $0 < \beta \leq 1$. Then the implicit difference equations for (3·6) become

$$\frac{1}{(\delta R)^2}\{\beta(\phi_{i+1} - 2\phi_i + \phi_{i-1}) + (1-\beta)(\theta_{i+1} - 2\theta_i + \theta_{i-1})\}$$

$$= F\left\{ i\delta R , t , u(R_i,t^*), \frac{\beta(\phi_{i+1} - \phi_{i-1}) + (1-\beta)(\theta_{i+1} - \theta_{i-1})}{2(\delta R)}, \frac{\phi_i - \theta_i}{\delta t} \right\} , \tag{3·7}$$

where $u(R_i, t^*)$ may denote θ_i, $\bar{\varphi}_i$, ϕ_i , etc . depending on the choice of β ; and the boundary conditions are replaced in a similar way. Rose [30] has shown , under certain conditions on F and its partial derivatives , that the solutions u^δ of (3·7) converge pointwise to the correct solution $u(R,t)$ of (3·6) if δR and δt tend to zero in such a way that $\frac{\delta t}{(\delta R)^2}$ remains constant . The existence of the solution u^δ and error estimates have also been established. Lees [20] has proved similar results under the additional assumption that the solution u^δ takes the correct values $u(R,t)$ on the boundaries $R = 0$ and $R = 1$.

On writing $p = \frac{\partial u}{\partial R}$ and $q = \frac{\partial u}{\partial t}$, the necessary conditions on F can be expressed as follows :

(i) $F(R, t, u, p, q)$ is a continuous function of R and t in $G = \{(R,t) ; 0 < R < 1 , 0 < t \leqslant T\}$; and F is a continuous function of u , p and q for all values of these variables determined by R and t in G .

(ii) F_u , F_p , F_q exist and are continuous , and satisfy the inequalities

$$
\begin{aligned}
0 < A_* \leqslant F_q \leqslant A^* &< \infty , \\
|F_p| \leqslant B &< \infty , \\
0 \leqslant C_* \leqslant F_u \leqslant C^* &< \infty ,
\end{aligned}
\qquad (3\cdot 8)
$$

where A_* , A^* , B , C_* and C^* are fixed constants . (The first inequality ensures the physical stability of the diffusion problem.) These conditions of boundedness and continuity make it possible to set up a difference equation in terms of the error $\varepsilon(R,t)$, where $\varepsilon(R,t) = u(R,t) - u^\delta(R,t)$, and to estimate the bounds of $|\varepsilon(R,t)|$.

---

§ 3 : On Implicit Difference Representations of the Problem :

There is clearly a practical difficulty in applying an implicit difference scheme to eq.(2·17) , because the infinite spatial range $0 \leq s < \infty$ leads to an infinite number of simultaneous equations to be solved at each time step . We therefore consider the possibility of transforming (2·17) in such a way that the new spatial range is finite. Let us apply to (2·17) the regular transformation

$$R = \frac{1}{s} \quad . \qquad (3\cdot9)$$

The problem for u(R,t) now becomes

$$\frac{a^2}{\alpha C_o^2}\frac{\partial u}{\partial t} = R^4\left[(1-u)^2 \frac{\partial^2 u}{\partial R^2} - 2(1-u)\left(\frac{\partial u}{\partial R}\right)^2 + \frac{(1-u)^2}{R}\frac{\partial u}{\partial R}\right] ,$$

$$0 < R \leq 1 \quad , \quad t \geq 0 \quad ,$$

subject to (3·10)

(i) $u(R,0) = 0 \quad , \quad 0 < R \leq 1 \quad ,$

(ii) $\frac{\partial u}{\partial R} = ah'(1-u) \quad , \quad R = 1 \quad , \quad t > 0 \quad ,$

(iii) $u(0,t) = 0 \quad .$

It would now appear natural to introduce a lattice of mesh $(\delta R , \delta t)$ in $G = \{(R,t) ; 0 < R \leq 1 , 0 < t \leq T\}$ and to set up and solve the appropriate difference equations on it . Using the notation of § 2 we find that

$$F(R , t , u , p , q) = \frac{a^2 q}{\alpha C_o^2 R^4 (1-u)^2} + \frac{2p^2}{1-u} - \frac{p}{R} \quad .$$

Since we know in advance that u(R,t) must satisfy $0 \leq u < 1$, $(R,t) \in G$, clearly F must satisfy the required continuity conditions.

Now

$$F_q = \frac{a^2}{\alpha C_o^2 R^4 (1-u)^2} \quad ,$$

$$F_p = \frac{4p}{1-u} - \frac{1}{R} \; ,$$

$$F_u = \frac{2a^2 q}{\alpha C_o^2 R^4 (1-u)^3} + \frac{2p^2}{(1-u)^2} \; ,$$

and clearly F_q , F_p , and F_u exist and are continuous for $(R,t) \in G$, but are not bounded as required by conditions (3·8) . Consequently we cannot expect convergence of the solutions of implicit difference equations as the mesh size $(\delta R \, , \, \delta t)$ tends to zero. The same result will also be true for any regular transformation function which transforms the infinite range $1 \leq s < \infty$ in-to a finite range.

Thus , to solve the problem at all by these methods , it will be necessary to truncate the spatial range near $R = 0$, and to re-define the problem in

$$0 < b \leq R \leq 1 \, ,$$

where b corresponds , in the physical system , to a large distance from the root. The condition (2·10)(iii) must be replaced by

$$u(b,t) = g(t) \; , \quad t \geq 0 \; , \qquad (3\cdot 11)$$

where the function $g(t)$ can in fact be determined from an asymptotic approximation of the differential equation. Appendix II ,§ 2 gives such an asymptotic solution valid for small times.

The idea of transforming the differential equation and using a rectangular mesh on the new spatial range shall be retained in preference to setting up difference equations using a rectangular mesh on

$$1 < s < S < \infty \; .$$

As $\frac{\partial u}{\partial s}$ must be estimated accurately at $s = 1$, it is desirable that the mesh points , equally spaced in $b < R < 1$, correspond in the physical system to many mesh points near $s = 1$ and relatively fewer at large distances from $s = 1$.

It is also desirable since the function $u(s,t)$ actually undergoes considerable change near $s = 1$ but relatively little elsewhere.

Most of the numerical work here has been done by utilizing the transformation (3·9) , but it is certainly also worthwhile to consider the transformation

$$R = \frac{\ln s}{\ln S} , \qquad (3\cdot12)$$

where $s = S$ marks the point at which the physical range has been truncated . Eq.(2·17) then becomes

$$\frac{a^2(\ln S)^2}{\alpha\, C_o^2} \frac{\partial u}{\partial t} = S^{-2R}[(1-u)^2 \frac{\partial^2 u}{\partial R^2} - 2(1-u)(\frac{\partial u}{\partial R})^2] ,$$

$$0 < R < 1 , \quad 0 < t \leqslant T ,$$

subject to

$$(i) \quad u(R,0) = 0 , \quad 0 \leqslant R \leqslant 1 ,$$

and the boundary conditions (3·13)

$$(ii) \quad \frac{\partial u}{\partial R} = -(\ln S)ah'(1-u) , \quad R = 0 , \; t > 0 ,$$

$$(iii) \quad u(1,t) = g(t) ,$$

where $g(t)$ has been determined either by using the asymptotic approximation , or simply by making the approximation $g(t) \equiv 0$.
Clearly the conditions (3·8) are again satisfied in the range $0 < R < 1$, $0 < t \leqslant T$.

A particular difference scheme may now be selected and a numerical solution attempted .

CHAPTER IV

The Numerical Treatment of the Problem

§ 1 : Detailed Description of Selected Difference Schemes :

Consider equation (2·17) and write

$$\tau = \frac{\alpha C_o^2 t}{a^2} \quad . \qquad (4\cdot1)$$

Using the transformation (3·9), the diffusion problem for $u(R,\tau)$ now becomes

$$\frac{\partial u}{\partial \tau} = R^4\left[(1-u)^2\frac{\partial^2 u}{\partial R^2} - 2(1-u)\left(\frac{\partial u}{\partial R}\right)^2 + \frac{(1-u)^2}{R}\frac{\partial u}{\partial R}\right] ,$$

$$0 < b \leqslant R \leqslant 1 \ , \ 0 < \tau < \tau^* ,$$

subject to (4·2)

(i) $u(R,0) = 0 \ , \quad 0 < R \leqslant 1 \ ,$

(ii) $\dfrac{\partial u}{\partial R} = ah'(1-u) \ , \ R = 1 \ , \ \tau > 0 \ ,$

(iii) $u(b,\tau) = G(\tau) \ , \ \tau \geqslant 0 \ ,$

where $G(\tau)$ is determined by the asymptotic solution given in Appendix II for some chosen b. Selecting the modified backward difference scheme (3·4) the difference equations for (4·2) become

$$\frac{\phi_i - \theta_i}{\delta\tau} = i^4(\delta R)^4\{(1-\theta_i)^2\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\delta R)^2} - \frac{1-\theta_i}{2(\delta R)^2}(\theta_{i+1} - \theta_{i-1})^2$$

$$+ \frac{(1-\theta_i)^2}{2\, i(\delta R)^2}(\theta_{i+1} - \theta_{i-1})\ \} \ ,$$

where we are now writing

$$u(R_i,\tau) = \theta_i \ , \ u(R_i,\tau + \tfrac{1}{2}\delta\tau) = \Phi_i \ , \text{ and } \ u(R_i,\tau + \delta\tau) = \phi_i \ .$$

Writing $\delta R = \frac{1}{n}$, where n = no. of divisions of the interval $0 < R < 1$, we obtain

$$\frac{2n^2}{\delta\tau}(\phi_i - \theta_i) = i^4\{(1-\theta_i)^2[2(\phi_{i+1} - 2\phi_i + \phi_{i-1}) + \frac{\theta_{i+1} - \theta_{i-1}}{i}]$$

$$- (1-\theta_i)(\theta_{i+1} - \theta_{i-1})^2\ \} \ . \qquad (4\cdot3)$$

If we now select $b = \frac{1}{n}$ and prescribe the values ϕ_1 by the condition (4·2)(iii), then we need only use the difference equations (4·3) for $i = 2, \dots, n-1$, the final equation of the set arising from (4·2)(ii) represented in terms of the ϕ's. The representation

$$\left[\frac{\partial u}{\partial R}\right]_{R=1} = \frac{\phi_n - \phi_{n-1}}{\delta R} + O(\delta R) , \qquad (4\cdot4)$$

is of course less accurate than the Milne formula

$$\left[\frac{\partial u}{\partial R}\right]_{R=1} = \frac{3\phi_n - 4\phi_{n-1} + \phi_{n-2}}{2(\delta R)} + O(\delta R)^2 , \qquad (4\cdot5)$$

but preserves the tridiagonal form of the resulting matrix.

Using (4·4) in condition (4·2)(ii) we obtain

$$-\phi_{n-1} + \phi_n\left(1 + \frac{ah'}{n}\right) = \frac{ah'}{n} , \qquad (4\cdot6)$$

and the matrix equation

$$A \underset{\sim}{\phi} = \underset{\sim}{\psi} ,$$

is such that the non-zero elements of A are

$$\begin{aligned}
a(1,1) &= 1 , \\
a(i,i-1) &= -2(1-\theta_i)^2 , \\
a(i,i) &= \frac{2n^2}{\delta\tau\, i^4} + 4(1-\theta_i)^2 , \\
a(i,i+1) &= -2(1-\theta_i)^2 , \qquad (i = 2, \dots, n-1) , \\
a(n,n-1) &= -1 , \\
a(n,n) &= 1 + \frac{ah'}{n} ;
\end{aligned} \qquad (4\cdot7)$$

and the components of $\underset{\sim}{\psi}$ are

$$\begin{aligned}
\psi(1) &= G(\tau) , \\
\psi(i) &= \frac{2n^2\theta_i}{\delta\tau\, i^4} + (1-\theta_i)^2 \frac{\theta_{i+1} - \theta_{i-1}}{i} \\
&\quad - (1-\theta_i)(\theta_{i+1} - \theta_{i-1})^2 ,
\end{aligned}$$

$$(i = 2 , \dots , n-1)$$

$$\psi(n) = \frac{ah'}{n} .$$

The solution of matrix equations of tridiagonal form is achieved by a modification of the method of Gaussian elimination [24] , as outlined in Appendix III .

If (4·5) is used in condition (4·2)(ii) , we obtain

$$\phi_{n-2} - 4\phi_{n-1} + (3 + \frac{2ah'}{n})\phi_n = \frac{2ah'}{n} ,$$

and the resulting matrix equation can then be solved by applying eqs.(C·11) and (C·12) of Appendix III , § 2 .

The Crank-Nicolson scheme for (4·2) can also be modified to yield linear difference equations . We represent one $\frac{\partial u}{\partial R}$ factor by

$$\frac{\partial u}{\partial R} \approx \frac{1}{4\,\delta R}[\phi_{i+1} - \phi_{i-1} + \theta_{i+1} - \theta_{i-1}] ,$$

and the other factor as

$$\frac{\partial u}{\partial R} \approx \frac{1}{2\,\delta R}[\Phi_{i+1} - \Phi_{i-1}] .$$

This idea of 'linearizing' $[\frac{\partial u}{\partial R}]^2$ has already been noted by Forsythe and Wasow [9] and others , but a strict mathematical analysis of the convergence and stability of this difference representation has not been attempted.

The difference equations for (4·2) become

$$\frac{\phi_i - \theta_i}{\delta\tau} = i^4(\delta R)^4 \Big\{ \frac{(1-\Phi_i)^2}{2(\delta R)^2}[\phi_{i+1} - 2\phi_i + \phi_{i-1} + \theta_{i+1} - 2\theta_i + \theta_{i-1}]$$

$$- \frac{(1-\Phi_i)}{4(\delta R)^2}[\phi_{i+1} - \phi_{i-1} + \theta_{i+1} - \theta_{i-1}][\Phi_{i+1} - \Phi_{i-1}]$$

$$+ \frac{(1-\Phi_i)^2}{4\,i(\delta R)^2}[\phi_{i+1} - \phi_{i-1} + \theta_{i+1} - \theta_{i-1}] \Big\} .$$

Again writing $\delta R = \frac{1}{n}$ we obtain

$$\frac{4n^2(\phi_i - \theta_i)}{\delta\tau} = i^4(1-\Phi_i)\{2[\phi_{i+1} - 2\phi_i + \phi_{i-1} + \theta_{i+1} - 2\theta_i + \theta_{i-1}]$$

$$- [\phi_{i+1} - \phi_{i-1} + \theta_{i+1} - \theta_{i-1}][\Phi_{i+1} - \frac{1-\Phi_i}{i} - \Phi_{i+1}]\},$$

for $i = 2, \ldots, n-1$.

Using (4·4) and writing $b = \frac{1}{n}$ as before , we obtain a new matrix equation

$$A\,\underset{\sim}{\phi} = \underset{\sim}{\psi} ,$$

where the non-zero elements of A are

$$\begin{aligned}
a(1,1) &= 1 , \\
a(i,i-1) &= -2(1-\Phi_i)^2 + [\Phi_{i-1} + \frac{1-\Phi_i}{i} - \Phi_{i+1}][1-\Phi_i] , \\
a(i,i) &= \frac{4n^2}{\delta\tau\, i^4} + 4(1-\Phi_i)^2 , \\
a(i,i+1) &= -2(1-\Phi_i)^2 - [\Phi_{i-1} + \frac{1-\Phi_i}{i} - \Phi_{i+1}][1-\Phi_i] , \\
& \qquad (i = 2, \ldots, n-1) , \qquad (4{\cdot}8) \\
a(n,n-1) &= -1 , \\
a(n,n) &= 1 + \frac{ah'}{n} ;
\end{aligned}$$

and the components of $\underset{\sim}{\psi}$ are

$$\begin{aligned}
\psi(1) &= G(\tau) , \\
\psi(i) &= \frac{4n^2\theta_i}{\delta\tau\, i^4} + 2(1-\Phi_i)^2(\theta_{i+1} - 2\theta_i + \theta_{i-1}) \\
&\quad - (1-\Phi_i)(\theta_{i+1} - \theta_{i-1})(\Phi_{i+1} - \Phi_{i-1}) + (1-\Phi_i)^2[\frac{\theta_{i+1} - \theta_{i-1}}{i}] , \\
& \qquad (i = 2, \ldots, n-1) , \\
\psi(n) &= \frac{ah'}{n} .
\end{aligned}$$

In this modification of the Crank-Nicolson scheme all derivatives are centred about the points $(R_i, \tau + \frac{1}{2}\delta\tau)$, but the boundary condition (4·2) (ii) must not be timewise centred at $\tau + \frac{1}{2}\delta\tau$, but should be represented in terms of the ϕ's alone . In the case of a linear boundary condition the tridiagonal or nearly tridiagonal matrix form is retained ; however for a non-linear boundary condition the corresponding algebraic equation will also become non-linear and a suitable iteration procedure must then be devised . The importance of treating the boundary condition in this manner has already been noted by others and Douglas (in ' Numerical Methods for Parabolic Equations') [1] has constructed a simple example demonstrating the uncontrolled oscillations which occur if $[\frac{\partial u}{\partial R}]_{R=1}$ is timewise centred . This effect is essentially due to truncation error .

---

§ 2 : The Starting Procedure :

As the rate of mass uptake of phosphorus is proportional to the concentration at the root surface , it is essential that the computations should for all times be accurate in this region. Therefore the effect of the initially discontinuous boundary condition must be carefully investigated. Certain authors , e.g. Albasiny , [2] , have found that , in obtaining a numerical solution of reasonable accuracy for large times , no special starting procedure is necessary and initial transient effects can be ignored . This method was tested by using the modified backward difference scheme described in § 1 to compute the ϕ's at $\tau = \delta\tau$ from $\theta_i = 0$, $i = 0, 1, \ldots, n$.

Numerical results were obtained over a small range of τ for several values of ah' , and these were compared with the corresponding values obtained from the asymptotic approximation outlined in Appendix II , § 2 , which is obtained by ignoring the non-linear terms of the equation

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial s^2} + \frac{1}{s}\frac{\partial u}{\partial s} - \left[(2u - u^2)\left[\frac{\partial^2 u}{\partial s^2} + \frac{1}{s}\frac{\partial u}{\partial s}\right] + 2(1 - u)\left[\frac{\partial u}{\partial s}\right]^2 \right] . \quad (4\cdot 9)$$

Let $V(s,\tau)$ denote the solution of the linear diffusion problem , where $V(s,\tau)$ is given by eq.(B·13). The check on the accuracy of taking $V(s,\tau)$ as the solution of the non-linear equation (4·9) is made at the boundary $s = 1$, where the effect of the non-linearity is greatest.

If $V(s,\tau)$ is to be a good approximation for eq.(4·9) then the non-linear terms in the square brackets can be approximated by

$$N(s,\tau) = -(2V - V^2)\left[\frac{\partial V}{\partial \tau}\right] - 2(1 - V)\left[\frac{\partial V}{\partial s}\right]^2 ,$$

and

$$N(1,\tau) = -(2V^* - V^{*2})\left[\frac{\partial V}{\partial \tau}\right]^* - 2(ah')^2(1 - V^*)^3 ,$$

where * indicates evaluation at $s = 1$.

Therefore the ratio of non-linear to linear terms is estimated by

$$L = V^{*2} - 2V^* - \frac{2\ ah'\ (1 - V^*)^3}{\left[\frac{\partial V}{\partial \tau}\right]^*} .$$

For sufficiently small τ , $V^*\left[\frac{\partial V}{\partial \tau}\right]^* \sim \frac{2(ah')^2}{\sqrt{\pi}}$; thus for any fixed value of ah' , we can make L of order V^* for some τ sufficiently small.

Computations were carried out for two different spatial intervals , viz., $\delta R = \frac{1}{20}$ and $\delta R = \frac{1}{40}$, and for a time step $\delta\tau = 10^{-4}$.
Fig. 2 shows how the computed $u(1,\tau)$ differs from the asymptotic estimate $V(1,\tau)$, which , in this time range , has an accuracy of two to three significant figures.

COMPARISON OF ASYMPTOTIC

ESTIMATE AND COMPUTED VALUES.

$ah' = 0.05$

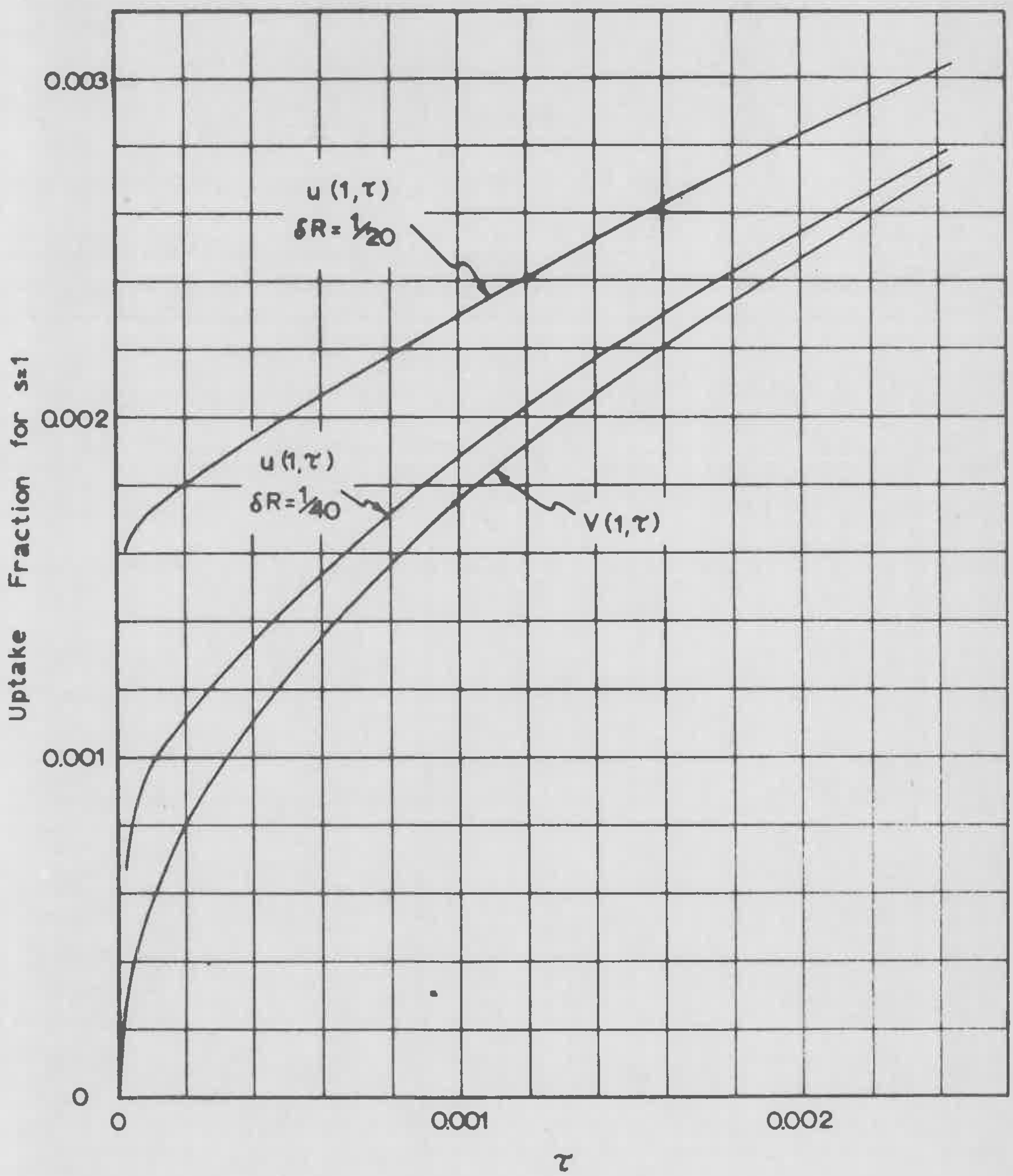


Fig. 2

COMPARISON OF ASYMPTOTIC

ESTIMATE AND COMPUTED VALUES.

$ah' = 0.05$

Initial Data: $V(s, 0.0005)$

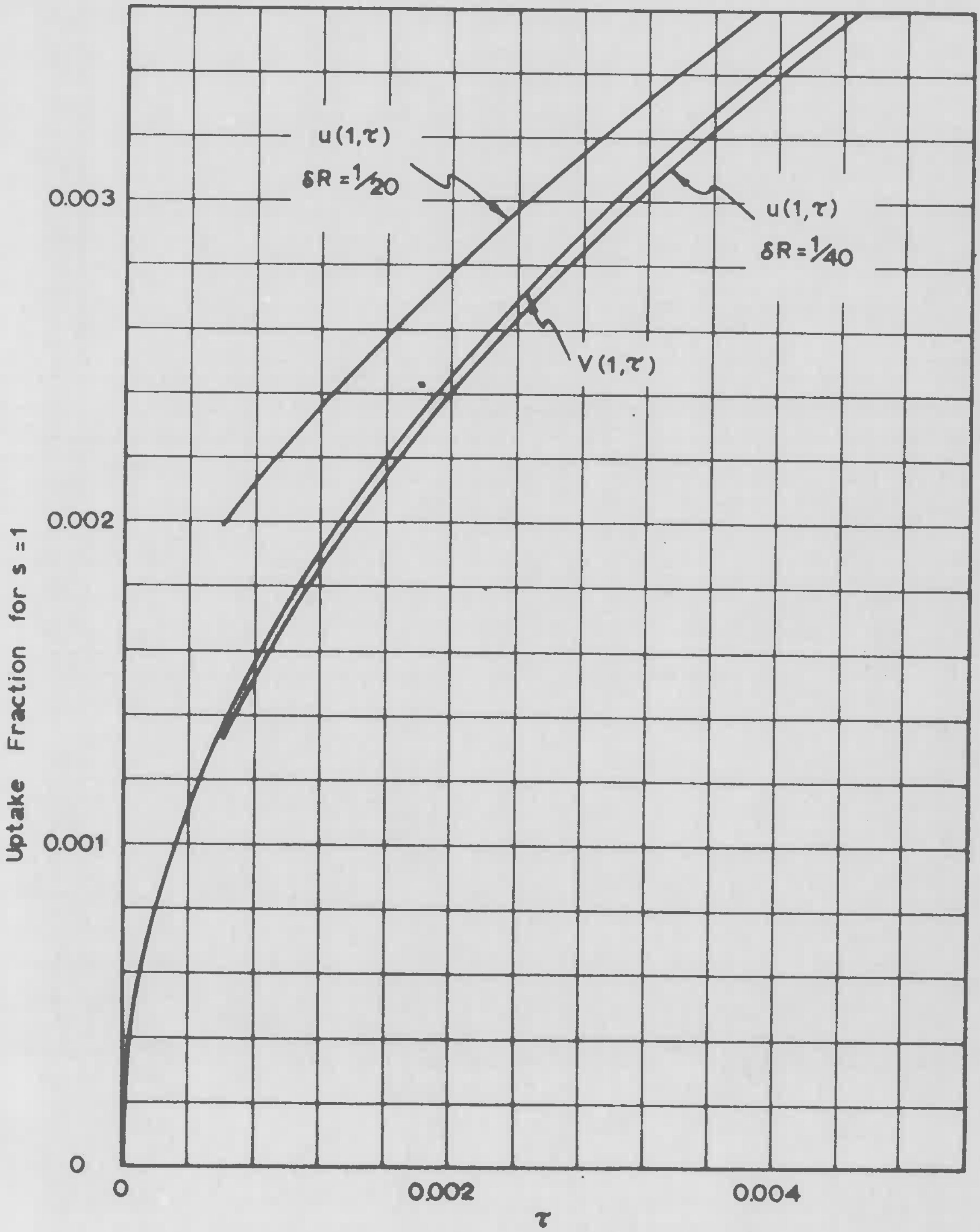


Fig. 3

The curves are drawn for $ah' = 0{\cdot}05$, but very similar results were obtained for other values of $ah' < 1$ and these are not displayed in this thesis. Comparing $u(s,\tau)$ with $V(s,\tau)$ at points for which $s > 1$ shows a great disparity – due to truncation and the initial discontinuity at $t = 0$ – which becomes larger as s increases. This disparity , however , diminishes and the results tend to become meaningful as τ increases . From fig. 2 , for $\delta R = \frac{1}{20}$ truncation and 'initial' error is very serious, but for $\delta R = \frac{1}{40}$ it seems that quite usable results (i.e. one or two figure accuracy) could be obtained for the mass uptake , given by eq.(2·11), for the time range of interest to Lewis [22].

Some improvement in the results is achieved by starting the solution of $u(s,\tau)$ at some $\tau = \tau_0 > 0$, where τ_0 is small enough for $V(s,\tau_0)$ to approximate the correct solution to a reasonable accuracy. However , an estimation of the ratio of non-linear to linear terms at $s = 1$ shows that an accuracy of three or four significant figures can only be obtained for values of τ_0 of the order of 10^{-6}. Fig. 3 gives a comparison of results in the case where $V(s, 0{\cdot}0005)$, as given by (B·13) , has been used as initial data ; the results for $\delta R = \frac{1}{20}$ are similar to those in fig. 2 , but for $\delta R = \frac{1}{40}$ there is no spurious effect and the function $\{V(s,\tau) - u(s,\tau)\}$ increases steadily with τ due the growth of the non-linear terms.

The results of fig. 2 show that a greater accuracy can be obtained by increasing the number of subdivisions of the spatial range $0 < R < 1$. However , improved accuracy can also be obtained without altering the mesh size. At the point $(R_i , \tau + \delta\tau)$ let us write

$$\frac{\partial u}{\delta \tau} = \frac{\phi_i - \theta_i}{\delta\tau} + \mathcal{C}(u_\tau)_i \quad ,$$

$$\frac{\partial u}{\partial R} = \frac{\phi_{i+1} - \phi_{i-1}}{2\,\delta R} + \mathcal{C}(u_R)_i \quad ,$$

$$\frac{\partial^2 u}{\partial R^2} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\delta R)^2} + \mathcal{C}(u_{RR})_i \quad ,$$

where $\mathcal{C}(u_\tau)_i$, ... are the higher correction terms which have so far been ignored . The usual practice is to make $\delta\tau$ sufficiently small for $\mathcal{C}(u_\tau)_i$ to be insignificant , since thèir inclusion adds greatly to the storage problem. The other correction terms can be included without affecting the linearity of the difference equations but the computing time now required at each time level will be significantly greater. Of interest in this respect is Albasiny's work [2] , which applies corrections to the spatial derivatives in a Crank-Nicolson representation of a linear radial diffusion problem.

Another possible way of obtaining better numerical results lies in finding an improved asymptotic approximation and the next section is devoted to this work .

---

§ 3 : An Improved Asymptotic Approximation :

Let us consider the linear problem

$$\frac{\partial v}{\partial \tau} = \frac{\partial^2 v}{\partial s^2} + \frac{1}{s}\frac{\partial v}{\partial s} - G(s,\tau) \quad ,$$

$$1 \leqslant s < \infty \;, \quad \tau > 0 \;,$$

subject to (4·10)

(i) $v(s,0) = 0 \;, \quad 1 \leqslant s < \infty \;,$

(ii) $\frac{\partial v}{\partial s} = -ah'(1 - v) \;, \quad s = 1 \;, \quad \tau > 0 \;,$

(iii) $v(s,\tau) \rightarrow 0$ as $s \rightarrow \infty$.

Applying the Laplace transform to eq.(4·10) we obtain the auxiliary equation , viz.,

$$\frac{d^2 \bar{v}}{ds^2} + \frac{1}{s}\frac{d\bar{v}}{ds} - q^2 \bar{v} = \bar{G}(s,p) ,$$

subject to the boundary condition (4·11)

$$\frac{d\bar{v}}{ds} = - ah'\left(\frac{1}{p} - \bar{v}\right) , \quad s = 1 ,$$

and

$$\bar{v} \to 0 \quad \text{as} \quad s \to \infty .$$

Solutions of the homogeneous equation are

$$\bar{v}_1 = K_o(qs) ,$$

$$\bar{v}_2 = I_o(qs) ;$$

thus , using the method of variation of parameters , the general solution of (4·11) becomes

$$\bar{v} = \left[M_1 - \int_1^s s' I_o(qs')\bar{G}(s',p)ds'\right]K_o(qs) + \left[M_2 + \int_1^s s' K_o(qs')\bar{G}(s',p)ds'\right] I_o(qs) , \tag{4·12}$$

where M_1 and M_2 are constants . On obtaining the values of M_1 and M_2 for the above boundary conditions we get

$$\bar{v} = \frac{ah' K_o(qs)}{p[qK_1(q) + ah'K_o(q)]} - \left[\int_s^\infty s'K_o(qs')\bar{G}(s',p)ds'\right] I_o(qs) - \left[\int_1^s s'I_o(qs')\bar{G}(s',p)ds'\right] K_o(qs) + \left[\int_1^\infty s'K_o(qs')\bar{G}(s',p)ds'\right] I_o(q)\frac{\left[ah' - \frac{q I_1(q)}{I_o(q)}\right]K_o(qs)}{[ah'K_o(q) + qK_1(q)]} . \tag{4·13}$$

The first term in eq.(4·13) is exactly the term obtained by putting $G(s,\tau) = 0$, and its inverse Laplace transform is given by eq.(B·13) , Using

$$\mathcal{L}\{\frac{1}{2\tau}\exp[-\frac{s^2+s'^2}{4\tau}]\, I_0(\frac{s\, s'}{2\tau})\} = \begin{cases} I_0(qs')K_0(qs) , & s > s' , \\ I_0(qs)K_0(qs') , & s < s' , \end{cases}$$

the inverse Laplace transform of the second and third terms is given by

$$W(s,\tau) = \int_0^\tau dt' \frac{\exp[-s^2/4(\tau-t')]}{2(\tau-t')} \int_1^\infty s'ds' G(s',t') I_0(\frac{s\, s'}{2(\tau-t')}) \ell^{-s'^2/4(\tau-t')} . \tag{4·14}$$

The first part of the fourth term gives

$$\int_0^\tau \frac{\partial V(s,\tau-t)}{\partial\tau} W(1,t)\, dt .$$

In the remaining part we write

$$\bar{N}(s,p) = \frac{I_1(q)\, K_0(qs)}{[I_0(q)K_1(q) + \frac{ah'}{q} I_0(q)K_0(q)]} ,$$

and expand $\bar{N}$ in powers of $\frac{1}{q}$.

Thus

$$\bar{N} = \frac{\ell^{-q(s-1)}}{\sqrt{s}}[1 - \frac{A}{q} + \frac{B}{q^2} \dots] + \text{higher order terms} ,$$

where

$$A = \frac{7}{8} + \frac{1}{8s} + ah'$$

$$B = \frac{41}{128} + \frac{7}{64s} + \frac{9}{128s^2} + \frac{11ah'}{8} + (ah')^2 + \frac{ah'}{8\, s} .$$

Thus we obtain

$$N(s,\tau) = \frac{s-1}{2\sqrt{(\pi s\tau^3)}}\exp[-\frac{(s-1)^2}{4\tau}] - \frac{A}{\sqrt{(\pi s\tau)}}\exp[-\frac{(s-1)^2}{4\tau}] + \frac{B}{\sqrt{s}}\,\mathrm{erfc}\,[\frac{s-1}{2\sqrt{\tau}}] + \dots . \tag{4·15}$$

Hence

$$v(s,\tau) = V(s,\tau) - W(s,\tau) + \int_0^\tau [\frac{\partial V(s,\tau-t)}{\partial\tau} - N(s,\tau-t)]W(1,t)dt . \tag{4·16}$$

As we want $G(s,\tau)$ to estimate the non-linear terms of eq.(4·9) we devise an iteration scheme as follows :

Write

$$G_1(s,\tau) = 0 ,$$
$$v_1(s,\tau) = V(s,\tau) ,$$
$$G_2(s,\tau) = (2v_1 - v_1^2)\left[\frac{\partial v_1}{\partial \tau}\right] + 2(1 - v_1^2)\left[\frac{\partial v_1}{\partial s}\right]^2 ,$$

and use eqs.(4·14) , (4·15) and (4·16) to find expressions for $W_2(s,\tau)$, $N_2(s,\tau)$ and $v_2(s,\tau)$. This procedure should then be iterated with the hope that $\lim_{n\to\infty} v_n(s,\tau)$ exists and equals $u(s,\tau)$, the solution of the non-linear diffusion equation (4·9) . Clearly if the existence of this limit can be proved , then existence and uniqueness of solutions of the non-linear equation (4·9) follow as a consequence of the existence and uniqueness of the solutions of the linear equation (4·10) .

However an attempt to utilize this approximation has not been attempted here as it would involve much additional computing .

---

§ 4 : A Further Note on Numerical Procedures :

The solution of the matrix equation (4·8) of the modified Crank-Nicolson scheme with initial data obtained from the simple asymptotic estimate (B·13) was also attempted , but the results , essentially similar to those obtained from the modified backward difference scheme , contributed but little to the study of the problem . Further computations were performed using the backward difference scheme (3·3) and consistent results obtained , however this scheme was then discarded because the solution of the resulting non-linear difference equations involved much additional computing time at each time level .

CHAPTER V

An Alternative Problem

§ 1: Numerical Procedure :

The alternative problem considered here replaces the boundary condition (4·1)(ii) which is discontinuous at $t = 0$ by the physically unrealistic exponential boundary condition

$$u(1,t) = 1 - e^{-mt}, \quad m \text{ const.},$$

which is continuous at $t = 0$, and is therefore easier to solve numerically. The problem is

$$\frac{a^2}{\alpha C_o^2}\frac{\partial u}{\partial t} = R^4\left[(1-u)^2\frac{\partial^2 u}{\partial R^2} - 2(1-u)\left[\frac{\partial u}{\partial R}\right]^2 + \frac{(1-u)^2}{R}\frac{\partial u}{\partial R}\right],$$

$$0 < b \leq R \leq 1, \quad 0 < t \leq T,$$

subject to (5·1)

(i) $u(R,0) = 0, \quad 0 < R \leq 1,$

(ii) $u(1,t) = 1 - e^{-mt}, \quad m$ const.,

(iii) $u(b,t) = g(t)$.

The constant m is chosen such that the concentration at the root surface after a period of five days is approximately 30 % of its initial value.

Interest in the numerical solution of this problem was stimulated by the desire of Lewis and Quirk, of the Waite Institute, to obtain some usable results, and computations were carried out in the early stages of this work, when b was taken to be zero, and (5·1)(iii) was replaced by

$$u(0,t) = 0, \quad t \geq 0, \qquad (5\cdot1)(\text{iiia})$$

Difference equations were set up according to the previously mentioned modification of the Crank-Nicolson scheme . The conditions (3·8) are not satisfied in this case , and we cannot prove the convergence of the difference equations to the correct solution as the mesh size (δR , δt) tends to zero. Nevertheless it is reasonable to suppose that , for the chosen mesh size , the numerical solution of the problem in which (5·1)(iii) has been applied correctly , will not differ widely from the one using (5·1)(iiia) .

Solutions were started by using a very small time step $\delta t'$ in conjunction with the initial data and estimated values at $t = \frac{1}{2}\delta t'$. A suitable larger time step was then chosen and computations were commenced with the initial data and the newly computed values at $t = \frac{1}{2}\delta t$. Throughout the computations a check was made to ensure that the multipliers λ_1 , as defined in Appendix III , satisfied the stability requirement.

Phosphorus mass uptake versus time relationships were computed for both main root and root hair dimensions at four different levels of added phosphate concentration , viz., 150 p.p.m. , 300 p.p.m., 600 p.p.m., and 1000 p.p.m.. The mass uptake $U = U(t)$ was computed by writing

$$R = \frac{a}{r} ,$$

in eq.(2·9) and then applying Simpson's rule . A check was made by evaluating $\frac{dU}{dt}$, as given by eq.(2·11) , at each time step and then integrating .

§ 2 : Summary of Results :

Clearly the problem (5·1) has no immediate bearing on the original problem (1·1) and its associated mathematical difficulties as it purposely avoids the discontinuous initial condition . A numerical solution of (1·1) for large times (up to five days) has not been attempted because of the large amount of computing time required by the methods of Chapter IV ; however in Chapter VI an attempt is made to obtain an asymptotic solution of eq.(4·9) valid for large times , and futher thought along these lines is still necessary .

Consequently no comparison of the results has yet been attempted and numerical results of eq.(5·1) and the results of the plant experiments of Lewis [22] are presented without due criticism .

Plant experiments conducted at the Waite Institute showed that the phosphorus uptake per plant per day was practically constant after the first two weeks of the plant's life . The measured uptake per plant per day for three levels of added phosphate concentration are given below :

150 p.p.m.	53 μgrams
600 p.p.m.	290 μgrams
2000 p.p.m.	530 μgrams

For eq.(5·1) the computed rates of uptake per m.m. of main root (or root hair) length per day were also fairly constant and are given below :

Conc. of added P (μgms P/ gm soil)	Uptake Rates (grams per day)	
	Main Root	Root Hair
150	$1{\cdot}6 \times 10^{-9}$	$1{\cdot}6 \times 10^{-10}$
300	$6{\cdot}8 \times 10^{-9}$	$7{\cdot}7 \times 10^{-10}$
600	32×10^{-9}	26×10^{-10}
1000		49×10^{-10}

———

The results of these computations are displayed in more detail in figs. 4 , 5 , 6 , and 7. Fig. 4 gives the computed phosphorus depletions for C_o = 150 p.p.m., and fig. 5 gives computed phosphorus depletions for C_o = 600 p.p.m. The percentage depletion has been plotted against the distance from the main root (or root hair) surface for 1 , 2 , 3 , and 5 days. Fig. 6 gives computed phosphorus uptakes for the root hair dimensions at 150 , 300 , 600 , and 1000 p.p.m. , and fig. 7 gives computed phosphorus uptakes for the main root dimensions at 150 , 300 , and 600 p.p.m.

Since each millimetre of active main root has about fifty root hairs each about 1 m.m. in length , the above results suggest that the root hairs are , per unit length , about four times as efficient as the larger main root , and that root hairs account for about 80 % of the total phosphorus uptake. Calculated lengths of active root are from 2 to 6 metres per plant ; but from the tables above , at 600 p.p.m. , 1·8 metres of root (together with its root hairs) would be required to account for the phosphorus absorbed by the plant. A similar length would be required at the other phosphate levels.

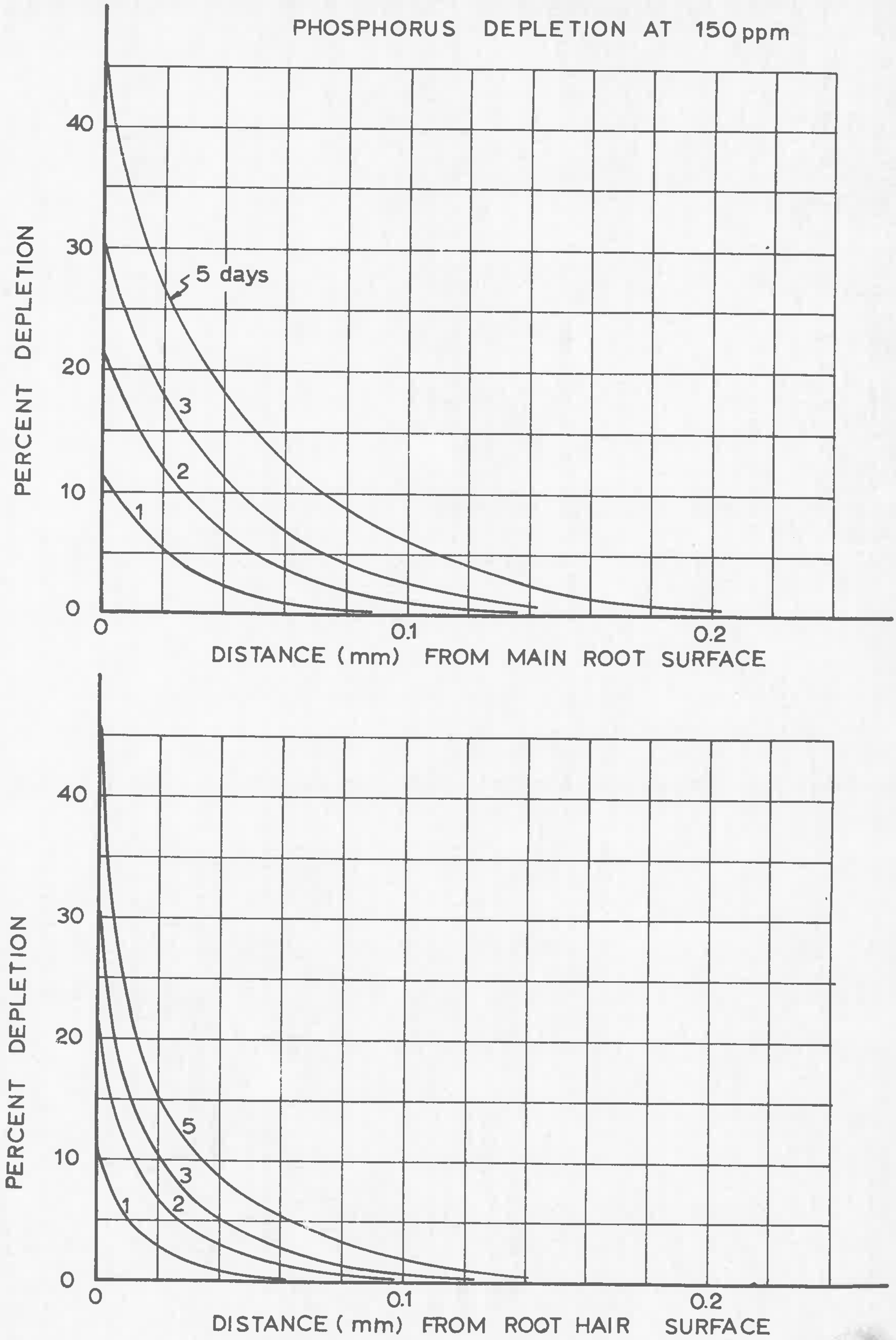
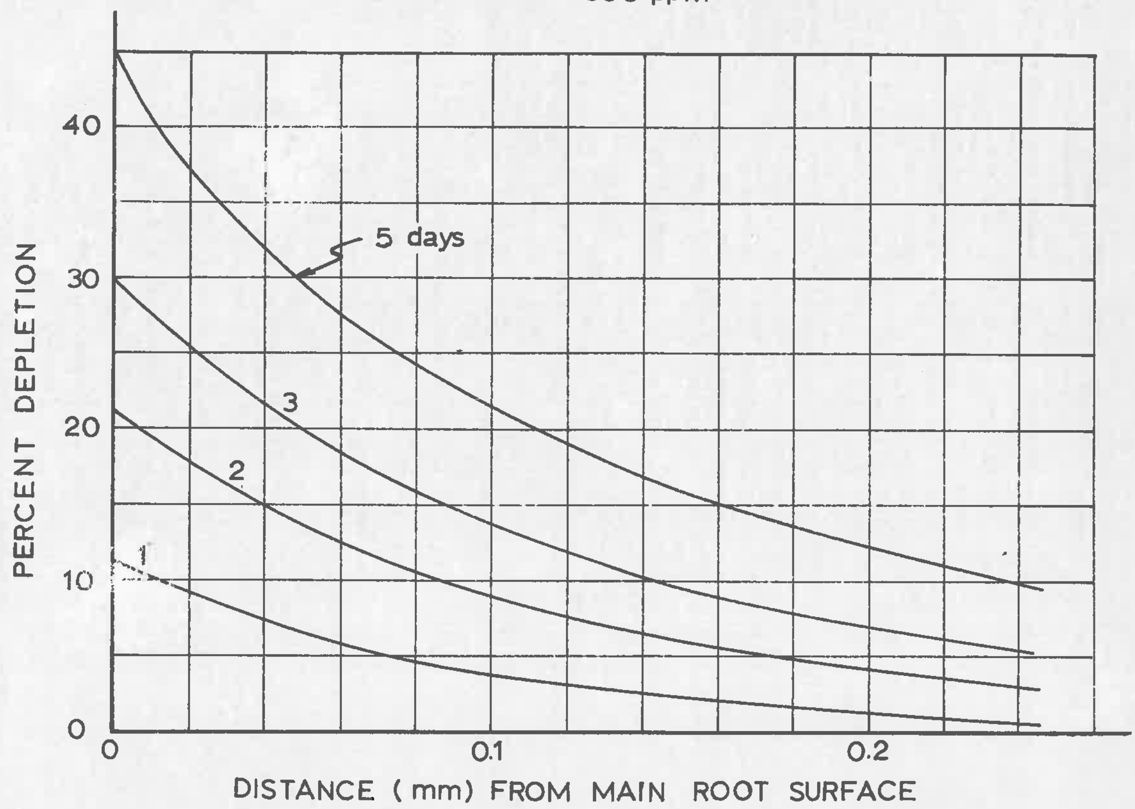

PHOSPHORUS DEPLETION AT 150 ppm
PERCENT DEPLETION
40
30
20
10
0
5 days
3
2
1
0
0.1
0.2
DISTANCE (mm) FROM MAIN ROOT SURFACE
PERCENT DEPLETION
40
30
20
10
0
5
3
2
1
0
0.1
0.2
DISTANCE (mm) FROM ROOT HAIR SURFACE

Fig. 4

COMPUTED PHOSPHORUS DEPLETIONS

AT 600 ppm



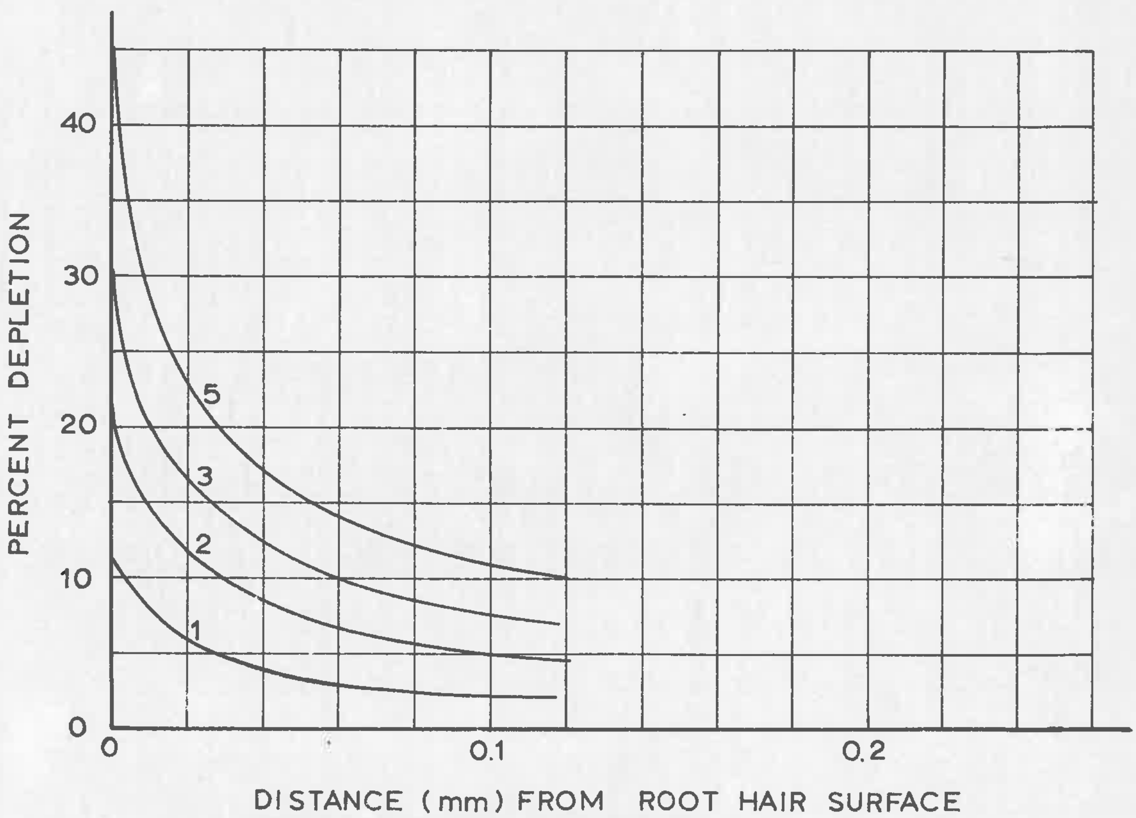


Fig.5

COMPUTED PHOSPHORUS UPTAKE

Root Hair Diameter = 0.01 mm

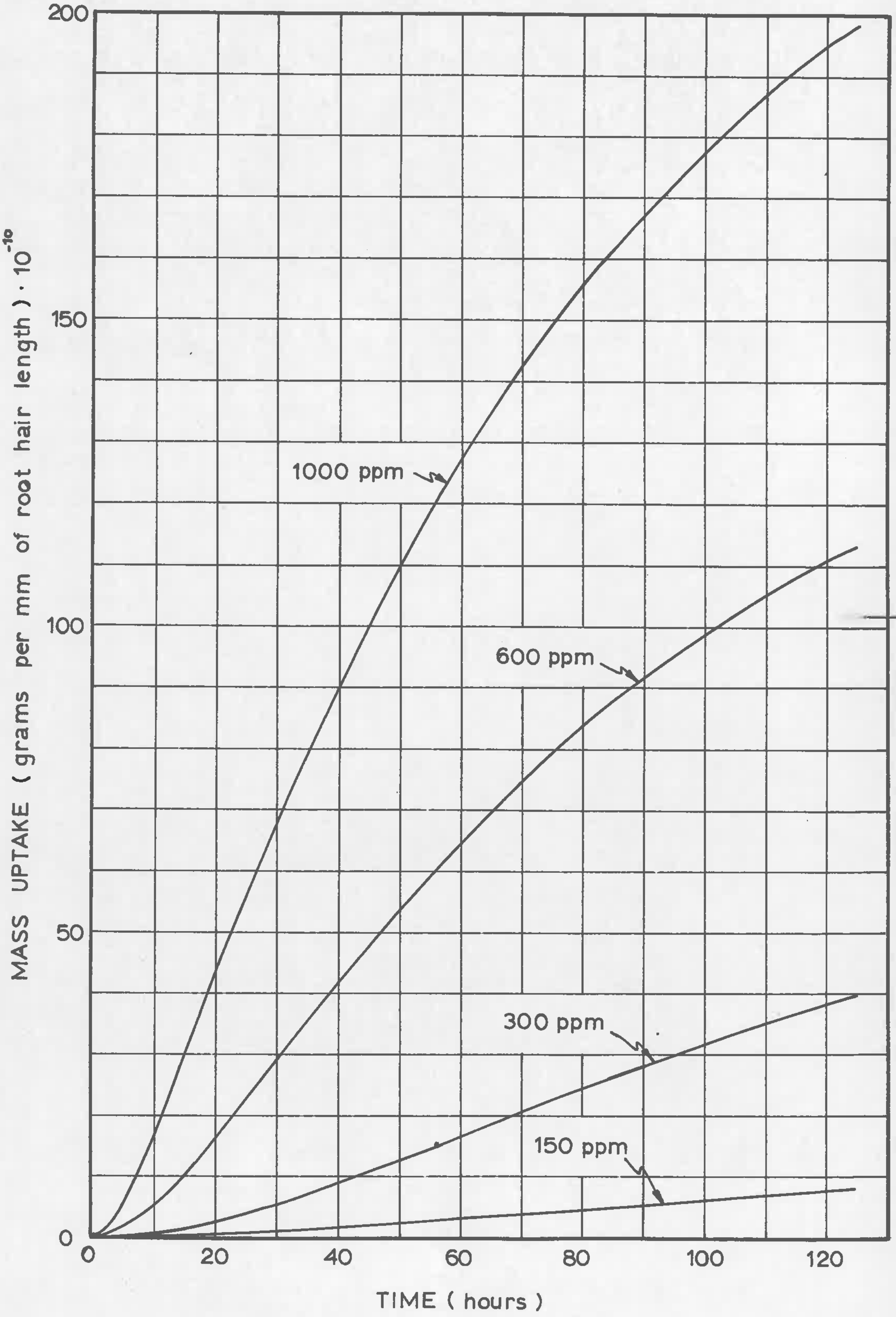


Fig. 6

COMPUTED PHOSPHORUS UPTAKE

Main Root Diameter = 0.4 mm

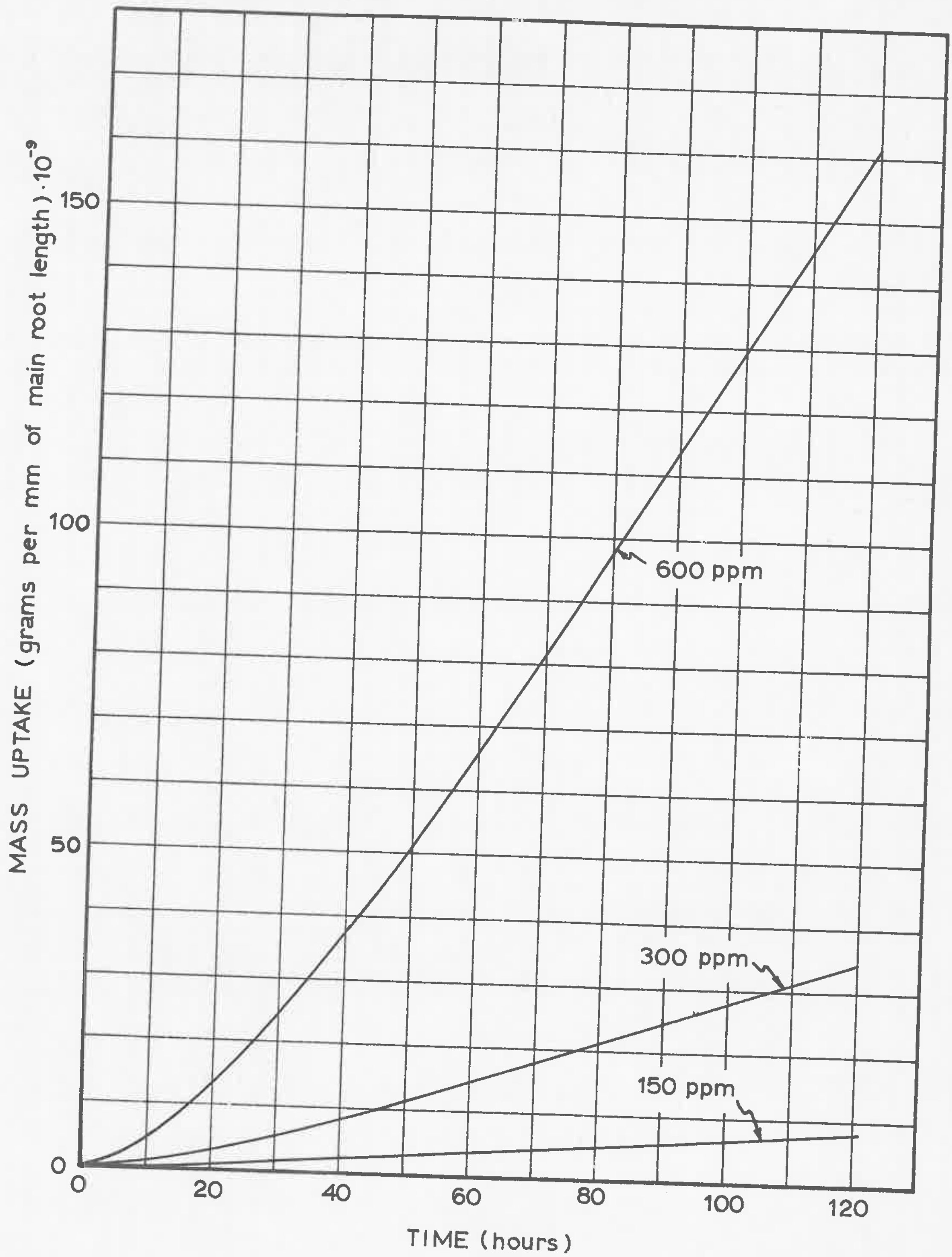


Fig.7

CHAPTER VI

Further Developments of the Problem

§ 1 : An Asymptotic Approximation for Large Times :

We investigate the solution of the linear diffusion problem (B·7) of Appendix II with the view of obtaining an asymptotic approximation, valid for large times, of the non-linear equation (4·9).

Writing $\varepsilon = ah'$ in eq.(B·9) we consider

$$\bar{\bar{V}} = \frac{\varepsilon K_0(qs)}{p[qK_1(q) + \varepsilon K_0(q)]} . \qquad (6\cdot1)$$

To obtain an approximate solution valid for large times we expand (6·1) for small q by utilizing the expansions

$$K_0(z) = -\ln(\tfrac{1}{2}Cz)I_0(z) + \frac{1}{4}z^2 + \frac{3}{128}z^4 + \ldots ,$$

$$K_1(z) = \ln(\tfrac{1}{2}Cz)I_1(z) - \frac{1}{4}(z - \frac{4}{z}) - \frac{1}{32}z^3 \ldots ,$$

$$I_\nu(z) = \sum_{r=0}^{\infty} \frac{(\frac{1}{2}z)^{\nu+2r}}{r!\,(\nu + r)!} , \quad \nu = 0, 1 ,$$

where $\ln C = \gamma = 0{\cdot}5772156649\ldots$.

The dominant term in the denominator of (6·1) is $\varepsilon K_0(q)$ for any positive ε however small.

Therefore (6·1) becomes

$$\bar{\bar{V}} = -\frac{\varepsilon\{\ln(\frac{1}{2}Cqs) + \frac{1}{4}s^2q^2[\ln(\frac{1}{2}Cqs) - 1] + \frac{1}{64}s^4q^4[\ln(\frac{1}{2}Cqs) - \frac{3}{2}]\ldots\}}{p\{-\varepsilon\ln(\frac{1}{2}Cq) + 1 + \frac{1}{2}q^2[\ln(\frac{1}{2}Cq) - \frac{1}{2}] - \frac{\varepsilon p}{4}[\ln(\frac{1}{2}Cq) - 1]\ldots\}} , \qquad (6\cdot2)$$

and the dominant term in the denominater of (6·2) is $-\varepsilon\ln(\frac{1}{2}Cq)$.

On removing this term as a factor we obtain

$$\bar{\bar{V}} = \frac{\{\ln(\frac{1}{2}Cqs) + \frac{1}{4}s^2p[\ln(\frac{1}{2}Cqs) - 1] + \ldots\}}{pL\{1 - \frac{1}{\varepsilon L} + \frac{p}{2\varepsilon}[1 - \frac{1}{2L}] + \frac{p}{4}[1 - \frac{1}{L}]\ldots\}} , \qquad (6\cdot3)$$

where $L = \ln(\tfrac{1}{2}Cq) = \tfrac{1}{2}\ln(\frac{C^2 p}{4})$.

Using the binomial theorem, and writing $\sigma = \ln s$, we then simplify (6·3) and obtain

$$\bar{V} = \frac{1}{p} + (\sigma + \frac{1}{\varepsilon})\frac{1}{pL} + \frac{1}{\varepsilon}(\sigma + \frac{1}{\varepsilon})\frac{1}{p\,L^2} + [\frac{(\sigma-1)(s^2-1)}{4} + \frac{s^2+2\sigma-3}{4\,\varepsilon} + \frac{1}{\varepsilon^2}]\,\frac{1}{L} \cdots \tag{6·4}$$

Eq.(6·4) is valid provided that s is not too large. However if s tends to infinity the previous expansion of $K_o(qs)$ becomes invalid and must be replaced by the expression given in (B·11) .

The Laplace transform inversion formula

$$f(t) = \frac{1}{2\pi i}\int_{c - i\infty}^{c + i\infty} e^{tp}\,\bar{f}(p)\,dp \quad ,$$

is now used to find the inverse Laplace transform of the function

$$\bar{f}(p) = \frac{1}{p \ln p} \quad , \tag{6·5}$$

for

$$0 < R(p) < 1 \quad .$$

We first note the result

$$\mathcal{L}\{\,\nu(t)\,\} = \frac{1}{p \ln p} \quad , \quad R(p) > 1 \quad ,$$

where $\nu(t)$ is defined by

$$\nu(t) = \int_0^\infty \frac{t^s\,ds}{\Gamma(s + 1)} \quad ,$$

(see Bateman Manuscript Project , Vols. 1 and 3) .

Clearly the same result is not true for $0 < R(p) < 1$ because $\bar{f}(p)$ has a singularity at $p = 1$. However the singularity can be removed and we consider

$$\bar{g}(p) = \frac{1}{p \ln p} - \frac{1}{p - 1} \quad ,$$

which has only a branch point at $p = 0$.

The contour of the complex integration is sketched in Appendix II , § 1 , where $0 < \mathcal{R}(p) < 1$ for the straight line path AB . It can easily be verified that the contributions from the small circle surrounding the origin , and the large semi-circle are both zero in the limit .

We write

$$p = x\ell^{i\pi} \quad \text{on CD} ,$$

$$p = x\ell^{-i\pi} \quad \text{on EF} ,$$

and hence obtain

$$g(t) = -\int_0^\infty \frac{\ell^{-xt}\,dx}{x[(\ln x)^2 + \pi^2]} .$$

But $\mathcal{L}^{-1}\{\frac{1}{p-1}\} = 0$ for $0 < \mathcal{R}(p) < 1$, $t > 0$,

therefore $\mathcal{L}^{-1}\{\frac{1}{p \ln p}\} = g(t)$, $0 < \mathcal{R}(p) < 1$.

We shall now define

$$\nu_*(t) = -\int_0^\infty \frac{\ell^{-xt}\,dx}{x[(\ln x)^2 + \pi^2]} ;$$

then we can set up a table of Laplace transforms valid for $0 < \mathcal{R}(p) < 1$ as follows :

$\nu_*(t)$	$\frac{1}{p \ln p}$
$\nu_*'(t)$	$\frac{1}{\ln p}$
$t\,\nu_*'(t)$	$\frac{1}{p(\ln p)^2}$
$\nu_*'(t) + t\,\nu_*''(t)$	$\frac{1}{(\ln p)^2}$

By use of the above transforms , eq.(6·4) can be inverted and $V(s,\tau)$ obtained . For the range of values of s for which eq.(6·4) is valid it is clear that $V(s,\tau) \to 1$ as $\tau \to \infty$, however a detailed study of the asymptotic behaviour of the functions $\nu_*(t)$, ... is still necessary .

For the range of values of s for which eq.(6·4) is not valid we obtain

$$\bar{V} = -\frac{\varepsilon}{pL}\left[\frac{\pi}{2qs}\right]^{\frac{1}{2}} \ell^{-qs}\left[1 - \frac{1}{8qs} + \ldots\right]\left[1 - \frac{1}{\varepsilon L} - \frac{p}{2\varepsilon}\left[1 - \frac{-1}{2L}\right] + \frac{p}{4}\left[1 - \frac{1}{L}\right]\right]^{-1},$$

of which the leading term is

$$\bar{V}_o = -\varepsilon\left[\frac{\pi}{2qs}\right]^{\frac{1}{2}} \frac{\ell^{-qs}}{p^{5/4}L} .$$

From the table of transforms of Carslaw and Jaeger [4]

$$\mathcal{L}^{-1}\{\ell^{-qs}\} = \frac{s}{2\sqrt{(\pi\tau^3)}}\exp[-s^2/4\tau] ;$$

and by complex integration , we obtain

$$\mathcal{L}^{-1}\left\{\frac{1}{p^{5/4}\ln p}\right\} = \frac{1}{\pi\sqrt{2}}\int_0^\infty \frac{\ell^{-tx}[\ln x + \pi]dx}{x^{5/4}[(\ln x)^2 + \pi^2]} .$$

Hence it can be shown that $V_o \rightarrow 0$ as $s \rightarrow \infty$, and thus the boundary condition (B·7)(iii) is satisfied .

The possibility of utilizing this 'large time' asymptotic approximation to obtain an asymptotic solution of eq.(4·9) still needs further investigation . However it is clear that the ratio of non-linear to linear terms in (4·9) tends to unity as $\tau \rightarrow \infty$, and there seems little chance of success in devising an iteration procedure for estimating the non-linear terms.

§ 2 : Conclusions :

The work covered in this thesis is in no way a complete numerical study of this particular non-linear diffusion equation , and no attempt has been made to study all of the many possible finite difference representations which can be used to obtain numerical solutions of parabolic partial differential equations . The selection of the best difference scheme for a particular problem is usually determined by the accuracy obtained for a given computing time and by other practical considerations . Most of the computations done here utilize a modified backward difference representation , which , in this case , gives rise to simple linear difference equations which can easily be solved numerically.

The numerical study of linear diffusion equations is clearly facilitated by the ease with which analytical solutions can be obtained , and the problem of an initially discontinuous boundary condition presents no difficulty . However for the non-linear diffusion equation discussed in this thesis , the need for good asymptotic approximations becomes clear as an analytical solution is not possible .

Our results show that a numerical solution can be obtained , at least for small values of the parameter ah' , without adopting any special starting procedure at $t = 0$, and that transient effects due to the initial discontinuity diminish with increasing time . However we are really more interested in the numerical solution for fairly large times (t in the order of days) and it is clear that some means of starting the computations well clear of $t = 0$ would be a great advantage .

The simple asymptotic approximation (B·13) , though valid for a very small $\tau_o > 0$ only , has been used successfully to overcome the effect of the discontinuity at $\tau = 0$; but it is felt that a more detailed study of the asymptotic approximation (4·16) could contribute much to the future numerical study of the problem .

APPENDIX I

Summary of Relevant Experimental Work

§ 1: Measurement and calculation of diffusion coefficient :

Various soils were used for the diffusion experiments at the Waite Institute [22] , but only Seddon sandy loam , a lateritic podzolic soil from Kangaroo Island , SouthA Australia is considered here. The relation between the diffusion coefficient (D) and the concentration of absorbable phosphorus (C) was established by means of a Perspex diffusion cell. Initially each half of the cell contained the same ^{31}P concentration , but one half of the cell contained a small known amount of ^{32}P in addition. Several samples over a wide range of ^{31}P concentration were prepared , and after a time of six hours the amount of ^{32}P transferred across the boundary was measured.

As established by Klute and Letey (1958) [18] , this is a linear diffusion problem , and if we define

$u = u(x,t) =$ concentration of ^{32}P ,

$D =$ diffusion coefficient ,

$\lambda =$ a constant depending on the rate of decay of the radio-active isotope ,

$t =$ time ,

$h =$ depth of the half-cell ,

the diffusion equation becomes

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - \lambda u ,$$

subject to

$$\frac{\partial u}{\partial x} = 0 , \quad x = 0 , \quad x = 2h , \qquad (A\cdot1)$$

and

$$u = 0 , \quad h < x < 2h , \quad t = 0 ,$$

$$u = u_0 , \quad 0 < x < h , \quad t = 0 .$$

The equation (A·1) is readily solved by separation of variables as Klute and Letey indicate , and an appropriate formula for $\frac{Q}{Q_\infty}$ is obtained , viz.,

$$\frac{Q}{Q_\infty} = 1 - \frac{8}{\pi^2}\sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp\left[- \frac{(2n+1)^2 \pi^2 D t}{4 h^2} \right] , \quad (A·2)$$

where

Q = amount of ^{32}P transferred across the boundary in time t ,

Q_∞ = amount of ^{32}P transferred at $t = \infty$.

If $\frac{Q}{Q_\infty} < 0·5$, the above relation can be replaced (vide [18]) by

$$\frac{Q}{Q_\infty} = \frac{2}{h}\sqrt{\frac{Dt}{\pi}} , \quad (A·3)$$

and it is from this very simple formula that D has actually been calculated , because eq.(A·2) does not permit D to be calculated directly.

---

§2 : The Experiment for the First Model :

The diffusion coefficient (D) is regarded as a function of the concentration C of 'absorbable' phosphorus , and a table of values of C and corresponding values of D was obtained by Lewis [22] by using the diffusion cell described in § 1 . It is important to note that the 'absorbable' phosphorus includes the phosphorus in the soil solution and also that amount of phosphorus in the soil which can be desorbed into the soil solution .

Table 1 : Water Content 20 %

C Conc. of added phosphorus (μgms P / gm soil)	D Diffusion coefficient ($\times 10^{-4}$ cm^2/day)
50	0·064 ± 22 %
100	0·16 ± 12 %
300	0·62 ± 10 %
1000	4·3 ± 7 %
2000	21·5 ± 7 %

In this diffusion coefficient experiment the treated soil containing the desired level of added phosphate was left moist for four days before sealing. It was considered that this was a long enough time for the soil solution concentration to reach a steady value. The sealed diffusion cell was then left for a six day period before separating the two halves of the cell and performing the necessary measurements for calculating D . The whole experiment was repeated for a diffusion time of fourteen days (instead of six days) and it was found that the new calculated values of D were 25 to 40 % lower than the ones previously obtained. One reason for this change might be that the four day settling period was inadequate ; however , more detailed suggestions for improving the experiment are given by Lewis [22] .

A law of the form

$$D = \alpha C^M ,$$

where α , M are constants to be determined , was fitted to the points in table 1 and plotted in fig. 1 ,(vide page 9). Quick calculations were made and the law

$$D = \alpha C^2 , \quad \alpha \text{ const.},$$

was proposed and the constant α then determined by minimizing

$$\sum_{\nu=1}^{5} [D_\nu - \alpha C_\nu^2]^2 ,$$

where (D_ν , C_ν) , $(\nu = 1 , .. 5)$ were the values in table 1 .

Hence

$$\alpha = 2560 .$$

---

§ 3 : The Experiment for the second Model :

The balance between the 'absorbable' phosphorus concentration , denoted by C in the first model and now denoted by C_1 , and the soil solution concentration , denoted by C can be related by a law of the form

$$C_1 = A C^N , \qquad (A \cdot 4)$$

where A and N are constants determined experimentally for each particular soil and given water content.

The Kangaroo Island soil samples have a fixed water content of 20 %, and the assumption is made that all added phosphate can eventually be desorbed into the soil solution.

Table 2:

C_1 Conc. of added phosphate (μgms P / gm soil)	C Conc. of soil solution (μgms P / gm soil sol$^{n.}$)
100	0·21
300	0·14
500	1·65
750	5·65
1000	10·6
1250	32·9
1500	68·2
2000	172·8

Full details of the actual experiment are given by Lewis [22] .

The values at 100 p.p.m. and 300 p.p.m. are unreliable due to low accuracy of measurements at low soil solution concentrations and have been omitted from the determination of the law. The method of least squares of fitting a linear law

$$Y = P X + Q ,$$

to a given set of values (Y_ν, X_ν) , $\nu = 1 , .. , n$, consists of minimizing the sum of squares

$$\sum_{\nu=1}^{n} [Y_\nu - P X_\nu - Q]^2 .$$

From our table of values ,

$$N = 0{\cdot}330 ,$$

$$A = 0{\cdot}0394 ;$$

and so (A·4) becomes

$$C_1 = 0{\cdot}0394\ C^{0\cdot330} . \qquad (A{\cdot}5)$$

APPENDIX II

Analytical and Asymptotic Solutions of the Linear Diffusion Equation

§ 1 : Solutions of Linear Diffusion Equations by Laplace Transforms :

In this appendix we find the analytical solutions of the linear diffusion problems having the same boundary conditions as the non-linear ones considered in this thesis . Goldstein [10] and Carslaw and Jaeger [4] have shown how readily the Laplace transformation method can be used to solve these problems.

Problem 1 :

Consider the equation

$$\frac{\partial C}{\partial t} = k\left[\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r}\right] ,$$

$$a \leqslant r < \infty , \quad t \geqslant 0 ,$$

subject to (B·1)

$$\text{(i)} \quad C(r,0) = C_o , \quad a \leqslant r < \infty ,$$

$$\text{(ii)} \quad C(a,t) = \phi(t) , \quad \phi(o) = C_o ,$$

$$\text{(iii)} \quad C(r,t) = C_o \quad \text{as } r \to \infty ,$$

where $\phi(t)$ is differentiable and the diffusion coefficient k is constant . Equation (B·1) is best solved in a non-dimensional form , and , rewritten in terms of $u(s,\tau)$, becomes

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial s^2} + \frac{1}{s}\frac{\partial u}{\partial s} ,$$

$$1 \leqslant s < \infty , \quad \tau \geqslant 0 ,$$

subject to (B·2)

$$\text{(i)} \quad u(s,0) = 0 , \quad 1 \leqslant s < \infty ,$$

$$\text{(ii)} \quad u(1,\tau) = \psi(\tau) , \quad \psi(0) = 0 ,$$

$$\text{(iii)} \quad u(s,\tau) \to 0 \quad \text{as } s \to \infty ,$$

where

$$u = \frac{C_o - C}{C_o} \quad , \qquad s = \frac{r}{a} \quad , \qquad \tau = \frac{k\,t}{a^2} \quad ,$$

and $\psi(\tau)$ is a differential function of τ determined from $\phi(t)$.

Writing

$$\bar{v} = \mathcal{L}\{ u(s,\tau) \} = \int_0^\infty e^{-p\tau}\, u(s,\tau)\, d\tau \quad , \quad p > 0 \quad ,$$

and multiplying eq.(B·2) by $e^{-p\tau}$ and integrating from 0 to ∞ , an ordinary differential equation is obtained , viz.,

$$\frac{d^2 \bar{v}}{ds^2} + \frac{1}{s}\frac{d\bar{v}}{ds} - q^2 \bar{v} = 0 \quad , \quad (q^2 = p) \quad ,$$

subject to (B·3)

(i) $\bar{v}(1,p) = \bar{\psi}(p)$,

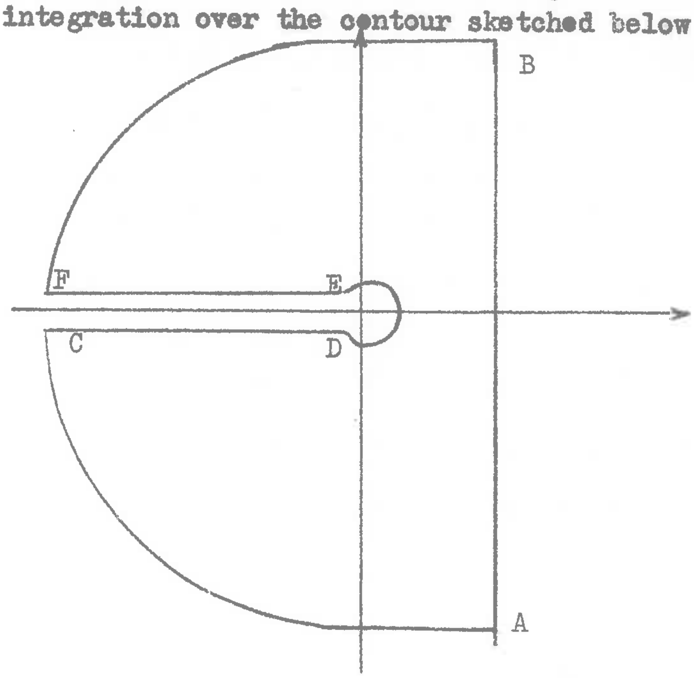
(ii) $\bar{v}(s,p) = 0$ as $s \to \infty$.

The solutions of eq.(B·3) are the modified Bessel functions $K_o(qs)$ and $I_o(qs)$, using the conventional notation .

Thus

$$\bar{v} = \bar{\psi}' \frac{K_o(qs)}{p\, K_o(q)} \quad , \qquad \text{(B·4)}$$

and the inverse Laplace transform of $\frac{K_o(qs)}{p\,K_o(q)}$ can be found by complex integration over the contour sketched below :



As in Carslaw and Jaeger [4] we find

$$\mathcal{L}^{-1}\left[\frac{K_o(qs)}{pK_o(q)}\right] = 1 + \frac{2}{\pi}\int_0^{\infty} e^{-x^2\tau}\,\frac{J_o(xs)Y_o(x) - Y_o(xs)J_o(x)}{x[J_o^2(x) + Y_o^2(x)]}\,dx .$$

Then using the convolution theorem for Laplace transforms we obtain the desired expression for $u(s,\tau)$, viz.,

$$u(s,\tau) = \psi(\tau) - \int_0^{\tau} dt\, \psi'(\tau - t)\int_0^{\infty} e^{-x^2 t}\,\frac{2[Y_o(xs)J_o(x) - J_o(xs)Y_o(x)]}{\pi\, x[J_o^2(x) + Y_o^2(x)]}\,dx . \qquad (B\cdot5)$$

<u>Problem 2</u> :

Consider the equation

$$\frac{\partial C}{\partial t} = k\left[\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r}\right] ,$$

$$a \leqslant r < \infty , \quad t \geqslant 0 ,$$

subject to (B·6)

(i) $C(r,0) = C_o , \quad a \leqslant r < \infty ,$

(ii) $\frac{\partial C}{\partial r} = h' C , \quad r = a , \quad t > 0 ,$

(iii) $C(r,t) \rightarrow C_o \quad \text{as} \quad r \rightarrow \infty .$

In non-dimensional form , the equation for $u(s,\tau)$ becomes

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial s^2} + \frac{1}{s}\frac{\partial u}{\partial s} ,$$

$$1 \leqslant s < \infty , \quad \tau \geqslant 0 ,$$

subject to (B·7)

(i) $u(s,0) = 0 , \quad 1 \leqslant s < \infty ,$

(ii) $\frac{\partial u}{\partial s} = -ah'(1 - u) , \quad s = 1 , \quad \tau > 0 ,$

(iii) $u(s,\tau) \rightarrow 0 \quad \text{as} \quad s \rightarrow \infty .$

The auxiliary equation is

$$\frac{d^2\bar{v}}{ds^2} + \frac{1}{s}\frac{d\bar{v}}{ds} - q^2\bar{v} = 0 ,$$

subject to

$$\frac{d\bar{v}}{ds} = -ah'\left(\frac{1}{p} - \bar{v}\right) , \quad s = 1 , \qquad \text{(B·8)}$$

$$\bar{v} \to 0 \quad \text{as} \quad s \to \infty ;$$

and the solution of (B·8) is

$$\bar{v} = \frac{ah' K_0(qs)}{p[qK_1(q) + ah'K_0(q)]} . \qquad \text{(B·9)}$$

By complex integration [4] over the contour of problem 1 , the inverse Laplace transform of $\bar{v}$ can be obtained , i.e.

$$u(s,\tau) = \frac{2\varepsilon}{\pi}\int_0^\infty \frac{dx}{x}\, e^{-x^2\tau}\, \frac{\{Y_0(xs)[xJ_1(x)+\varepsilon J_0(x)] - J_0(xs)[xY_1(x)+\varepsilon Y_0(x)]\}}{\{(xJ_1(x)+\varepsilon J_0(x))^2 + (xY_1(x)+\varepsilon Y_0(x))^2\}} ,$$

where $\varepsilon = ah'$.

---

§ 2 : An asymptotic Solution of the Non-linear Diffusion Problem :

The non-linear diffusion problem (1·1) can be written in the non-dimensional form

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial s^2} + \frac{1}{s}\frac{\partial u}{\partial s} - \left[(2u - u^2)\left(\frac{\partial^2 u}{\partial s^2} + \frac{1}{s}\frac{\partial u}{\partial s}\right) + 2(1-u)\left(\frac{\partial u}{\partial s}\right)^2\right] ,$$

subject to (B·10)

(i) $u(s,0) = 0 , \quad 1 < s < \infty ,$

(ii) $\frac{\partial u}{\partial s} = -\varepsilon(1-u) , \quad s = 1 , \tau > 0 ,$

(iii) $u(s,\tau) \to 0 \quad \text{as} \quad s \to \infty .$

Clearly the contribution of the non-linear terms in the square brackets in (B·10) will be small if ε and τ are also small , and a good approximation to the non-linear problem will be given by the linear diffusion problem (B·7) .

To obtain an asymptotic approximation valid for small times we therefore expand (B·9) in powers of $\frac{1}{q}$. Using

$$K_o(z) = [\frac{\pi}{2z}]^{\frac{1}{2}} \ell^{-z}\{1 - \frac{1}{8z} + \frac{9}{128 z^2} - O(\frac{1}{z^3})\} ,$$

$$K_1(z) = [\frac{\pi}{2z}]^{\frac{1}{2}} \ell^{-z}\{1 + \frac{3}{8z} - \frac{15}{128 z^2} + O(\frac{1}{z^3})\} , \qquad (B\cdot11)$$

$$K_o'(z) = - K_1(z) ,$$

we obtain

$$\bar{v} = \frac{\varepsilon \ell^{-q(s-1)}}{pq\sqrt{s}}\{1 - \frac{A}{q} + \frac{B}{q^2} - \frac{C}{q^3} + O(\frac{1}{q^4})\} , \qquad (B\cdot12)$$

where

$$A = \frac{1}{8s} + \frac{3}{8} + \varepsilon ,$$

$$B = \frac{33}{128} + \frac{7\varepsilon}{8} + \varepsilon^2 + \frac{9}{128s^2} + \frac{3}{64s} + \frac{\varepsilon}{8s} ,$$

$$C = \varepsilon^3 + \frac{11\varepsilon^2}{8} + \frac{105\varepsilon}{128} + \frac{279}{1024} + \frac{75}{1024s^3} + \frac{33}{1024s} + \frac{7\varepsilon}{64s}$$

$$+ \frac{\varepsilon^2}{8s} + \frac{27}{1024s^2} + \frac{9\varepsilon}{128s^2} .$$

Now if

$$\bar{v}_n = \frac{\ell^{-q(s-1)}}{p^{1+\frac{1}{2}n}} , \qquad n = 1 , 2 , \ldots ,$$

then the inverse Laplace transform v_n is given by

$$v_n = (4\tau)^{\frac{1}{2}n} \; i^n \operatorname{erfc} \frac{s-1}{2\sqrt{\tau}} ,$$

where $i^n \operatorname{erfc} \frac{s-1}{2\sqrt{\tau}}$ is the n-th repeatdd integral of the error function. Laplace transforms and properties of the functions $i^n\operatorname{erfc} x$ are given in [4] and tables have been constructed by Kaye[17] .

Thus we obtain

$$v(s,\tau) = \frac{\varepsilon}{\sqrt{s}}\{ 2\sqrt{\tau}\; i \operatorname{erfc} \frac{s-1}{2\sqrt{\tau}} - 4A\tau\; i^2\operatorname{erfc} \frac{s-1}{2\sqrt{\tau}} + 8B\tau^{3/2} i^3\operatorname{erfc} \frac{s-1}{2\sqrt{\tau}}$$

$$- 16C\tau^2\; i^4 \operatorname{erfc} \frac{s-1}{2\sqrt{\tau}} \} \qquad (B\cdot13)$$

This expansion is valid for small τ over the whole range $1 \leq s < \infty$.

APPENDIX III

Useful Modifications of the Method of Gaussian Elimination

§ 1 : Matrices of Tridiagonal Form :

The method of Gaussian elimination is employed in the numerical solution of the matrix equation

$$A \underset{\sim}{\phi} = \underset{\sim}{\psi} , \qquad (C\cdot1)$$

where the $n \times n$ matrix $A = [a(i,j)]$ and the vector $\underset{\sim}{\psi} = [\psi(i)]$, $(i = 1, .., n)$ are both known. However it is well known that the numerical work can be simplified considerably if the matrix A is of tridiagonal form, and (C·1) can be written as

$$p_i\phi_{i-1} - q_i\phi_i + r_i\phi_{i+1} = \psi_i , \qquad (C\cdot2)$$

$$(i = 1, 2, \ldots, n) ,$$

where $r_n = 0$, $p_1 = 0$, $\phi_o = 0$.

From (C·2) we find

$$\phi_{i+1} = \frac{q_i\phi_i - p_i\phi_{i-1} + \psi_i}{r_i} , \qquad (C\cdot3)$$

for $i = 1, 2, \ldots, n$.

But we can use similar relations to substitute successively for ϕ_{i-1}, ϕ_{i-2}, ... respectively in eq.(C·3). Thus eq.(C·3) can also be written as

$$\phi_{i+1} = \frac{\alpha_i\phi_i + S_i}{r_i} , \qquad (C\cdot4)$$

where α_i and S_i are to be determined.

For $i = 1$,

$$\alpha_1\phi_1 + S_1 = q_1\phi_1 - p_1\phi_o + \psi_1 .$$

Hence

$$\alpha_1 = q_1 ,$$

$$S_1 = \psi_1 .$$

For $i = 2$,

$$\alpha_2\phi_2 + S_2 = q_2\phi_2 - p_2\phi_1 + \psi_2 ,$$

$$= q_2\phi_2 - \frac{p_2}{\alpha_1}(r_1\phi_2 - S_1) + \psi_2 .$$

Hence

$$\alpha_2 = q_2 - \frac{p_2 r_1}{\alpha_1} ,$$

$$S_2 = \psi_2 + \frac{p_2 S_1}{\alpha_1} .$$

Assuming

$$\alpha_i = q_i - \frac{p_i r_{i-1}}{\alpha_{i-1}} ,$$

$$S_i = \psi_i + \frac{p_i S_{i-1}}{\alpha_{i-1}} , \qquad (C\cdot5)$$

are true , it can easily be shown that this set of equations also holds for $i+1$ in place of i . Hence by induction (C·5) is valid for all values $i = 2 , \ldots , n$.

From eq.(C·4) , putting $i = n$, we get

$$\phi_n = -\frac{S_n}{\alpha_n} ,$$

and also

$$\phi_i = \frac{r_i\phi_{i+1} - S_i}{\alpha_i} , \qquad (C\cdot6)$$

for $i = n-1 , n-2 , \ldots , 2 , 1$.

The success of the method , i.e. its numerical stability , depends on the condition that the multipliers

$$\lambda_i = \frac{p_i}{\alpha_{i-1}} , \quad i = 2 , \ldots , n ,$$

satisfy

$$|\lambda_i| < 1 . \qquad (C\cdot7)$$

These multipliers determine the numbers α_i and S_i which must be computed before evaluating (C·6) .

§ 2 : Matrices with Five Diagonals of Non-zero Elements :

The same procedure as in § 1 also applies in the case when eq.(C·1) can be written as

$$m_i\phi_{i-2} + p_i\phi_{i-1} - q_i\phi_i + r_i\phi_{i+1} + s_i\phi_{i+2} = \psi_i \ , \qquad (i = 1, 2, \ldots, n) \ , \tag{C·8}$$

where $m_1 = m_2 = p_1 = s_{n-1} = s_n = r_n = \phi_{-1} = \phi_o = 0$.

From eq.(C·8) we find

$$\phi_{i+2} = \frac{\psi_i - m_i\phi_{i-2} - p_i\phi_{i-1} + q_i\phi_i - r_i\phi_{i+1}}{s_i} \ , \tag{C·9}$$

for $i = 1, 2, \ldots, n$,

and we can use similar relations to substitute successively for ϕ_{i+1}, ϕ_i, ... respectively in eq.(C·9) .

Thus eq.(C·9) can also be written as

$$\phi_{i+2} = \frac{T_i + \alpha_i\phi_i + \beta_i\phi_{i+1}}{s_i} \ , \tag{C·10}$$

where α_i, β_i and T_i are to be determined .

For $i = 1$,

$$\psi_1 + q_1\phi_1 - r_1\phi_2 = T_1 + \alpha_1\phi_1 + \beta_1\phi_2 \ .$$

Thus

$$T_1 = \psi_1 \ , \quad \alpha_1 = q_1 \ , \quad \beta_1 = -r_1 \ .$$

Similarly for $i = 2$,

$$T_2 = \psi_2 + \frac{p_2}{\alpha_1} T_1 \ ,$$

$$\alpha_2 = q_2 + \frac{p_2}{\alpha_1}\beta_1 \ ,$$

$$\beta_2 = -r_2 - \frac{p_2}{\alpha_1} s_1 \ ,$$

and for $i = 3$,

$$T_3 = \psi_3 + \frac{m_3}{\alpha_1} T_1 + \left(p_3 - \frac{m_3 \beta_1}{\alpha_1} \right) \frac{T_2}{\alpha_2} ,$$

$$\alpha_3 = q_3 - \frac{m_3}{\alpha_1} s_1 + \left(p_3 - \frac{m_3 \beta_1}{\alpha_1} \right) \frac{\beta_2}{\alpha_2} ,$$

$$\beta_3 = - r_3 - \left(p_3 - \frac{m_3 \beta_1}{\alpha_1} \right) \frac{s_2}{\alpha_2} .$$

Straightforward induction shows that

$$T_i = \psi_i + \frac{m_i}{\alpha_{i-2}} T_{i-2} + \left(p_i - \frac{m_i \beta_{i-2}}{\alpha_{i-2}}\right) \frac{T_{i-1}}{\alpha_{i-1}} ,$$

$$\alpha_i = q_i - \frac{m_i}{\alpha_{i-2}} s_{i-2} + \left(p_i - \frac{m_i \beta_{i-2}}{\alpha_{i-2}}\right) \frac{\beta_{i-1}}{\alpha_{i-1}} , \qquad (C\cdot 11)$$

$$\beta_i = - r_i - \left(p_i - \frac{m_i \beta_{i-2}}{\alpha_{i-2}} \right) \frac{s_{i-1}}{\alpha_{i-1}} ,$$

hold for $i = 3 , \ldots , n$.

Putting $i = n$ in eq . (C·10) , we get

$$\phi_n = - \frac{T_n}{\alpha_n} ,$$

and putting $i = n-1$ in eq.(C·10) , we get

$$\phi_{n-1} = - \frac{T_{n-1} + \beta_{n-1}\phi_n}{\alpha_{n-1}} , \qquad (C\cdot 12)$$

and so

$$\phi_i = \frac{s_i \phi_{i+2} - \beta_i \phi_{i+1} - T_i}{\alpha_i} ,$$

for $i = n-2$, $n-3$, ... , 2 , 1 .

The numbers T_i , α_i , and β_i ($i = 1 , \ldots , n$) are first computed from (C·11) ; then ϕ_n , ϕ_{n-1} , .. ϕ_1 can be calculated .

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