RECEIVED BY DTIE OCT 10 1967

OAK RIDGE NATIONAL LABORATORY

operated by

UNION CARBIDE CORPORATION

NUCLEAR DIVISION

for the

U.S. ATOMIC ENERGY COMMISSION

MASTER

ORNL - TM - 1970

130

**NUMERICAL SOLUTION OF THE ISOTHERMAL FISSION-PRODUCT
DEPOSITION EQUATIONS: THE PROGRAM PREDEP-II**

T. S. Kress
Paul Nelson, Jr.

NOTICE This document contains information of a preliminary nature and was prepared primarily for internal use at the Oak Ridge National Laboratory. It is subject to revision or correction and therefore does not represent a final report.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

- A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or
- B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

ORNL-TM-1970

Contract No. W-7405-eng-26

UNIT PRICES

MATHEMATICS DIVISION

H.C. \$ 3.00 MN 65

NUMERICAL SOLUTION OF THE ISOTHERMAL FISSION-PRODUCT

DEPOSITION EQUATIONS: THE PROGRAM PREDEP-II

T. S. Kress

Paul Nelson, Jr.

OCTOBER 1967

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee
operated by
UNION CARBIDE CORPORATION
for the
U.S. ATOMIC ENERGY COMMISSION

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

CONTENTS

	Page
Abstract.....	1
I. Introduction.....	1
II. Dimensionless Variables.....	5
a. Physically Convenient Dimensionless Variables.....	5
b. Dimensionless Variables for Computation.....	7
III. The Method of Solution.....	11
a. Transformation to a System of Integral Equations...	11
b. The Finite-Difference Scheme.....	12
c. Discussion.....	14
IV. The Program PREDEP-II.....	17
Acknowledgment.....	23
References.....	24
Appendix - The Steady-State Problem.....	25

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

109

NUMERICAL SOLUTION OF THE ISOTHERMAL FISSION-PRODUCT

DEPOSITION EQUATIONS: THE PROGRAM PREDEP-II

T. S. Kress
Paul Nelson, Jr.

ABSTRACT

The heat-mass analogy was previously used to develop a semilinear system of partial differential equations to describe the isothermal deposition of fission products. In this report this system is transformed into a system of integral equations in computationally convenient variables, and a finite-difference method for the solution of the integral equation system is described. A brief description is given of the computer program PREDEP-II, which accepts data in terms of physically convenient dimensionless variables, transforms these to the computational variables for means of solving the finite-difference equations, and finally reports the results in terms of the physical variables.

I. INTRODUCTION

Kress and Neill [2, Eqs. 7 and 8] proposed the system of partial differential equations,

$$\frac{\partial \bar{N}}{\partial t} + \bar{U}_x \frac{\partial \bar{N}}{\partial x} + \left\{ \lambda + \frac{4h}{D} - \frac{4h^2}{D[h + \sigma \text{Kr}(1 - M/M_S)]} \right\} \bar{N} - \left\{ \frac{4h\theta}{D[h + \sigma \text{Kr}(1 - M/M_S)]} \right\} M = 0, \quad (1)$$

and

$$\frac{\partial M}{\partial t} + \left\{ \theta + \lambda - \frac{\sigma \text{Kr}(1 - M/M_S)\theta}{[h + \sigma \text{Kr}(1 - M/M_S)]} \right\} M - \left\{ \frac{h \sigma \text{Kr}(1 - M/M_S)}{[h + \sigma \text{Kr}(1 - M/M_S)]} \right\} \bar{N} = 0, \quad (2)$$

to describe the deposition of fission products from a carrier stream onto an isothermal conduit surface. Here $\bar{N}$ and M , the stream volume

density and wall areal density of fission products, respectively, are functions of time, t , and distance x along the conduit. The other quantities in Eqs. (1), (2) are physical constants described fully in [2]. The notation of [2] is followed as closely as possible in the present report, but, for completeness, various constants appearing in the above equations and in §IIa are defined briefly in the following list:

D - conduit equivalent diameter

g_c - proportionality constant

h - mass transfer coefficient

Kr - gross collision rate term = $(RTg_c/2\pi m)^{1/2}$

m - molecular weight of the fission product

M_S - saturation limit of fission-product surface concentration

R - universal gas constant

T - absolute temperature

$\bar{U}_x$ - carrier stream bulk mean axial velocity

θ - desorption coefficient; rate of desorption from conduit surface
= θM

λ - fission-product decay constant

μ - carrier stream viscosity

ν - carrier stream kinematic viscosity ($= \mu/\rho$)

ρ - carrier stream density

σ - fraction of those molecules striking bare conduit surface which are adsorbed

τ_w - wall shearing stress

The partial differential equations (1), (2) are to be solved for the unknowns $\bar{N}(x,t)$, $M(x,t)$, subject to the auxiliary conditions

$$\bar{N}(0,t) = \bar{N}_0, \quad (3)$$

$$\bar{N}(x,0) = 0, \quad 0 < x, \quad (4)$$

and

$$M(x,0) = 0, \quad 0 \leq x. \quad (5)$$

Here $\bar{N}_0$ is a constant density for an assumed uniform source.

The present report describes a method developed for numerically solving the initial-boundary problem defined by Eqs. (1)-(5). In Chapter II we describe two transformations of the problem into equivalent problems defined in terms of dimensionless variables. The first transformation allows us to define the minimal number of independent, physically meaningful, parameters. The resulting dimensionless variables are convenient for comparison with physical intuition and with the existing literature, but are not convenient for computational purposes. Consequently we introduce a further change of variables which does result in a computationally convenient formulation of the problem. Data may then be accepted in terms of the first set of dimensionless variables, transformed to the second set for purposes of computation, and transformed back into the physically convenient variables.

The method of solution is described and discussed in Chapter III. The semilinear system (1), (2) is connected into a pair of coupled integral equations of the second kind by formally integrating along the characteristics of the system, and the integral equations are then solved by a finite-difference scheme. This basic method is well-known

(for example [1, §8.3]), but there is some freedom in choosing the system of integral equations and in choosing the difference scheme to be used. We made a considerable effort to select procedures which promise to give good results for the initial-boundary problem defined by Eqs. (1)-(5). Some discussion of the reasons for these choices is given in section c of Chapter III, along with a description of some possible alternate choices and refinements of the selected scheme.

Chapter IV contains a description and discussion of typical results obtained using the numerical method described earlier. Some attention is given there to various practical problems encountered in using the numerical method on a computing machine. The computer program was written in FORTRAN/360 for the IBM 360/75 at the Oak Ridge National Laboratory. A listing of the computer program may be obtained from the authors.

II. DIMENSIONLESS VARIABLES

a. Physically Convenient Dimensionless Variables

The following is adapted from reference [2], especially pp.5-6. Symbols not defined explicitly here are explained in the preceding chapter.*

We define new independent variables by

$$t_* = t(\tau_w g_c / \mu), \quad x_* = x/D, \quad (6)$$

and new dependent variables by

$$\bar{N}_*(x_*, t_*) = \bar{N}(x, t) / \bar{N}_O, \quad (7)$$

$$M_*(x_*, t_*) = M(x, t) \sqrt{\tau_w g_c / \rho} / \bar{N}_O v.$$

In addition we define

$$\left. \begin{aligned} D_* &= D \sqrt{\tau_w g_c / \rho} / v, \quad \theta_* = \theta / (\tau_w g_c / \mu), \\ U_* &= U_* / \sqrt{\tau_w g_c / \rho}, \quad \lambda_* = \lambda / (\tau_w g_c / \mu), \\ M_{S_*} &= M_S \sqrt{\tau_w g_c / \rho} / \bar{N}_O v, \quad h_* = h / \sqrt{\tau_w g_c / \rho}, \\ Kr_* &= (RT g_c / 2\pi m)^{1/2} / \sqrt{\tau_w g_c / \rho} = Kr / \sqrt{\tau_w g_c / \rho} \end{aligned} \right\} \quad (8)$$

In terms of these new variables and constants, the equations (1) and (2) are

$$\frac{\partial \bar{N}_*}{\partial t_*} + \frac{U_*}{D_*} \frac{\partial \bar{N}_*}{\partial x_*} + \left\{ \lambda_* + \frac{4h_*}{D_*} - \frac{4h_*^2}{D_* [h_* + \sigma Kr_* (1 - M_*/M_{S*})]} \right\} \bar{N}_* - \left\{ \frac{4h_* \theta_*}{D_* [h_* + \sigma Kr_* (1 - M_*/M_{S*})]} \right\} M_* = 0, \quad (1*)$$

$$\frac{\partial M_*}{\partial t_*} + \left\{ \theta_* + \lambda_* - \frac{\theta_* \sigma Kr_* (1 - M_*/M_{S*})}{[h_* + \sigma Kr_* (1 - M_*/M_{S*})]} \right\} M_* - \left\{ \frac{h_* \sigma Kr_* (1 - M_*/M_{S*})}{[h_* + \sigma Kr_* (1 - M_*/M_{S*})]} \right\} \bar{N}_* = 0, \quad (2*)$$

and the auxiliary conditions (3) - (5) are

$$\bar{N}_* (0, t_*) = 1, \quad (3*)$$

$$\bar{N}_* (x_*, 0) = 0, \quad 0 < x_* , \quad (4*)$$

$$M (x_*, 0) = 0, \quad 0 \leq x_* . \quad (5*)$$

We further introduce the Blasius friction coefficient, C_f , in terms of which

$$U_* = 1/\sqrt{C_f}, \quad (9)$$

and

$$D_* = \sqrt{C_f N_{Re}}, \quad (10)$$

where N_{Re} is the Reynolds number of the physical system.

The friction coefficient can be expressed as a function of the Reynold's number, N_{Re} , and the relative roughness, k_* ,

$$C_f = G(N_{Re}, k_*) . \quad (11)$$

In particular for a smooth surface C_f is well-represented by the formula

$$C_f = C_{fo} = 0.316/8(N_{Re})^{1/4} . \quad (12)$$

Furthermore the dimensionless mass transfer film coefficient, h_* , can be expressed as a function of C_f , N_{Re} , and the Schmidt number, N_{Sc}

$$h_* = H(C_f, N_{Re}, N_{Sc}) . \quad (13)$$

Inspection of Eqs. (9) - (13) show that we can now select the seven independent paramcters θ_* , λ_* , σKr_* , M_{S*} , N_{Re} , N_{Sc} and k_* as fundamental for the problem defined by Eqs. (1*) - (5*).

b. Dimensionless Variables for Computation

We expect M_* to vary between 0 and M_{S*} , $\bar{N}_*$ between 0 and 1. Equation (2*) and the auxiliary conditions (3*) - (5*) show that $(\partial M_*/\partial t)_0 = h_* \sigma Kr_*/(h_* + \sigma Kr_*)$ at $(x, t) = (0, 0)$. Thus a characteristic time (in terms of the dimensionless time t_*) for the variation of M_* between 0 and M_{S*} is given by

$$\tau = \frac{(h_* + \sigma Kr_*) M_{S*}}{h_* \sigma Kr_*} \quad (14)$$

Letting L be the length of the conduit under consideration, we define new independent variables by

$$\tilde{t} = t_*/\tau, \quad \tilde{x} = x_*D/L = x/L, \quad (15)$$

and new dependent variables by

$$\tilde{N}(\tilde{x}, \tilde{t}) = \bar{N}_*(\tilde{x}L/D, \tilde{t}\tau) = \bar{N}_*(x_*, t_*) , \quad (16)$$

$$\tilde{M}(\tilde{x}, \tilde{t}) = M_*(\tilde{x}L/D, \tilde{t}\tau)/M_{S*} = M_*(x_*, t_*)/M_{S*} .$$

We also define the following constants:

$$D_0 = D/L , \quad (17)$$

$$\epsilon = D_*/\tau U_* D_0 ,$$

$$\lambda_1 = \lambda_* D_*/D_0 U_* ,$$

$$\alpha = 4M_{S*}/U_* D_0 \tau ,$$

$$A = \sigma K r_* \tau / M_{S*} = 1 + \frac{\sigma K r_*}{h_*} \quad (18)$$

$$B = \theta_* \tau$$

$$a = \sigma K r_*/h_* = A-1$$

$$\lambda_2 = \lambda_* \tau .$$

In terms of these new variables and the constants defined by (18), the equations (1*) and (2*) become

$$\frac{\partial \tilde{N}}{\partial \tilde{x}} + \epsilon \frac{\partial \tilde{N}}{\partial \tilde{t}} + \left\{ \lambda_1 + \frac{\alpha A(1-\tilde{M})}{1+a(1-\tilde{M})} \right\} \tilde{N} - \frac{\alpha B \tilde{M}}{1+a(1-\tilde{M})} = 0, \quad (1')$$

$$\frac{\partial \tilde{M}}{\partial \tilde{t}} + \left\{ \lambda_2 + \frac{B}{1+a(1-\tilde{M})} \right\} \tilde{M} - \frac{A(1-\tilde{M}) \tilde{N}}{1+a(1-\tilde{M})} = 0, \quad (2')$$

where, for brevity, the arguments $(\tilde{x}, \tilde{t})$ are omitted everywhere. The auxiliary conditions (3*) - (5*) are transformed into

$$\tilde{N}(0, \tilde{t}) = 1, \quad 0 \leq \tilde{t} \quad (3')$$

$$\tilde{N}(\tilde{x}, 0) = 0, \quad 0 < \tilde{x} \leq 1, \quad (4')$$

and

$$\tilde{M}(\tilde{x}, 0) = 0, \quad 0 \leq \tilde{x} \leq 1. \quad (5')$$

The problem now is to solve the system (1'), (2') of partial differential equations on $0 \leq \tilde{x} \leq 1$, $0 \leq \tilde{t}$, subject to the auxiliary conditions (3') - (5'). From the interpretation of τ as a characteristic time for deposition of the fission product of interest, we expect the solution $\tilde{M}(\tilde{x}, \tilde{t})$ to essentially reach a steady-state for values of $\tilde{t}$ somewhat larger than unity, say certainly for $\tilde{t} \approx 10$.

The above development shows that the solution of the problem depends on seven independent parameters, namely, those defined by Eqs. (18). These parameters can, in turn, be calculated in terms of the seven fundamental parameters of the previous section and the additional parameter D_0 defined by (17). The introduction of the "extra" parameter D_0 is essentially the price one must pay to limit the range of values of x to the fixed bounded set $0 < \tilde{x} < 1$.

III. THE METHOD OF SOLUTION

a. Transformation to a System of Integral Equations

We will work only with the problem defined by (1')-(5') henceforth and, for convenience, will delete the tildes in referring to the variables in these equations. The equations (1') and (2') form a semilinear hyperbolic first-order system of two partial differential equations in two independent variables and two unknowns. The characteristic curves of this system are the lines $C_{\bar{t}} = \{(x, t) | t - \epsilon x = \bar{t}\}$ for an arbitrary nonnegative constant $\bar{t}$, and the lines $x = \text{constant}$. Integrating Eq. (1') along an arbitrary line $C_{\bar{t}}$, $\bar{t} \geq 0$, we find, on using the condition (3'),

$$N(x, \bar{t} + \epsilon x) = \exp \left\{ - \int_0^x \left[\lambda_1 + \frac{\alpha A [1 - M(s, \bar{t} + \epsilon s)]}{1 + a [1 - M(s, \bar{t} + \epsilon s)]} \right] ds \right. \\ \left. + \alpha B \int_0^x \left\{ \frac{M(s, \bar{t} + \epsilon s)}{1 + a [1 - M(s, \bar{t} + \epsilon s)]} \right\} \exp \left\{ - \int_s^x \left[\lambda_1 + \frac{\alpha A [1 - M(y, \bar{t} + \epsilon y)]}{1 + a [1 - M(y, \bar{t} + \epsilon y)]} \right] dy \right\} ds \right\}, \quad \bar{t} \geq 0, \quad (19)$$

Similarly, integrating (2') along a line of constant x , $0 \leq x \leq 1$ and using (5'), we find

$$M(x, t) = A \int_{\epsilon x}^t \frac{[1 - M(x, s)]}{1 + a [1 - M(x, s)]} N(x, s) \exp \left\{ - \int_s^x \left[\lambda_2 + \frac{B}{1 + a [1 - M(x, y)]} \right] dy \right\} ds, \quad (20)$$

The condition (4') has been used implicitly in obtaining Eq. (20). This condition along with (5') imply, as may easily be shown, that the solutions M and N are identically zero in the part of the xt -plane under the characteristic C_0 , and thus we may write ϵx rather than 0 for the lower limit in the first integral in (20).

Equations (19) and (20) are a coupled pair of integral equations for the unknowns M and N on the set $D = \{(x, t) | 0 \leq x \leq 1, \epsilon x \leq t\}$. These equations form the basis for our further analysis.

b. The Finite-Difference Scheme

We let $0 = x_1 < x_2 < \dots < x_n = 1$, $0 = t_1 < t_2 < \dots < t_j < t_{j+1} < \dots$, be partitions of the unit interval on the x -axis and the positive t -axis, respectively. It is not necessary that the points of these partitions be equispaced, although this will normally be the most convenient arrangement. The points $(x_i, t_j + \epsilon x_i)$ are the grid points in the xt -plane for a finite-difference approximation to Eqs. (19) and (20). Equations (19) and (20) easily yield, respectively

$$N(x_{i+1}, t_j + \epsilon x_{i+1}) = N(x_i, t_j + \epsilon x_i) \exp \left\{ - \int_{x_i}^{x_{i+1}} \left[\lambda_1 + \frac{\alpha A[1-M(s, t_j + \epsilon s)]}{1 + \alpha[1-M(s, t_j + \epsilon s)]} \right] ds \right\} \quad (21)$$

$$+ \alpha B \int_{x_i}^{x_{i+1}} \left\{ \frac{M(s, t_j + \epsilon s)}{1 + \alpha[1-M(s, t_j + \epsilon s)]} \right\} \exp \left\{ - \int_s^{x_{i+1}} \left[\lambda_1 + \frac{\alpha A[1-M(y, t_j + \epsilon y)]}{1 + \alpha[1-M(y, t_j + \epsilon y)]} \right] dy \right\} ds ,$$

$$M(x_i, t_{j+1} + \epsilon x_i) = M(x_i, t_j + \epsilon x_i) \exp \left\{ - \int_{t_j + \epsilon x_i}^{t_{j+1} + \epsilon x_i} \left[\lambda_2 + \frac{B}{1 + \alpha[1-M(x_i, s)]} \right] ds \right\} \quad (22)$$

$$+ A \int_{t_j + \epsilon x_i}^{t_{j+1} + \epsilon x_i} \left\{ \frac{[1-M(x_i, s)]}{1 + \alpha[1-M(x_i, s)]} N(x_i, s) \right\} \exp \left\{ - \int_s^{t_{j+1} + \epsilon x_i} \left[\lambda_2 + \frac{B}{1 + \alpha[1-M(x_i, y)]} \right] dy \right\} ds .$$

Alternatively, these equations may be obtained directly from Eqs. (1') and (2') by integrating from $(x_i, t_j + \epsilon x_i)$ to $(x_{i+1}, t_j + \epsilon x_{i+1})$ along the

characteristic C_{t_j} , and from $(x_i, t_j + \epsilon x_i)$ to $(x_i, t_{j+1} + \epsilon x_i)$ along the characteristic $x = x_i$, respectively.

We denote the finite-difference approximation to $N(x_i, t_j + \epsilon x_i)$ by $N_{i,j}$, and similarly for M . We define the finite-difference approximation to (21) by replacing $M(x_i, s)$, $x_i \leq s \leq x_{i+1}$, on the right-hand side by $M_{i,j}$. The result is

$$\begin{aligned} N_{i+1,j} = N_{i,j} \exp \left\{ - \left[\lambda_1 + \frac{\alpha A(1-M_{i,j})}{1+a(1-M_{i,j})} \right] (x_{i+1} - x_i) \right\} \\ + \frac{\alpha B M_{i,j}}{\lambda_1 + (a\lambda_1 + \alpha A)(1-M_{i,j})} \left\{ 1 - \exp \left\{ - \left[\lambda_1 + \frac{\alpha A(1-M_{i,j})}{1+a(1-M_{i,j})} \right] (x_{i+1} - x_i) \right\} \right\}. \end{aligned} \quad (23)$$

Similarly the finite-difference approximation to (22) is defined by replacing $M(x_i, s)$ and $N(x_i, s)$ on the right-hand side by $M_{i,j}$ and $N_{i,j}$, respectively, the result being

$$\begin{aligned} M_{i,j+1} = M_{i,j} \exp \left\{ - \left[\lambda_2 + \frac{B}{1+a(1-M_{i,j})} \right] (t_{j+1} - t_j) \right\} \\ + \frac{A(1-M_{i,j}) N_{i,j}}{\lambda_2 [1+a(1-M_{i,j})] + B} \left\{ 1 - \exp \left\{ - \left[\lambda_2 + \frac{B}{1+a(1-M_{i,j})} \right] (t_{j+1} - t_j) \right\} \right\}. \end{aligned} \quad (24)$$

Equations (23) and (24) are solved with j as the "marching" index. Given $M_{i,j}$ for $i = 1, \dots, n$ and some fixed j , and also given $N_{1,j}$, we first obtain $N_{i,j}$, $i = 2, \dots, n$, from (23), and then $M_{i,j+1}$, $i = 1, \dots, n$, from (24). The starting conditions are defined by

$$M_{i,1} = 0, \quad i = 1, \dots, n, \quad (25)$$

and the $N_{1,j}$ are defined by

$$N_{1,j} = 1, \quad j = 1, \dots \quad (26)$$

The equations (23)-(26) define a completely explicit finite-difference scheme.

c. Discussion

The system (1')-(5') could be converted to a system of integral equations in many ways. The most obvious is to simply integrate Eqs. (1') and (2') along their respective characteristics, rather than so integrating after multiplication by an integrating factor as was done in obtaining Eqs. (19) and (20). The resulting equations could then be solved by an "Euler-like" finite-difference scheme. However the present treatment should be more accurate, particularly if the parameters and step sizes are such that the exponential terms on the right-hand sides of (23) and (24) are significantly smaller than unity.

One could develop more accurate numerical solutions to Eqs. (19)-(20) than that described in the preceding section, at the cost of increased complexity. For example the finite-difference analogs of (19) and (20) could be written as implicit equations (linear or nonlinear) in the $N_{i,j+1}$, $M_{i,j+1}$ for known $N_{i,j}$, $M_{i,j}$, or the equations could be solved numerically by some predictor-corrector method similar to those for ordinary differential equations. For the range of physical parameters of interest in the present study, the method of §IIIb seems to work reasonably well, although there are some "stability" difficulties which might be alleviated by slightly varying the difference method (see Chapter IV). One should be aware that major modifications might be advantageous or even necessary in other parameter ranges.

The problem of convergence of the difference method of §IIIb has not been considered. There is some question as to whether such questions

are really relevant to physical problems, except perhaps as an aside to obtaining error estimates. In any event these matters are quite difficult, and hardly seem worth pursuing in view of the present lack of knowledge regarding the validity of the basic equations.

It seems worth mentioning that Eqs. (1)-(5) can be transformed directly into a problem of the form (1')-(5'), but with values of the variables and parameters different from those given by Eqs. (14)-(18). Specifically, if we define

$$\tau' = \frac{(h + \sigma Kr) M_S}{h \sigma Kr}, \quad (14')$$

$$\tilde{t}' = t/\tau', \quad \tilde{x}' = x/L = \tilde{x}, \quad (15')$$

$$\left. \begin{aligned} \tilde{N}'(\tilde{x}', \tilde{t}') &= \bar{N}(x, t)/N_0, \\ \tilde{M}'(\tilde{x}', \tilde{t}') &= M(x, t)/M_S, \end{aligned} \right\} \quad (16')$$

substitute these into (1) and (2), and drop the primes, the resulting equations are of the form (1'), (2'), with

$$\left. \begin{aligned} \epsilon &= L/\tau' \bar{U}_x, \\ \lambda_1 &= L\lambda/\bar{U}_x, \\ \alpha &= 4 L M_S/(\bar{U}_x N_0 D \tau'), \\ A &= \sigma Kr N_0 \tau'/M_S, \\ B &= \theta \tau', \\ a &= \sigma Kr/h, \\ \lambda_2 &= \lambda \tau'. \end{aligned} \right\} \quad (18')$$

The transformation described in section IIb, and that given here, are useful in different ways, as follows. If the interest is in making a parametric study of the problem while varying a minimal number of physically meaningful parameters, then the problem (1')-(5') should be solved with the parameters defined by (18). However, if the interest is in writing a computer program which will solve the problem for any specific physical problem, defined by a nonminimal set of directly accessible physical parameters, then Eqs. (1')-(5') should be solved with the parameters defined by (18'). In either case the computational problem to be solved is given by Eqs. (1')-(5').

IV. THE PROGRAM PREDEP-II

The computer program PREDEP-II was written to accept sets of values of the seven parameters θ_* , λ_* , σKr_* , M_{S*} , N_{Re} , N_{Sc} , and k_* , compute the resulting values of the parameters defined by (18), and solve the corresponding difference equations (23) and (24). This program was intended to allow a parametric study of the problem. The program could be easily modified to yield a program which accepts as input the physical parameters appearing in Eqs. (1) - (5) and solves the corresponding problem (see §III c).

In this chapter we discuss the program PREDEP-II and the difference equations (23), (24) from a computational and numerical point of view. Specific results of the calculation will be mentioned only to show typical results and to illustrate numerical phenomena. The results of the parametric study will be presented elsewhere.

PREDEP-II accepts as input up to six different values of each of the parameters θ_* , λ_* , σKr_* , M_{S*} , N_{Re} , N_{Se} , k_* , D_o , and T_* , where T_* is the maximum value of t_* for which the calculation is to be carried out. The only other required input is the number K of x -points for which the computation is to be carried out, where the x -step Δx is taken as the constant $1/(K-1)$. The output is the value of $M_*(x_*, T_*)$ at the values of x_* corresponding to $x = j/(K-1)$, $j = 0, \dots, K-1$, for each combination of the eight input parameters listed above. A CALCOMP plot of $M_*(x_*, T_*)$ vs. x_* is generated for each combination of parameters, with the curves for different T_* and a fixed combination of the other parameters being shown on the same

graph. The constant value of the time step $\Delta t = t_{j+1} - t_j$ is selected internally as $\min \{ .01, 0.1T_*/\tau \}$. Typical results from PREDEP-II are shown in Figs. 1, 2, and 3.

For small Δx and Δt there is obviously the possibility of a large cancellation error occurring in the second terms on the right sides of Eqs. (23) and (24). This is avoided in PREDEP-II by writing x for $1 - e^{-x}$ if $0 \leq x < .01$.

One problem which recurred frequently in numerically implementing Eqs. (23) and (24) is as follows. If $N(x, t)$, $M(x, t)$ are the solutions of the problem defined by (1') - (5'), then these functions should increase monotonically in t for fixed x and approach the steady-state solutions $n(x)$, $m(x)$ (see Appendix), respectively, as $t \rightarrow \infty$. However, because of discretization and round-off errors, the difference equations (23), (24) will sometimes yield values of $M_{i,j}$ which are slightly larger than the corresponding value of $m(x)$. If this erroneous value $M_{i,j}$ is such that $\lambda_2 + \beta / [1 + a(1 - M_{i,j})]$ is positive then the difference equations (23), (24) are stable against the perturbation, and no great harm is done; however if $\lambda_2 + \beta / [1 + a(1 - M_{i,j})]$ is negative, then the difference equations begin to predict exponential growth of M because the argument of the exponential function in (24) becomes, and remains, positive, and likewise a rapid decrease in the calculated values of N occurs because of the second term on the right of (23). The latter situation is particularly likely to occur if λ_2 is small, a is large compared to unity, and $m(x)$ is near one. Indeed if a is large enough and λ_2 small enough there will be no machine number x sufficiently near 1

from above so that $\lambda_2 + \beta / [1 + a(1-x)]$ is nonnegative. Since $\lambda_2 = 0$ and $a \geq 10^3$ are of interest, and $m(x)$ can lie very near one, it can be seen that this instability is a very real problem. In PREDEP-II this problem is avoided by simply setting $M_{i,j+1}$ equal to the minimum of one and the value obtained from Eq. (24).

Since $M(x,t)$ is increasing in t , the quadrature formula by which Eq. (22) was converted to (24) will tend to cause the values obtained from (24) to be overestimates. This tends to increase the frequency of occurrence of the instability described in the preceding paragraph. One way of underestimating would be to replace (24) by the "predictor-corrector" method

$$\bar{M}_{i,j} = M_{i,j} g_1(M_{i,j}) + g_2(M_{i,j}) ,$$

$$M_{i,j+1} = M_{i,j} g_1(\bar{M}_{i,j}) + g_2(\bar{M}_{i,j}) ,$$

where $g_1(M_{i,j})$ is the exponential term and $g_2(M_{i,j})$ the second term on the right side of (24). This was not implemented for PREDEP-II because it was felt that an overestimate of M is more satisfactory than an underestimate for engineering purposes.

Fig. 1. Typical Results from PREDEP-II

Fig. 2. Typical Results from PREDEP-II

Fig. 3. Typical Results from PREDEP-II

ACKNOWLEDGMENTS

The authors wish to express their thanks to Messrs. A. R. Jenkins and D. R. Winkler, both of the ORNL Mathematics Division, for their very capable assistance in coding the computer program PREDEP-II.

REFERENCES

1. George E. Forsythe and Wolfgang R. Wasow, Finite-Difference Methods for Partial Differential Equations, Wiley, New York, 1960.
2. T. S. Kress and F. H. Neill, "A Model for Fission Product Transport and Deposition under Isothermal Conditions", ORNL-TM-1274, Oak Ridge National Laboratory, October 1965.

APPENDIX

The Steady-State Problem

The steady-state problem corresponding to equations (1')-(5') is

$$\frac{dn}{dx} + \lambda_1 n + \alpha \lambda_2 m = 0, \quad (A1)$$

$$\left\{ \lambda_2 + \frac{B}{1+a(1-m)} \right\} m - \frac{A(1-m)n}{1+a(1-m)} = 0, \quad (A2)$$

$$n(0) = 1, \quad (A3)$$

where $n(x) = \tilde{N}(x, \infty)$, $m(x) = \tilde{M}(x, \infty)$. Equation (A2) can be solved for m in terms of n (see the remark below), yielding

$$m(x) = \begin{cases} \frac{\lambda_2(1+a) + B + An - \sqrt{\{\lambda_2(1+a) + B + A'n\}^2 - 4\lambda_2 aAN}}{2a\lambda_2}, & a\lambda_2 \neq 0 \\ An/(B+An+\lambda_2) & , \quad a\lambda_2 = 0. \end{cases} \quad (A4)$$

If this result is substituted into (A1), then the resulting equation is a differential equation for n which is to be solved subject to the "initial" condition (A3). After finding n by solving this initial-value problem, $m(x)$ is found from (A4).

The manipulations described are particularly easy to carry out in the case $\lambda_1 = \lambda_2 = 0$. In this event the solution of the initial-value problem defined by Eqs. (A1), (A4) and (A3) is obviously $n(x) \equiv 1$, and the corresponding value of m is $m(x) \equiv A/(A+B)$. The range of parameters of interest includes $A \geq \sim 10^3$, $0 \leq B \leq \sim 10^{-1}$, and thus $m(x)$

can be very near one. In such situations one is very likely to encounter the instability problem mentioned in Chapter IV.

We remark that (A2) is equivalent to a quadratic equation in m , with coefficients depending on n . Both roots of this quadratic equation are positive. In writing (A4) we selected the smallest root because we are interested in the steady-state solution which is the limit of the solution $M(x,t)$ of (1'), (2') satisfying $M(x,0) = 0$. If we were interested in the steady-state solution corresponding to $M(x,0)$ a sufficiently large positive number, then the correct root of (A2) would be the largest root. This is another instance of the frequently occurring situation in which some knowledge of the underlying transient problem is necessary in order to select the "correct" steady-state solution.

INTERNAL DISTRIBUTION

1. R. D. Ackley	39. A. P. Malinauskas
2. D. W. Altom	40. H. C. McCurdy
3. D. E. Arnurius	41. A. B. Meservey
4. S. E. Beall	42. A. J. Miller
5. M. Bender	43. W. L. Morris
6. J. P. Blakely	44-54. F. H. Neill
7. A. L. Boch	55. C. W. Nestor, Jr.
8. W. E. Browning, Jr.	56. L. G. Overholser
9. J. R. Buchanan	57. G. W. Parker
10. S. Cantor	58. L. F. Parsley, Jr.
11. D. W. Cardwell	59. A. M. Perry
12. R. S. Carlsmith	60. M. W. Rosenthal
13. R. M. Carroll	61. A. W. Savolainen
14. S. T. Carroll	62. J. L. Scott
15. H. P. Carter	63. M. D. Silverman
16. W. B. Cottrell	64. O. Sisman
17. A. M. Craig	65. M. J. Skinner
18. F. L. Culler, Jr.	66. I. Spiewak
19. D. M. Eissenberg	67. J. G. Sullivan
20. W. K. Ergen	68. E. R. Taylor
21. M. Feliciano	69. D. B. Trauger
22. M. H. Fontana	70. W. C. Ulrich
23. A. P. Fraas	71. J. L. Wantland
24. D. L. Gray	72. G. M. Watson
25. W. O. Harms	73. G. D. Whitman
26. P. N. Haubenreich	74. C. S. Williams
27. A. S. Householder	75. D. R. Winkler
28. J. O. Kalb	76. E. I. Wyatt
29. S. I. Kaplan	77. W. D. Yuille
30. R. B. Korsmeyer	78-79. Central Research Library (CRL)
31-35. T. S. Kress	80-81. Document Reference Section (DRS)
36. M. I. Lundin	82-92. Laboratory Records (LRD)
37. R. N. Lyon	93. Laboratory Records - Record Copy (LRD-RC)
38. R. E. MacPherson	94-103. Mathematics Division
	104. Nuclear Safety Information Center

EXTERNAL DISTRIBUTION

- 105. W. E. Bell, General Atomic
- 106. H. W. Brishen, GENMPO, Evandale, Ohio
- 107. W. E. Bull, University of Tennessee
- 108. D. F. Bunch, AEC-IDO
- 109. R. M. Fryar, General Atomic
- 110. D. H. Imhoff, GEAP, San Jose
- 111. A. R. Jenkins, 2412 Pierce Ave., Apt. 902-E, Nashville, Tennessee
- 112. R. F. Kirkpatrick, AEC-Washington
- 113-117. Paul Nelson, Jr., Dept. of Math., Univ. of New Mexico, Albuquerque
- 118. M. N. Ozisik, North Carolina State University
- 119. R. E. Pahler, AEC-Washington
- 120. J. B. Radcliffe, AEC-SAN
- 121. G. E. Raines, BMI
- 122. J. H. Russell, LAMS
- 123. J. P. Waggner, The Franklin Institute
- 124. L. R. Zumwalt, North Carolina State University
- 125-126. General Atomic Library (Attention: R. B. Duffield and D. V. Ragone)
- 127. Laboratory and University Division, AEC-ORO
- 128-129. Reactor Division, AEC-ORO
- 130-144. Division of Technical Information (DTIE)