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TITLE

A MATHEMATICAL MODEL FOR PREDICTING VAPOUR DOSAGES ON AND DOWNWIND OF CONTAMINATED AREAS OF GRASSLAND

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SUFFIELD TECHNICAL PAPER NO. 386

A MATHEMATICAL MODEL FOR PREDICTING VAPOUR DOSAGES ON AND DOWNWIND OF CONTAMINATED AREAS OF GRASSLAND (U)

by

J. Monaghan and W.R. McPherson

PROJECT NO. 20-20-32

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ERRATA:

Abstract Page - last sentence - amend to read:

Le modèle est employé pour donner des exemples de calculs desquels quelques relations approximateurs sont deduites qui peuvent être employées pour développer des méthodes graphiques plus simples de calcul.

Page 4 - Equation (7) - amend to read:

$$\text{Peak } C(x,z) = C(x,z) \text{ erf } (Y/2^{\frac{1}{2}}\sigma_y(x)); \; Y = y_o/2, \qquad (7)$$

Page 31 - Line 13 - amend to read:

------ value as P/P_1 or P/P_a increases.

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ABSTRACT

Th~~is paper discusses~~ The problems of the evaporation of liquids sprayed on a rough natural surface which may absorb the sprayed material in both the liquid and vapour phases and the subsequent atmospheric diffusion of the vapour evolved, is discussed

A mathematical model for predicting vapour dosages downwind of contaminated areas of grassland is presented together with a description of numerical methods and the computer program employed to obtain solutions of the diffusion equations. Examples are given of calculations with the model from which approximate relations are deduced that can be used to develop simpler graphical methods of computation.

RÉSUMÉ

Ce document discute les problèmes de l'évaporation des liquides vaporisés sur un terrain accidenté (une surface naturelle accidentée) qui peut absorber la matière pulvérisée dans toutes les deux phases de liquide et de vapeur et la diffusion atmosphérique ultérieure du dégagement de gaz.

Un modèle mathématique pour prédire les dosages de vapeur dans la direction du vent des étendues de prairie contaminées est présenté accompagné d'une description de méthodes numériques et du programme d'ordinateur utilsé pour obtenir des solutions des équations de diffusion. Le modèle est employé pour donner des exemples de calculs desquels qui peuvent être employées pour développer des méthodes graphiques plus simples de calcul.

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INTRODUCTION

In chemical warfare the spraying of a target with a toxic agent challenges the target population with a liquid and a vapour hazard. The vapour hazard can be divided into two phases; that from vapour (or fine aerosol) evolved during spraying and that due to the evaporation of the deposited liquid. This paper applies to the latter, or persistent, phase of the vapour challenge and proposes a mathematical model for quantifying it in terms of vapour dosage accumulation with time on and downwind of the target area.

The model was developed in response to a need for a method of predicting vapour hazards for agents that are sorbed in both the liquid and vapour phases by natural terrain; this sorption effect is characteristic, to varying degrees, of the nerve agents on vegetation and bare ground. Besides sorption effects, account has been taken of the three-dimensional nature of the rough natural surface, and the discrete form of liquid deposits on the roughness elements of the surface in the formulation of expressions for vapour transfer between the air and the surface, and for evaporation rate. Atmospheric diffusion of the vapour was described by a modified form of the classical K theory with appropriate boundary conditions. Numerical solutions of the diffusion equations were obtained using a novel finite difference approximation method and a digital computer, and from these were developed simpler graphical methods for the calculation of vapour dosages. Data were acquired from supporting field experiments, and from other sources, from which parameter values were derived.

The theory of the model, the numerical solution of the diffusion equations, for which a computer program is provided, and simplified calculating procedures are described below. Tests and validation of the model against field data are dealth with in a separate paper.

THE PROBLEM

Open grassland is a complicated rough surface. Above the soil substrate there is a mat of older vegetation from which extend individual stems and blades of grass mingled with which are small plants. Liquid droplets sprayed on grassland impact at various depths in the vegetation and spread to form liquid films which may overlap and coalesce to an extent dependent upon the rate of application; however, unless the ground is flooded with liquid it is reasonable to suppose that the films together will never cover more than half the total surface of the vegetation.

Many substances including the nerve agents are absorbed by vegetation, and the plants behave internally as sinks of the absorbed material; special ambient conditions of humidity such as dew, associated with the opening of stomata are required for agent desorption. In general then, since the surface is never completely covered with liquid, a sprayed area of grassland is a complicated system of sources and sinks of agent; vapour evolved from the liquid film is diffused in the turbulent airstream from which it is absorbed by the dry fraction of the surface, at the same time the vegetation absorbs agent from the films. Downwind of the sprayed area the situation is relatively simpler since only absorption of vapour by the vegetation from the airstream is involved.

Local evaporation rates, or source strength per unit area of substrate, will generally decrease with time as individual films disappear at times determined by their initial thicknesses and positions above the substrate; however there will be a period following spraying when the area of the total evaporating surface of liquid will remain constant, or decrease so slowly, that the evaporation rates will remain practically constant. Vapour concentrations in the airstream above the surface will reflect source strength, so that following initially steady values they too will gradually decrease with time. We have made the problem of calculating vapour dosages above and downwind of grassland tractable by means of simplifying assumptions concerning the flux of material between the surface and the airstream in an initial steady state of atmospheric diffusion, and the relationship between vapour concentrations during and following the steady state; the latter based on a semi-empirical model for evaporation from a rough surface.

STEADY-STATE MODEL

The total surface area of the roughness elements per unit area of the substrate is defined as the total specific surface S and is assumed to be uniform for the area under consideration. The liquid films over unit area of substrate together form initially a specific surface S_1, also uniform, and from the previous discussion $S_1 < S$.

If P_a is the mean transport velocity of vapour between the rough surface and the turbulent airstream and P is the transport velocity of vapour between the surface and the internal sink, then the evaporation flux F_1 and the sorptive flux F_2 per unit area of substrate are:

$$\lim_{z \to 0} F_1(x,z) = S_1 \left\{ C_S - C(x,z) \right\} P_a, \qquad (1)$$

$$\lim_{z \to 0} F_2(x,z) = -(S-S_1)C(x,z)PP_a/(P+P_a); \qquad (2)$$

$$S_1 = 0 \text{ for } x > x_0,$$

and the net flux is

$$\lim_{z \to 0} F(x,z) = F_1(x,z) + F_2(x,z), \qquad (3)$$

where z is measured from the lower boundary of the turbulent airstream. C_S is saturated vapour concentration at the temperature of the liquid surface, and x_0 is the downwind dimension of the sprayed area.

Diffusion of vapour in the turbulent airstream can be described by the steady-state diffusion equation. Although the area has a finite crosswind dimension y_0, which theoretically requires a three-dimensional diffusion equation, the effect of crosswind diffusion on crosswind concentrations is negligible on the sprayed area, thus a simpler two-dimensional form could be used there with little loss of accuracy. Downwind, the interest in hazard evaluation is in the peak crosswind value of concentration at a given downwind distance. For areas where y_0 is equal to or greater than x_0, concentrations calculated from the two-dimensional equation do not vary significantly from the peak values from the three-dimensional form until x is equal to $5y_0$ or greater, where the source area begins to approximate a finite line source. Thereafter, corrections based on Pasquill's (1961) observations of lateral cloud spread provide sufficient accuracy.

The two-dimensional atmospheric diffusion equation is

$$u(z) \frac{\partial C(x,z)}{\partial x} = \frac{\partial}{\partial z} \left\{ K(z) \frac{\partial C(x,z)}{\partial z} \right\} \qquad (4)$$

where u(z) is the horizontal windspeed and K(z) the eddy diffusion coefficient, both functions of height. We assume that the turbulent airstream is bounded above by the non-turbulent atmosphere at z = H, a height determined by atmospheric stability. The boundary conditions for equation (4) are

$$\lim_{z \to 0} K(z) \; \partial C(x,z)/\partial z = -F(x,z) \qquad (5)$$

from equation (3) above, and

$$\lim_{z \to H} K(z)\, \partial C(x,z)/\partial z = o \tag{6}$$

Given functional forms for $K(z)$, $u(z)$ and P_a (a function of windspeed), and a value for P equation (4) can be solved for $C(x,z)$. At extended downwind distances $C(x,z)$ is corrected for finite crosswind dimension to give peak $C(x,z)$, as follows:

$$\text{Peak } C(x,z) = C(x,z) \text{ erf } (Y/2\sigma_y(x));\ Y = y_o/2, \tag{7}$$

where σ_y is the standard deviation of the crosswind distribution of concentration derived from Pasquill's parameters for cloud widths from point sources.

A novel finite-difference approximation method is employed to solve the diffusion equation numerically; details of which are given under "Finite Difference Approximation to the Diffusion Equation". A semi-empirical method is used for calculating the decay of concentration with time and dosage accumulation. The method is based on the following rough surface evaporation model.

ROUGH SURFACE EVAPORATION MODEL

Droplets sprayed on grassland impact on the roughness elements at various heights above the substrate. It is reasonable to suppose that ventilation of the surface will increase with height above the substrate with consequent increase in evaporation rates of the impacted films. Thus films with the same liquid loading, mass per unit area of film, would be expected to persist longer towards the bottom of the rough surface, and the life of an individual film will depend upon its initial liquid loading and its position above the substrate.

If P_l is the vapour transport velocity from liquid at a height l above the substrate to the turbulent airstream, its rate of evaporation is

$$e_l(x) = \left\{ C_S - \lim_{z \to o} C(x,z) \right\} P_l \tag{8}$$

and if it is absorbed at a rate $C_S P$, it will disappear at a time given by

$$t_l = M/(e_l + C_S P) \tag{9}$$

where M is its liquid loading and is assumed uniform throughout the film. Given functions for P_l and the initial distributions of liquid area and loading on the surface, equations (8) and (9) could be employed to calculate the rate of evaporation from the area.

In the steady state diffusion model, the mean transport velocity P_a is the same for both evaporation and absorption; simple hypotheses consistent with this assumption are that P_l is a linear function of height and that the distribution of film area is uniform with height. Appeal was made to experimental data on vapour recovery to deduce a form for the initial distribution of liquid loading; see "Vapour Recovery" below. Using the foregoing hypotheses it was found that a satisfactory fit to vapour recovery-time data was achieved when M was assumed to be a decreasing linear function of height above the substrate. Thus we assume that

$$P_l = P_o + (P_1 - P_o)l/l_1;\ P_1 > P_o, \tag{10}$$

$$M_l = M_o + (M_1 - M_o)l/l_1;\ M_o > M_1 \tag{11}$$

where suffix o applies to the bottom and suffix 1 to the top of the rough surface of height l_1.

Calculations with the steady state model show that $\lim_{z \to o} C(x,z)$ varies very slowly with x, and over the period of evaporation will have a mean value approximately an order less than C_S. It is convenient therefore either to regard it as a small fixed fraction of C_S or to ignore it, and to calculate a mean evaporation rate for the area as a whole. On this basis, the rate of evaporation from unit area of the substrate will be approximated by $S_1 C_S P_a$ initially and this rate will be maintained until the area of liquid film begins to shrink at a time T given by

$$T = M_1/C_S(P_1 + P) \tag{12}$$

Thereafter the evaporation rate decreases until all liquid has gone at time τ, where

$$\tau = M_o/C_S(P_o + P) \tag{13}$$

The rate of evaporation is found by integration of equation (8) with height, ignoring the limit-term, thus

$$E(t) = \int_o^l \frac{S_1}{l_1} e_l \, dl = \frac{C_S S_1}{l_1} \int_o^l P_l \, dl$$

where l at time t is derived from equation (9). Using the relationships (10), (11), (12) and (13) the following expressions are obtained:

$$E(t) = S_1 C_S P_a; \; o<t\le T, \tag{14}$$

$$E(t) = S_1 C_S \left[A^2 - 2PA - (P_o{}^2 - P^2) \right] /2(P_1 - P_o); \tag{15}$$

$$T<t\le\tau,$$

$$A = (\Delta P \; M_o - (P_o + P)\Delta M)/(\Delta P \; C_S t - \Delta M). \tag{16}$$

where $\Delta P = P_1 - P_o$, $\Delta M = M_1 - M_o$, $(M_o > M_1)$.

Integration of expressions (14) and (15) with time gives equations for the mass of liquid evaporated in a given time. If CD is the mass of liquid sprayed per unit area of substrate, or contamination density, the mass evaporated per unit area in a given time is CD $R_e(t)$ where $R_e(t)$ the fraction of the deposit evaporated is given by:

$$R_e(t) = \frac{M_1}{M_1+M_o} \quad \frac{P_1+P_o}{P_1+P} \; \frac{t}{T} \; ; \; o<t\le T \; , \tag{17}$$

$$R_e(t) = \frac{M_1}{M_1+M_o} \left[\frac{P_1+P_o}{P_1+P} + \frac{P_1+P}{P_1-P_o} \left\{ B^2 \left(\frac{1}{C-t/T} - \frac{1}{C-1} \right) - \frac{2PB}{P_1+P} \ln \left(\frac{C-t/T}{C-1} \right) + \frac{P_o{}^2 - P^2}{(P_1+P)^2} \; (1-t/T) \right\} \right] \; ; \tag{18}$$

for $T<t\le\tau$, and

$$B = \frac{M_o}{M_1} - \frac{(P_o+P)\Delta M}{M_1 \Delta P} \; , \quad C = \frac{\Delta M (P_1+P)}{M_1 \Delta P} \; .$$

In expression (18) time is normalized in terms of T, further normalization can be effected by normalizing P_o and P to P_1, and M_o to M_1.

Contamination density is related to liquid loading by

$$CD/S_1 = (M_1+M_o)/2 = \bar{M} \quad ; \tag{19}$$

$\bar{M}$ is of course the mean liquid loading.

VAPOUR RECOVERY

The equation for total mass balance in the diffusion model is

$$\int_0^H u(z)\ C(x,z)\ dz = \lim_{z \to 0} \int_0^x F(x,z) dx, \qquad (20)$$

where the left hand integral gives the horizontal advective flux per unit crosswind width through the crosswind vertical plane at a downwind distance x, and $\lim_{z \to 0} F(x,z)$ is the net vertical flux per unit area of substrate at the lower boundary. Vapour recovery is defined as the integral of the horizontal advective flux with time, thus in an interval of time t after spraying,

$$\text{Vapour Recovery } (x,t) = \int_0^H u(z)\ D(x,z,t)\ dz, \qquad (21)$$

where D(x,z,t) is vapour dosage. Vapour recovery can be calculated from field data on vertical profiles of vapour dosage and wind speed, using a quadrature equivalent to the above integral, and when calculated at the downwind edge of contamination will be equal to the time integral of the net vertical flux for the whole area. When the surface is impermeable to an agent, the net vertical flux is equal to the evaporative flux, and if $R_v(t)$ is the fraction of the total liquid deposit recovered as vapour in time t,

$$R_v(t) \cong R_e(t)\ ;\ P = o \qquad (22)$$

This relationship can be used to deduce a simple functional form for the initial distribution of liquid loading in the evaporation model by fitting curves of $R_e(t)/R_e(\tau)$, calculated from equations (17) and (18), to plots of $R_v(t)/R_v(\tau)$ against time derived from field data.

When an agent is absorbed by the surface the net vertical flux is less than the evaporative flux. In the steady state

$$R_v(x,t) \cong R_e(t) \lim_{z \to 0} \int_0^x (F(x,z)/F_1(x,z))dx, \qquad (23)$$

$$\cong R_e(t)\ R_f(x). \qquad (24)$$

Both the net and the evaporative flux will decrease with time thereafter; as a first approximation we assume that they decrease in such a way that $R_f(x_o)$ remains constant and hence equations (23) and (24) apply as well to the non-steady state, so that the total fraction of deposited liquid recovered as vapour is given by

$$R_v(x,\tau) \cong R_e(\tau)\ R_f(x) \qquad (25)$$

VAPOUR CONCENTRATION IN THE NON-STEADY STATE

It is implicit in equation (24) that the horizontal advective flux is directly proportional to the mean rate of evaporation from the sprayed area at any given time, we therefore assume that vapour concentrations over the area are also directly related to the mean evaporation rate. Thus if C(x,z,T) is a steady state concentration, the concentration at some time t is related to it by

$$C(x,z,t) = C(x,z,T)\ E(t)/E(T) \qquad (26)$$

through equations (14) and (15).

DOSAGE ACCUMULATION

An expression for dosage accumulation is obtained by integrating equation (26) with time. Referring to equations (14) to (18), the equation for dosage accumulation is

$$D(x,z,t) \cong C(x,z,T)\ R_e(t)\ CD/S_l C_S P_a \quad (o<t\leq\tau) \qquad (27)$$

where C(x,z,T) is the steady-state concentration. Downwind of the sprayed area there will be a time lag before the vapour cloud arrives. Equations (24) to (27) will require the addition of a lag-time to the left hand term based on a mean translational speed for the cloud, as a first correction. For materials that persist for several hours this simple correction is assumed to be adequate to at least the distance downwind where crosswind diffusion becomes significant, i.e. a distance of the order of 10 x_o.

FUNCTIONS FOR THE PARAMETERS

Functional forms of K(z), u(z), P_a, P_l and M_l are used in the models; those we have adopted are discussed below. It is emphasized that we do not consider them or any other forms to be unique for the solutions of the diffusion and evaporation equations in the present state of knowledge concerning vertical diffusion in extended downwind travel and vapour transport between natural surfaces and the turbulent airstream.

Values of H, S, S_1 and P are given, those for the latter two derived from field data.

K(z), u(z) and H

Theoretical expressions for K(z) and u(z) are available in meteorological literature. The most familiar are logarithmic and power-law functions for u(z), from which K(z) functions are derived through the relationship

$$K(z)\ du/dz = u_{\star}^{2}\ . \tag{28}$$

These equations are applicable strictly to the layer of constant shearing stress in contact with the ground. Estimates of the upper limit of this layer vary about a value of 50m, which is well below the upper boundary, H, of the turbulent boundary layer in most categories of atmospheric stability, and below the top of the cloud of diffusing material at extended downwind distances of practical interest. Tyldesley (1966) discusses the shortcomings of some modified forms of the theoretical expressions in the prediction of the vertical spread of diffusing material for downwind travel in excess of 100m. For stability categories other than neutral he found that empirical adjustment to the K(z) function was necessary to fit calculated values of cloud height to Pasquill's (1961) data. He noted further that these functions were not necessarily unique in providing the fit. The empirically adjusted functions given are not directly applicable to the bounded turbulent boundary layer assumed in the diffusion model. However, our approach to the problem has been similar in that Pasquill's data have been used as a criterion for testing calculations of vertical cloud spread at downwind distances greater than 5 x_0, where the source approximates a line source, using various functions for u(z), K(z) and P_a. At the same time calculations of vertical and horizontal profiles of vapour concentration on and downwind of rectangular contaminated areas were tested against available field data. In this way we selected functions for use in the model that would best predict vapour diffusion for short and long distance downwind travel in Pasquill's stability categories C, D, E and F. These were:

$$K(z) = A(z+\Delta l)u(2) \tag{29}$$

where A is a different constant for each category, Δl is a length of the same order as the roughness length z_0 of the surface; and u(2) is the wind speed at 2m; and

$$u(z) = u(2)\ (z/2)^{p}, \tag{30}$$

z is given in metres and is measured from the lower boundary of the turbulent airstream; p is a stability parameter, values of which were deduced from observed wind speed profiles in the four stability categories.

In using a finite-difference approximation to the diffusion equation, H may be chosen at a level where vapour concentrations are expected to become negligible, this height will increase with travel downwind, provided this is not above a physically apparent "lid" such as a subadiabatic layer or an inversion. We have chosen maximum values of H to coincide roughly with the average depths of the dry adiabatic layer or the heights of inversions in the various categories.

The suggested values of the constants in equations (29) and (30) and of H are given in Table I below.

TABLE I

STABILITY CATEGORY	VALUES OF CONSTANTS A	Δl m	p	u(2) m/s	H m
C	0.08	0.025	0.2	2-4	1000
D	0.04	0.025	0.23	~3	500
E	0.03	0.025	0.3	1.5-3	200
F	0.02	0.025	0.5	1.5-2	100

It will be noted that the value of A for category D will give practically the same values for K(z) as given by the classical equation $K(z) = ku_*z$, derived from equation (28) and the logarithmic wind profile function, since $k = 0.4$ and u_* is approximately equal to $u(2)/10$ in neutral conditions.

P_a and P_l

A report by Chamberlain (1966) on the transport of gases to and from grass and grasslike surfaces was the source of data on vapour transport velocities. Chamberlain derived values of the sublayer Stanton number B which he related to r_i the resistance to transport of gas to and from the surface by

$$B^{-1} = u_* \, r_i/S. \tag{31}$$

P_a is the reciprocal of r_i. Although B^{-1} was dependent upon u_* for various types of rough surfaces cited, in the experiments with long grass he found no significant dependence; this indicates that

$$P_a = u_*/B^{-1}S. \tag{32}$$

A value of 7.7 for B^{-1} was obtained for long grass but S was not measured, however from measurements quoted for his artificial grass it is assumed that S lay between 1 and 2. Since u_* is approximately one tenth of the mean wind speed at 2m, P_a appears to be two orders less than u(2). In the model we have adopted the simple equation

$$P_a = 0.01\ u(2) \tag{33}$$

for all stability categories.

There is no direct information on transport velocity as a function of height above the substrate. However, data are given for one experiment where the distribution of absorbed thorium vapour with height in a stand of artificial grass was determined by cutting the blades into segments and measuring the activity. Since the blade surfaces acted as sinks of vapour it can be assumed that the deposits were directly related to P_l. If the deposits are plotted against height in the form of a histogram, Fig. 1, there appears to be some support for a simple linear function of P_l with height in this idealized rough surface.

We have assumed that P_o in equation (10) is the transport velocity in conditions of slight air movement. In these conditions the major factor in vapour transport to the surrounding air may well be molecular diffusion through a sublayer. From various estimates of the thickness of the sublayer and the molecular diffusivities of agents of interest, P_o would therefore be of the order of 0.1 cm/s. Because dosages contain units of minutes we have selected a rounded value of

$$P_o = 5\ \text{cm/min} \tag{34}$$

S, S_1, M_l

No attempt has yet been made to relate S to grassland of various types. The total specific surface will obviously vary with the density of vegetation, which in turn will depend upon season, climate and soil properties. It is plausible to assume that unless the growth is sparse, S will exceed 1, taking into account the mat close to the substrate. For want of specific information we have accepted Chamberlain's artificial grass as a reasonable facsimile, with respect to S, to natural grass, for which S = 2.

Values of initial liquid specific surface have been derived experimentally from calculations of vapour recovery at the downwind edge of sprayed areas. The initial rate of vapour recovery, IR, was found from plots of vapour recovery against time, and in general,

$$IR(x) = x_o S_1 C_S P_a R_f(x), \tag{35}$$

see equations (14) and (24). For poorly absorbed agents $R_f(x)$ approaches a value of 1, and data for these agents were used to determine values of S_1 initially. In general, two effects on S_1 were observable: the first due to the size of the sprayed droplets; the second due to the level of contamination density; but a functional relationship remains to be found. For spray applied at rates between 1 and 5 g/m^2 with nominal mass median diameters between 200

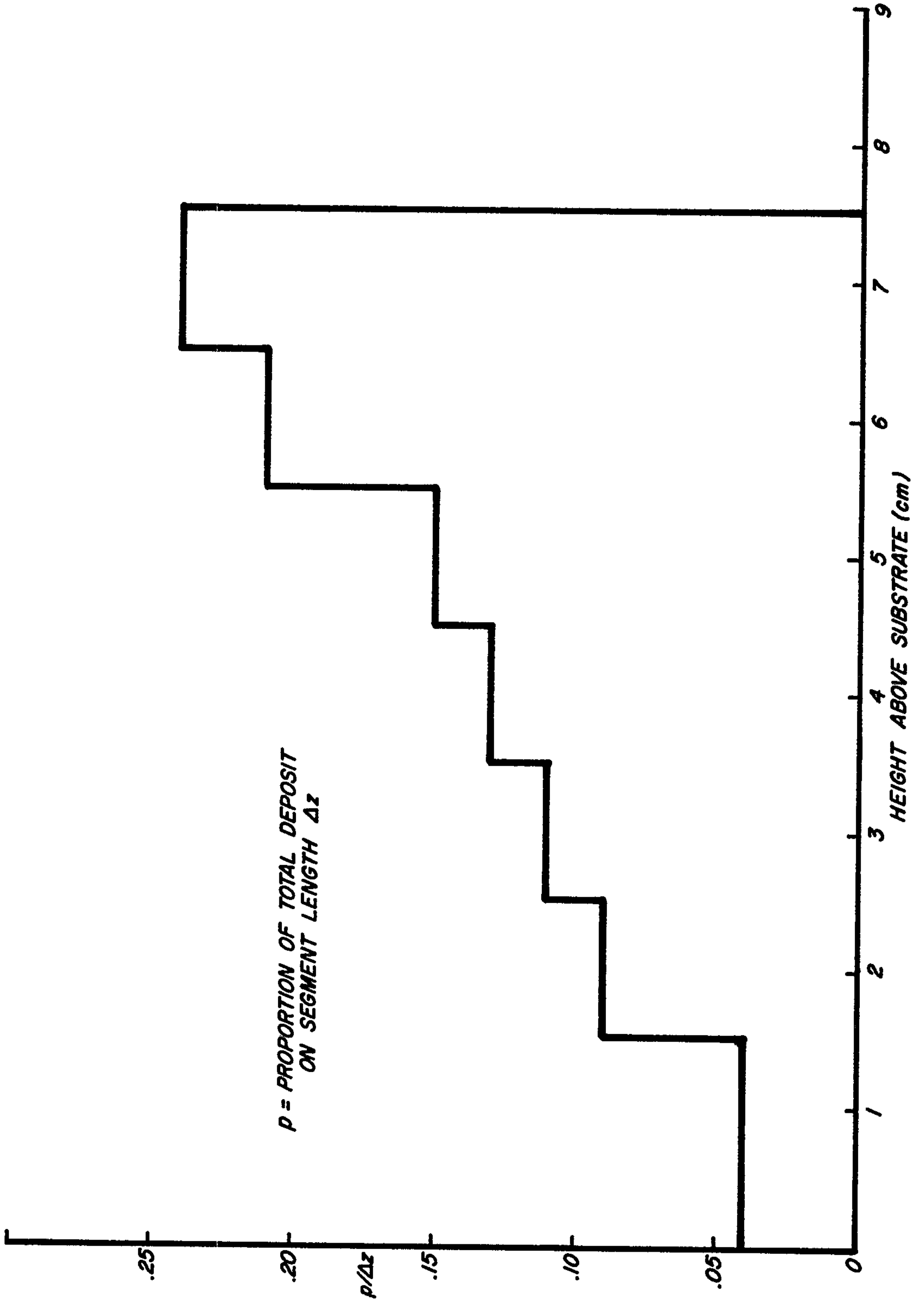

FIG. I VAPOUR DEPOSIT V. HEIGHT WITHIN STAND OF ARTIFICIAL GRASS
(Chamberlain's Data)

and 500 microns, values of S_1 were between 0.04 and 0.09 per g/m^2. At larger spray mmd's of 0.5-1mm applied at 10 to 15 g/m^2, values of S_1 ranged between 0.02 and 0.03 per g/m^2. At these contamination densities which are in a range expected in CW, S_1 rarely exceeded a value of 0.04.

The mean liquid loading $\bar{M}$ is related to S_1 and CD by

$$\bar{M} = CD/S_1. \tag{36}$$

As explained above under "Vapour Recovery", the magnitude of the assumed linear gradient of M_1 was deduced from experimental recovery data. The value of M_0/M_1 for spray mmd's between 200 and 1000 microns, applied at rates, between 1 and 15 g/m^2, is 10, whence

$$\bar{M}_1 = M/5.5. \tag{37}$$

P

Values of P vary with the agent used. Within the family of nerve agents, P decreases with increasing agent volatility and ranges from 5 to 200 cm/min.

Values of the parameter were deduced from laboratory and field data on vapour recovery from turf and grassland respectively, by comparison with values calculated from the model.

FINITE-DIFFERENCE APPROXIMATION TO THE DIFFUSION EQUATION

A standard scheme for approximating the parabolic equation (4) using finite-differences is illustrated in Fig. 2.

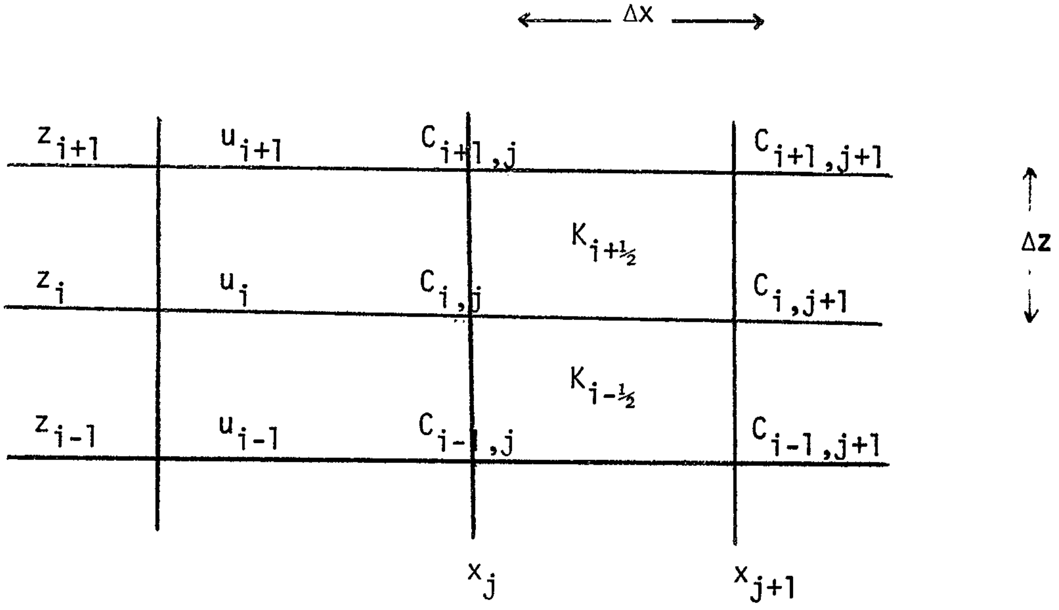

FIGURE 2

and since we assume resistance in all slices is the same we have

$$R(z_3) - R(z_2) = \frac{1}{A} \ln \left(\frac{z_3+\Delta \ell}{z_2+\Delta \ell} \right) = \frac{1}{A} \ln \left(\frac{z_2+\Delta \ell}{\Delta \ell} \right)$$

or

$$z_3 = \Delta \ell \left\{ \left(\frac{z_2+\Delta \ell}{\Delta \ell} \right)^2 - 1 \right\} .$$

By induction it can be shown that

$$z_i = \Delta \ell \left\{ \left(\frac{z_2+\Delta \ell}{\Delta \ell} \right)^{i-1} - 1 \right\} \qquad i=1,2,\ldots,L. \tag{39}$$

and that

$$\Delta z_i = z_i - z_{i-1} = \left(\frac{z_2+\Delta \ell}{\Delta \ell} \right)^{i-2} z_2 \qquad i=2,\ldots,L. \tag{40}$$

For convenience, let $\eta = \left(\frac{z_2+\Delta \ell}{\Delta \ell} \right)$. By assumption

$$R(z_i) - R(z_{i-1}) = \frac{\Delta z_i}{K_{i-\frac{1}{2}}} = \frac{1}{A} \ln (\eta) = \text{a constant } i=2,\ldots,L$$

Since K, the coefficient of eddy diffusivity is measured as an average within each atmospheric slice, it will be necessary to have an equational form for $\Delta z_{i+\frac{1}{2}}$

Now $z_{i+\frac{1}{2}}$ is that position such that

$$R(z_{i+\frac{1}{2}}) - R(z_i) = \tfrac{1}{2}(R(z_{i+1}) - R(z_i)) = \frac{1}{2A} \ln (\eta)$$

or upon simplifying

$$R(z_{i+\frac{1}{2}}) = \frac{1}{A} \ln (\eta^{i-\frac{1}{2}})$$

and $z_{i+\frac{1}{2}} = \Delta \ell \, (\eta^{i-\frac{1}{2}}-1)$ (41)

Therefore

$$\Delta z_{i+\frac{1}{2}} = z_{i+\frac{1}{2}} = \eta^{\frac{1}{2}}\Delta z_i \tag{42}$$

The two approaches of solving the diffusion equation have been used at DRES. The standard method as outlined by Figure 2 was employed in the development work of the model but as the requirement for long distance runs became necessary, the previously mentioned shortcomings of this approach became apparent. Therefore, the more economical diffusive resistance approach was developed. Both methods will give identical solutions when the input parameters are the same. The second approach, however, can be adapted to fit within the capacity of a very small computer, say 8K while for reasonably accurate and detailed output, the standard scheme would require core storage of 32K. In addition, the diffusive resistance solution of the problem provides a better physical interpretation of the diffusion process.

DISCRETIZATION OF THE DIFFUSION EQUATION

Equation 4 was approximated according to the discretization scheme given in Figure 3.

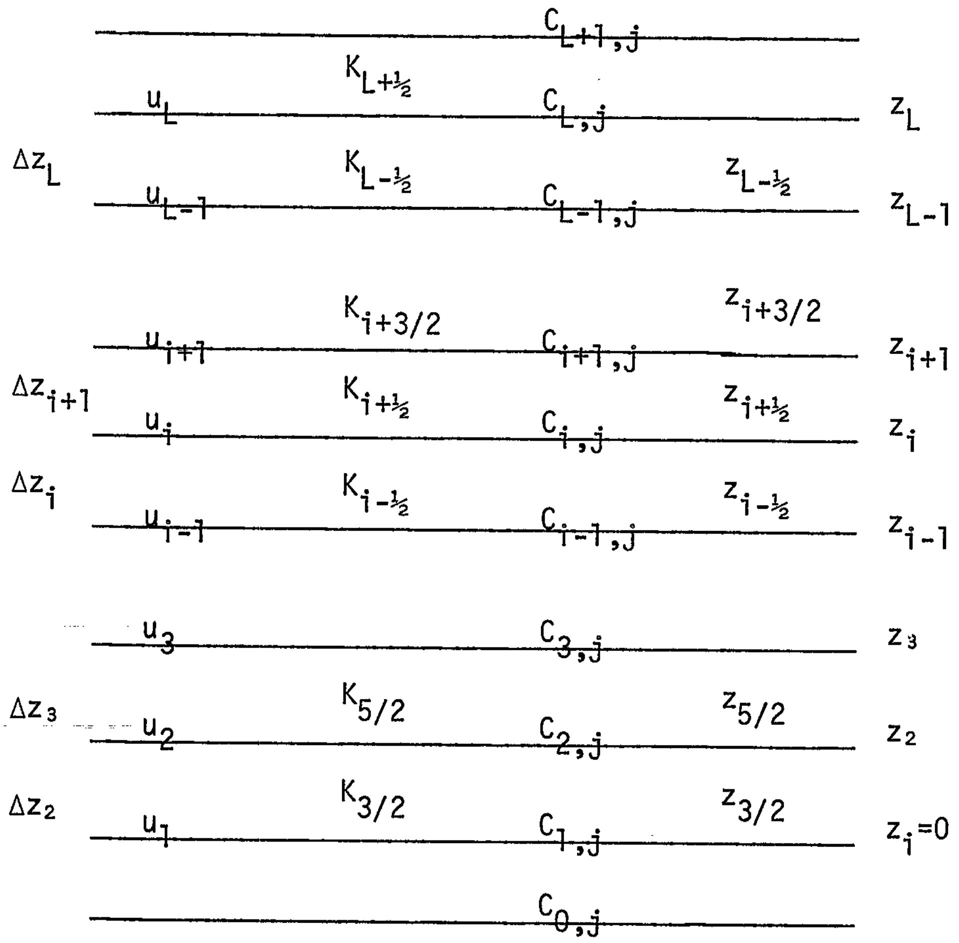

Figure 3: Discretization Scheme

The approximation to the right hand side of equation 4 was developed in the following manner. If for the moment we ignore the indices in the horizontal direction, and approximate C_{i+1} and C_i at the point $i+\frac{1}{2}$ by the Taylor approximation, then

$$C_{i+1} = C_{i+\frac{1}{2}} + (z_{i+1}-z_{i+\frac{1}{2}}) \left.\frac{\partial C}{\partial z}\right|_{i+\frac{1}{2}} + \frac{1}{2!} (z_{i+1}-z_{i+\frac{1}{2}})^2 \left.\frac{\partial^2 C}{\partial z^2}\right|_{i+\frac{1}{2}} +$$

$$\frac{1}{3!} (z_{i+1}-z_{i+\frac{1}{2}})^3 \left.\frac{\partial^3 C}{\partial z^3}\right|_{i+\frac{1}{2}} + \ldots\ldots$$

and

$$C_i = C_{i+\frac{1}{2}} + (z_i-z_{i+\frac{1}{2}}) \left.\frac{\partial C}{\partial z}\right|_{i+\frac{1}{2}} + \frac{1}{2!} (z_i-z_{i+\frac{1}{2}})^2 \left.\frac{\partial^2 C}{\partial z^2}\right|_{i+\frac{1}{2}} +$$

$$\frac{1}{3!} (z_i-z_{i+\frac{1}{2}})^3 \left.\frac{\partial^3 C}{\partial z^3}\right|_{i+\frac{1}{2}} + \ldots\ldots$$

Subtracting these two equations, dividing by $(z_{i+1}-z_i) = \Delta z_{i+1}$ and rearranging some terms we have

$$\left.\frac{\partial C}{\partial z}\right|_{i+\frac{1}{2}} = \frac{C_{i+1}-C_i}{\Delta z_{i+1}} - \frac{1}{2!} \left\{ \frac{(z_{i+1}-z_{i+\frac{1}{2}})^2 - (z_i-z_{i+\frac{1}{2}})^2}{\Delta z_{i+1}} \right\} \left.\frac{\partial^2 C}{\partial z^2}\right|_{i+\frac{1}{2}} -$$

$$\frac{1}{3!} \left.\left\{ \frac{(z_{i+1}-z_{i+\frac{1}{2}})^3 - (z_i-z_{i+\frac{1}{2}})^3}{\Delta z_{i+1}} \frac{\partial^3 C}{\partial z^3} \right\}\right|_{i+\frac{1}{2}} - \ldots\ldots$$

Similarly

$$\left.\frac{\partial C}{\partial z}\right|_{i-\frac{1}{2}} = \frac{C_i-C_{i-1}}{\Delta z_i} - \frac{1}{2!} \left\{ \frac{(z_i-z_{i-\frac{1}{2}})^2 - (z_{i-1}-z_{i-\frac{1}{2}})^2}{\Delta z_i} \right\} \left.\frac{\partial^2 C}{\partial z^2}\right|_{i-\frac{1}{2}} -$$

where $$\Delta_z^2 K(z_i)C_{i,j} = \left\{ \frac{K_{i+\frac{1}{2}}}{\Delta z_{i+1}} (C_{i+1,j}-C_{i,j}) - \frac{K_{i-\frac{1}{2}}}{\Delta z_i} (C_{i,j}-C_{i-1,j}) \right\} \frac{1}{\Delta z_{i+\frac{1}{2}}} \;.$$

The index j defines the grid position in the horizontal direction.

This equation can be further simplified by substituting:

$$\frac{K_{i+\frac{1}{2}}}{\Delta z_{i+1}} = \frac{A}{\ln(\eta)}$$

$$\Delta z_{i+\frac{1}{2}} = \Delta Z \eta^{i-3/2}(\eta-1)$$

$$\therefore \; \Delta_z^2 K(z_i)C_{i,j} = \frac{A}{\Delta Z \eta^{i-3/2}(\eta-1)\ln(\eta)} \left\{ C_{i+1,j} - 2C_{i,j} + C_{i-1,j} \right\}$$

Equation (44) now simplifies to

$$C_{i,j+1} - C_{i,j} = \frac{\Delta x}{2u_i} \left\{ C_{i+1,j} - 2C_{i,j} + C_{i-1,j} + C_{i+1,j+1} - 2C_{i,j+1} + C_{i-1,j+1} \right\} \frac{A}{\Delta Z \eta^{i-3/2}(\eta-1)\ln(\eta)}$$

Letting $$\xi_i = \frac{(\Delta Z)^{p+1} \eta^{i-3/2}(\eta-1)(\eta^{i-1}-1)^p \ln(\eta^2)}{2^p A \Delta x} > 0 \quad i=2,\ldots,L$$

where p is the exponent of the windspeed profile, then

$$-C_{i-1,j+1} + (2+\xi_i)\, C_{i,j+1} - C_{i+1,j+1} = C_{i-1,j} - (2-\xi_i)\, C_{i,j} + C_{i+1,j} \qquad i=2,\ldots,L-1 \tag{45}$$

where

$$\Delta_z^2 K(z_1)C_{1,j} = \left\{ \frac{K_{3/2}}{\Delta z_2} (C_{2,j}-C_{1,j}) + S_1 P_a C_{o,j} - \Psi P_a C_{1,j} \right\} / l \qquad l = \text{some length.}$$

$C_{o,j} = C_s$ and without loss of generality it can be taken to be 1.

Let $\xi_1 = \frac{\ln \eta}{A} > 0$ and simplifying, the lower boundary is approximated by

$$(1 + \xi_1 \Psi P_a)C_{1,j+1} - C_{2,j+1} = C_{2,j} - (1 + \xi_1 \Psi P_a)C_{1,j} + \xi_1 S_1 P_a (C_{o,j} + C_{o,j+1}) \qquad (47)$$

SOLUTION OF THE DIFFUSION EQUATION

The difference scheme which we have just outlined can now be represented by the following matrix equation

$\tilde{A}\,\vec{C}_{j+1} = \tilde{B}\,\vec{C}_j + \vec{d}$ where $\vec{d}$ is the source vector

and $\tilde{A}$ and $\tilde{B}$ are tridiagonal matrices. The components of $A = (a_{ij})$ are

$$a_{11} = 2+(\xi_1 \Psi P_a - 1)$$

$$a_{ii} = 2+\xi_i \qquad i=2,\ldots,L-1$$

$$a_{LL} = 2+(\xi_L - 1)$$

$$a_{i,i-1} = -1 \qquad i=2,\ldots,L$$

$$a_{i,i+1} = -1 \qquad i=1,\dots,L-1$$

$$a_{i,j} = 0 \qquad j\neq i,\ i-1,\ i+1$$

and the components of $\tilde{B} = (b_{ij})$

$$b_{11} = -2+(-\xi_1\Psi P_a+1)$$

$$b_{ii} = -2+\xi_i \qquad i=2,\dots,L-1$$

$$b_{LL} = -2+(\xi_L+1)$$

$$b_{i,i-1} = 1 \qquad i=2,\dots,L$$

$$b_{i,i+1} = 1 \qquad i=1,\dots,L-1$$

$$b_{i,j} = 0 \qquad j\neq i,\ i-1,\ i+1$$

The components of $\vec{d} = (d_i)$ are

$$d_1 = \xi_1 S_1 P_a(C_{o,j}+C_{o,j+1})$$

$$d_i = 0 \qquad i=2,\dots,L$$

Let $\vec{D}_j = \tilde{B}\,\vec{C}_j + \vec{d}$ and the matrix equation reduces to

$$\tilde{A}\,\vec{C}_{j+1} = \vec{D}_j$$

Since $\tilde{A}$ is a tridiagonal matrix, its inverse can be readily calculated by the Gauss elimination method (Forsythe and Wasow, 1967). The solution of equation 4 at the j+1 increment in the x direction is

$$\vec{C}_{j+1} = \tilde{A}^{-1} \vec{D}_j$$

STABILITY AND CONVERGENCE

It is important to know that the solution of the finite-difference equations is a reasonably accurate approximation to the solution of the corresponding partial differential equation. The conditions associated with an understanding of accuracy are the stability and convergence of the approximation method.

Stability is that type of error associated with round-off error. Let $\vec{e}$ denote the error vector. Then

$$\vec{e}_j = \vec{C}_j - \vec{C}_{j_{est.}} \qquad \text{and}$$

$\vec{e}_j = E^j \vec{e}_0$ where it has been assumed that the source vector is a constant. In order to show that our approximation method is stable, it is necessary to prove that the $\vec{e}_j$ remain bounded as j increased indefinitely. It can be shown (Smith, 1965) that the errors will not increase exponentially with j provided the eigenvalue of E with the largest modulus has a modulus less than or equal to unity.

The matrix E is equal to

$$E = (2I-F+G)^{-1} (-2I+F+G') \quad \text{where}$$

I_{LxL} is the identity matrix, $F=(f_{ij})$ is of the form

$$f_{i,i-1} = f_{i,i+1} = 1 \qquad i=1,L$$

$$f_{i,j} = 0 \qquad \text{otherwise}$$

$G = (g_{ij})$ and $G' = (g'_{ij})$ are diagonal matrices where

$$g_{11} = \xi_1\Psi P_a-1 \qquad g'_{11} = \xi_1\Psi P_a+1$$

$$g_{ii} = \xi_i \qquad g'_{ii} = \xi_i \qquad i=2,\ldots,L-1$$

$$g_{LL} = \xi_L-1 \qquad g'_{LL} = \xi_L+1$$

The eigenvalues of E then are

$$\lambda_1 = \frac{1-\xi_1\Psi P_a - 4\sin^2\left(\frac{\pi}{2(L+1)}\right)}{-1+\xi_1\Psi P_a + 4\sin^2\left(\frac{\pi}{2(L+1)}\right)} \equiv -1.$$

$$\lambda_i = \frac{\xi_i - 4\sin^2\left(\frac{i\pi}{2(L+1)}\right)}{\xi_i + 4\sin^2\left(\frac{i\pi}{2(L+1)}\right)} \qquad \text{and since } \xi_i>0 \quad |\lambda_i|<1$$

$$i=2,..,L-1$$

$$\lambda_L = \frac{\xi_L + 1 - 4\sin^2\left(\frac{L\pi}{2(L+1)}\right)}{\xi_L - 1 + 4\sin^2\left(\frac{L\pi}{2(L+1)}\right)}$$

$|\lambda_L|<1$ for $\xi_L>0$ and $L>1$

Therefore, our approximation is stable, and since our equations are consistent, we are assured of convergence (Douglas, 1961).

The only equation that restricts this method from being universally stable is the equation of the lower boundary condition. This limitation suggests that while the errors may not increase exponentially they will persist as linear combinations of the initial errors. This error however was found to be negligible when we checked the mass balance by means of the relationship given by equation (20).

There is one instance in which the formulation of the lower boundary does not adequately describe the situation being simulated. If one assumes that P=0 and attempts to estimate concentration downwind of the source, then equation (47) reduces to

$$C_{1,j+1} - C_{2,j+1} = C_{2,j}-C_{1,j}$$

Now if $C_{2,j} - C_{1,j} = 0$ implies $C_{1,j+1} - C_{2,j+1} = 0$ for all i

If however $C_{2,j} - C_{1,j} > 0$ then $C_{1,j+1} > C_{2,j+1}$ and

$C_{1,j+2} < C_{2,j+1}$ etc.

Therefore if $(C_{2,j} - C_{1,j}) = \delta \neq 0$ oscillation will occur between the first two concentration calculations. Under most circumstances δ has been found to be so small that this effect could be ignored. This problem requires some further study and a reformulation of the boundary condition for the case of an impermeable surface.

THE COMPUTER PROGRAM

The computer program used to calculate vapour concentrations on and downwind of the contamination is written in the basic Fortran IV language of the DRES 1130 Model 2C computer (16K words of core storage). The program in its present form requires approximately 9K of core storage. The input requirements of this program are given in detail in Appendix A along with a listing of the latest version of the program. A sample run is also included.

The input to the program consists of a definition of the absorptive characteristics of the material, a description of the contamination and the meteorological situation being simulated, and the form of the output required. Velocity parameters, wind speed, P_a and P are normalized in terms of u(2), the 2m windspeed; inputs describing the area of contamination and the downwind extent of calculation, as well as information concerning output are in absolute units, in our case in metres.

One parameter required for input to the program which has not yet been described is z_2. In order to define the vertical array z_i, two of the three parameters L, z_L, or z_2 must be given. The relationship between these parameters, following from equation (39) is

$$L = 1 + \frac{\ln\left(\frac{z_L + \Delta z}{\Delta z}\right)}{\ln\left(\frac{z_2 + \Delta z}{\Delta z}\right)} \, .$$

z_L which is denoted by H in Table 1 is an input to the simulation since it is the definition of the atmospheric lid, and will change according to the atmospheric stability category. z_2 is an arbitrary reference height chosen according to some criterion of economy of computation and degree of precision suitable to users' requirements. Figure 4 illustrates the size of the z_i array for various values of z_L and z_2. It was found that an appropriate value for our purposes was $z_2 = 0.0075$, since it provided approximately 10 grid points in the region 0.-1.0 metres and a further 10 in the range 1.0-10.0 metres. In addition a total of only 40 grid positions is required to simulate an atmosphere of 1000 metres in depth. Test runs have shown that there was only a slight difference between normalized concentration calculations for values of z_2 ranging from 0.01 to

0.002 at the estimated 0.5 metre position so that the choice of z_2 is not critical.

A few test runs were made to assess the effect on accuracy of different values of Δx. These runs suggested that the error introduced by increasing Δx was constant in the vertical direction, maximum within the first few iterations, and converged towards zero with downwind distance. No work was carried out on the rate of convergence. We have used values of Δx equal to 1 for runs with downwind dimensions of hundreds of metres and 10 for downwind distances in the thousands of metres.

Concentrations are normalized to the saturated vapour concentration, and hence output is in the form of vertical profiles of normalized concentration at selected positions on and downwind of the contaminated area.

In addition to the normalized concentration profiles at selected positions, calculations of normalized evaporative and absorptive flux from the area upwind are given by TVAØF and VAREA respectively, i.e.,

$$\mathrm{TVA\emptyset F} = \int_0^x F_1 dx/C_s u(2) \qquad \text{and}$$

$$\mathrm{VAREA} = \int_0^x F_2 dx/C_s u(2) \quad .$$

The recovery factor R_f can then be calculated from

$$R_f = (\mathrm{TVA\emptyset F} - \mathrm{VAREA})/\mathrm{TVA\emptyset F} \quad .$$

Since the array z_i as given by equation (39) is exponential in form, the concentration profiles as calculated by the computer are not in a convenient form for usage. In order that we might have as output from the computer concentration profiles of a specified degree of resolution, we wrote an interpolation routine. Bessels interpolation formula was used to transform the data from the exponential array into the required linear array. If $f(z_i + \theta\delta z)$ is the function value required and f_0 is the calculated value nearest to it such that $|\theta|$ is a minimum then

$$f(z_i+\theta\delta z) \cong \frac{1}{2}\ (f_0+f_1) + (\theta-0.5)\delta f_{\frac{1}{2}} + B^{ii}(\theta)\ (\delta^2 f_0+\delta^2 f_1)$$

$$+\ B^{iii}(\theta)\delta^3 f_{\frac{1}{2}}$$

where $B^{ii} = \theta(\theta-1)/4$

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$$+ B^{iii}(\theta)\delta^3 f_{\frac{1}{2}}$$

where $B^{ii} = \theta(\theta-1)/4$

$$B^{iii} = \theta(\theta-\tfrac{1}{2})\ (\theta-1)/6$$

$$\delta f_{\frac{1}{2}} = f_o+f_1$$

$$\delta^2 f_o = f_1-f_{-1}$$

$$\delta^2 f_1 = f_2-2f_1+f_{-1}$$

$$\delta^3 f_{\frac{1}{2}} = \delta^2 f_1-\delta^2 f_o$$

RESULTS FROM THE MODEL AND SIMPLIFIED CALCULATING PROCEDURES

Calculations with both components of the model indicate simple approximate relationships, some of which can be adopted to reduce the computational effort required to cover a variety of situations and to develop graphical methods for summarizing and interpolating results.

CALCULATIONS WITH THE STEADY STATE DIFFUSION MODEL

An example of a calculation with the diffusion model is illustrated in Fig. 5. Curves of normalized concentration $C(x,z,T)/C_s$, at heights 0 to 2m above ground, and of R_f, against downwind distance to 2500m, are shown for a contaminated area 250m in downwind dimension and infinite crosswind length. The ratio $P/P_a = 1.0$ is independent of windspeed, since both P and P_a are normalized to u(2) in the model, and represents strongly sorbed materials in the range of wind speeds appropriate to stability category D, see Table I. A value of $S_1 = 0.2$ was chosen as a mean value for aircraft spray.

On the contaminated area, the concentration at z=o is an order less than C_s, and increases very slowly with downwind distance. As height increases concentration decreases, and the downwind relative increase of concentration becomes greater. The vertical gradient of concentration, downwind of the area, is reversed at these lower levels, as a result of vapour sorption by the rough surface. Values of R_f fall at a decreasing rate downwind on the contaminated area and indicate that about half of the vapour evolved is absorbed; downwind of the area the curve reflects the effect of vapour sorption by the "clean" surface.

VARIATION OF $C(x,z,T)$ WITH P/P_a

When P/P_a alone is varied over a wide range of values, it is found that relative vertical profiles of concentration ($C(x,z)/C(x,z_1)$, where z_1 is a fixed reference level) on the contaminated area change very little, as indicated in Table 2. Downwind of the area, the relative profiles vary significantly reflecting the varying degrees of vapour sorption by the surface. It is also found that C(x,z) for a given downwind distance and height over the contaminated area is approximately directly proportional to $R_f(x)$. This is shown in

Table 3 where $C(x,z,T)/C_s R_f(x)$ is tabulated against height and P/P_a. The direct proportionality between $R_f(x)$ and $C(x,z)$ does not hold downwind of the contaminated area.

TABLE 2

VARIATION OF RELATIVE VERTICAL CONCENTRATION PROFILES WITH P/P_a. STABILITY CATEGORY D

	$x=x_0=250m$				$x=500m$, $c_0=250m$			
	$C(z)/C(0.5)$				$C(z)/C(0.5)$			
P/P_a	0	0.1	0.5	1.0	0	0.1	0.5	1.0
z(m)								
0	2.178	2.168	2.150	2.143	1.024	.904	.694	.602
.1	1.554	1.550	1.542	1.539	1.012	.953	.848	.801
.3	1.184	1.182	1.180	1.179	1.008	.989	.955	.939
.5	1	1	1	1	1	1	1	1
1.0	.748	.750	.753	.754	.978	1.004	1.051	1.072
1.5	.603	.606	.610	.611	.953	.994	1.066	1.099
2.0	.504	.506	.511	.513	.927	.968	1.067	1.107

TABLE 3

RELATIONSHIP BETWEEN $C(x,z,T)/C_s$, P/P_a and $R_f(x)$

$x = x_0 = 250m$. CATEGORY D

$C(x,z)/CsR_f(x)$

P/P_a	0	0.05	0.1	0.5	1.0
z(m)					
0	.2186	.2208	.2226	.2289	.2314
.1	.1560	.1577	.1591	.1641	.1662
.3	.1188	.1203	.1213	.1404	.1273
.5	.1004	.1017	.1027	.1064	.1080
1.0	.0751	.0762	.0770	.0801	.0814
1.5	.0606	.0615	.0610	.0649	.0660
2.0	.0506	.0514	.0520	.0544	.0554
20.0	.0011	.0012	.0012	.0013	.0013
$R_f(x)$	1	.9065	.8353	.5796	.4786

evaporated, $R(\tau)$, for a given value of P/P_a, varies only slightly with wind speed. A value calculated for a wind speed of 5 m/s would be less than 5% in error at either extreme of the wind speed range.

Fig. 8 is a plot of $R_e(t)/R_e(\tau)$ against t/T for four values of P/P_a. It shows that the normalized time at which a given value of $R_e(t)/R(\tau)$ is reached increases with P/P_a. The effect of wind speed on the fraction is greatest for a non-absorbed agent, but as shown the value of $R_e(t)/R_e(\tau)$ varies by less than 5% in the chosen range of wind speed. The effect at the other values of P/P_a is too small to be discriminated graphically. Similar effects can be shown for E(t)/E(T) against t/T.

The normalized time to complete evaporation is obtained from equations (12) and (13) which indicate that τ/T is directly proportional to wind speed for a non-absorbed material and approaches a constant value as P/P or P/P_a increases.

$R_e(t)$ is used in equations 25 and 27 for the calculation of vapour recovery and dosage respectively. A single curve of $R_e(\tau)$ v P/P_a, as in Fig. 7 can be used to calculate total values for a given P/P_a at all wind speeds with little error. Fig. 9 shows curves of total vapour recovery against P/P_a, calculated from Fig. 7, and curves of $R_f(x)$. Partial vapour dosages and recoveries are obtained from the total values using $R_e(t)/R_e(\tau)$. For strongly absorbed materials, $P/P_a = 0.1$ and greater, single curves as in Fig. 8 can be used for the range of wind speeds covered by stability categories C to F. Two curves might be used for each value of P/P_a less than 0.1; one for wind speeds greater than 3 m/s, the other for lower wind speeds. We have adopted values of 5 m/s and 2 m/s for this purpose. A set of curves for suitable values of P/P_a permits interpolation in P/P_a and t/T. A similar procedure can be followed for E(t)/E(T) against t/T, to obtain values for calculating vapour concentrations following the steady state of evaporation, equation 26.

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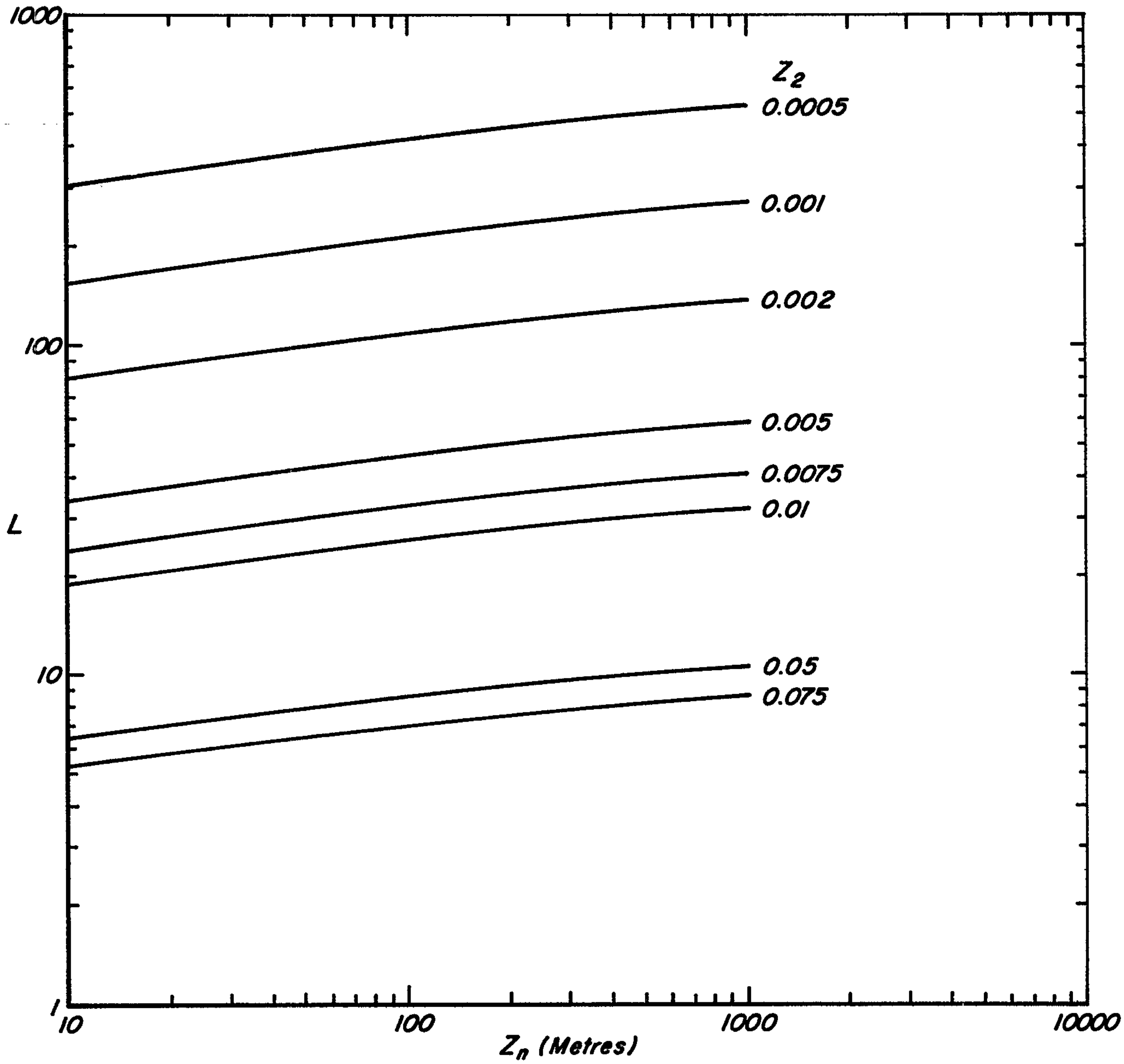

FIG. 4 MESH SIZE V. H FOR VARIOUS VALUES OF Z_2

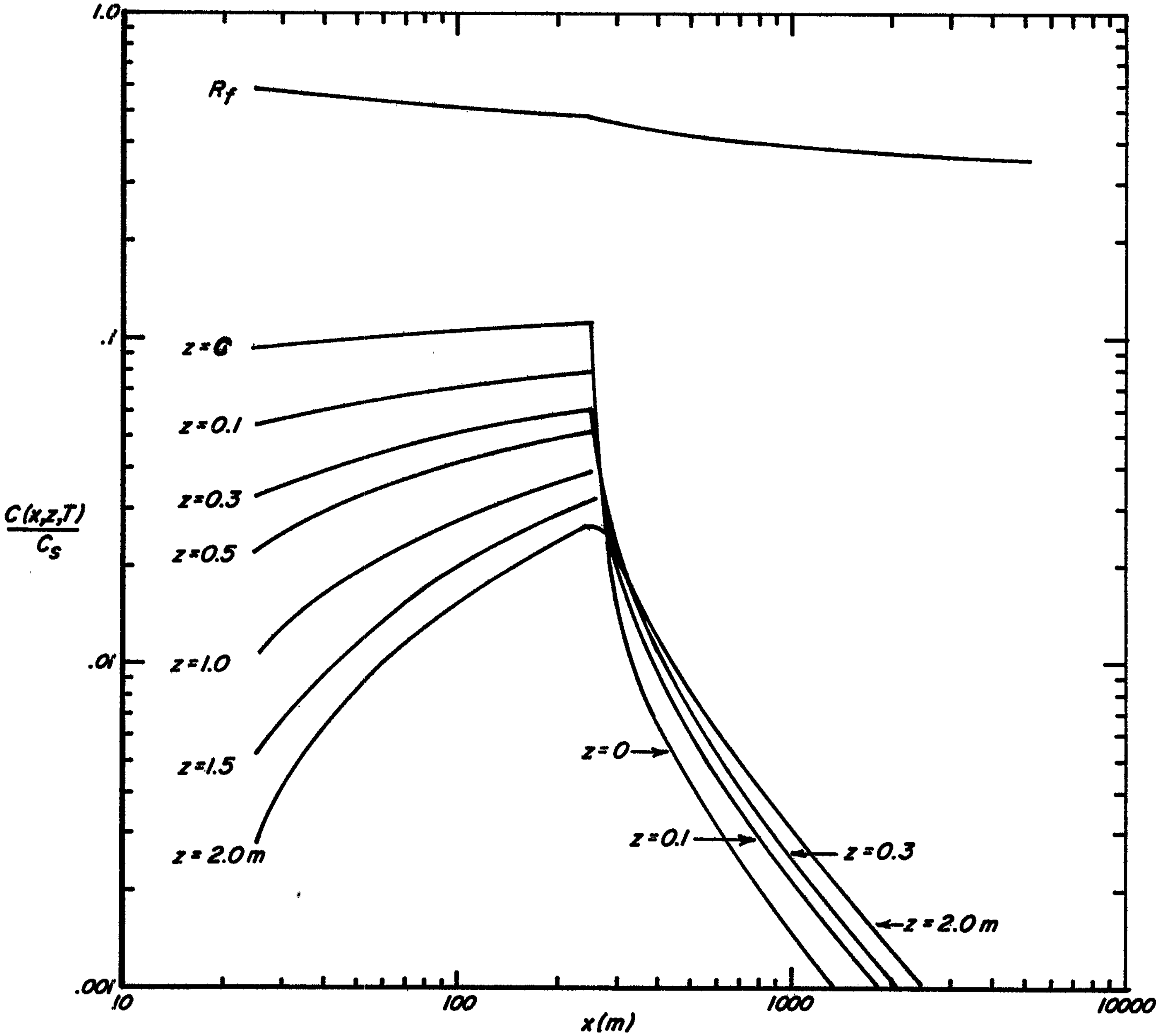

FIG. 5 NORMALIZED CONCENTRATION AND R_f v. DOWNWIND DISTANCE: $x_0 = 250m$; $P/P_a = 1.0$; $S_1 = 0.2$; STABILITY CATEGORY D.

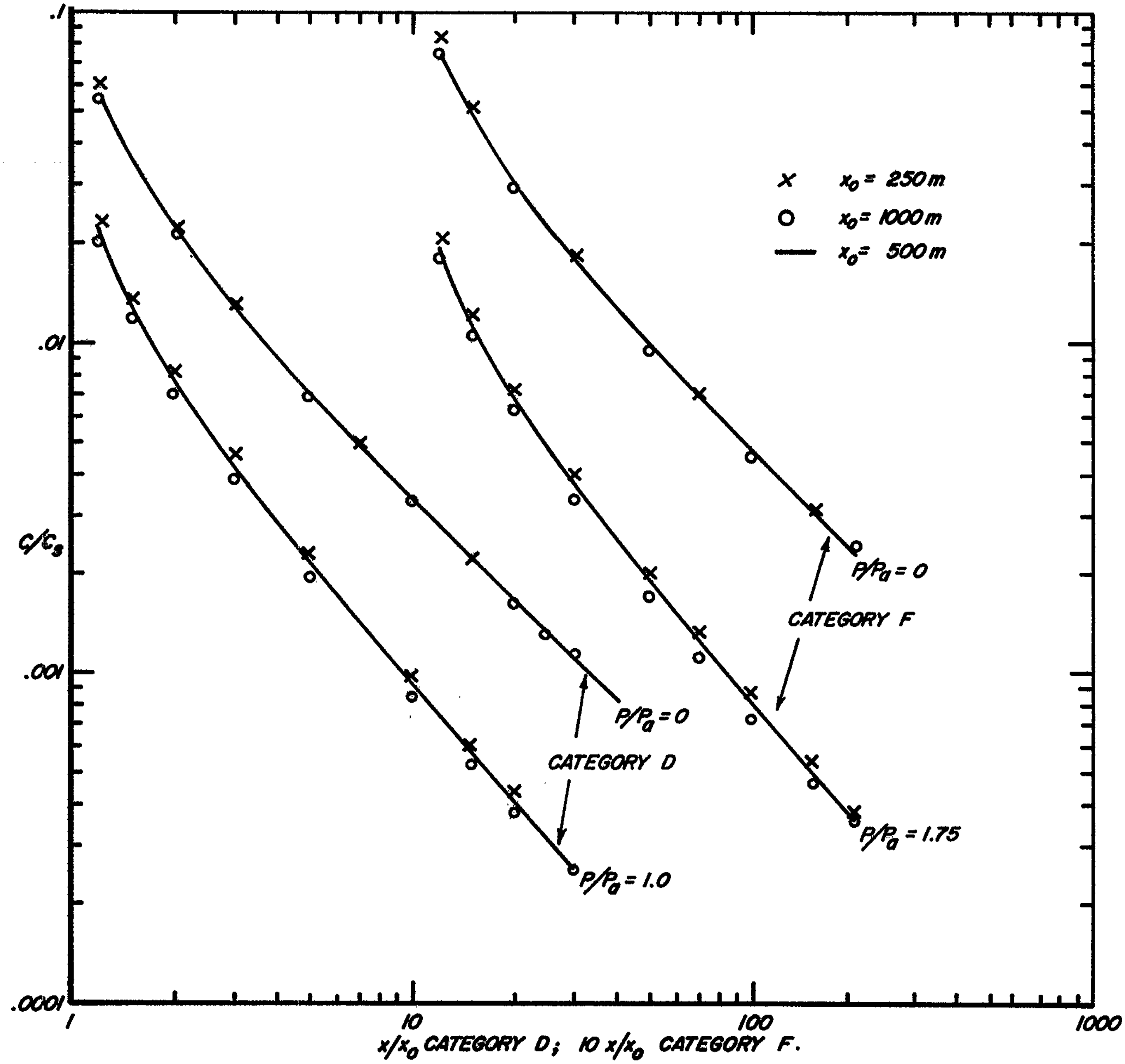

FIG. 6 NORMALIZED CONCENTRATION OF SORBED AND NON-SORBED MATERIALS DOWNWIND OF SPRAYED AREAS OF VARIOUS DOWNWIND DIMENSIONS; MAXIMUM VALUES OF C/C_s; $z = o$ TO $z = 2m$, v. x/x_0, CATEGORY D AND F, $S_1 = 0.2$.

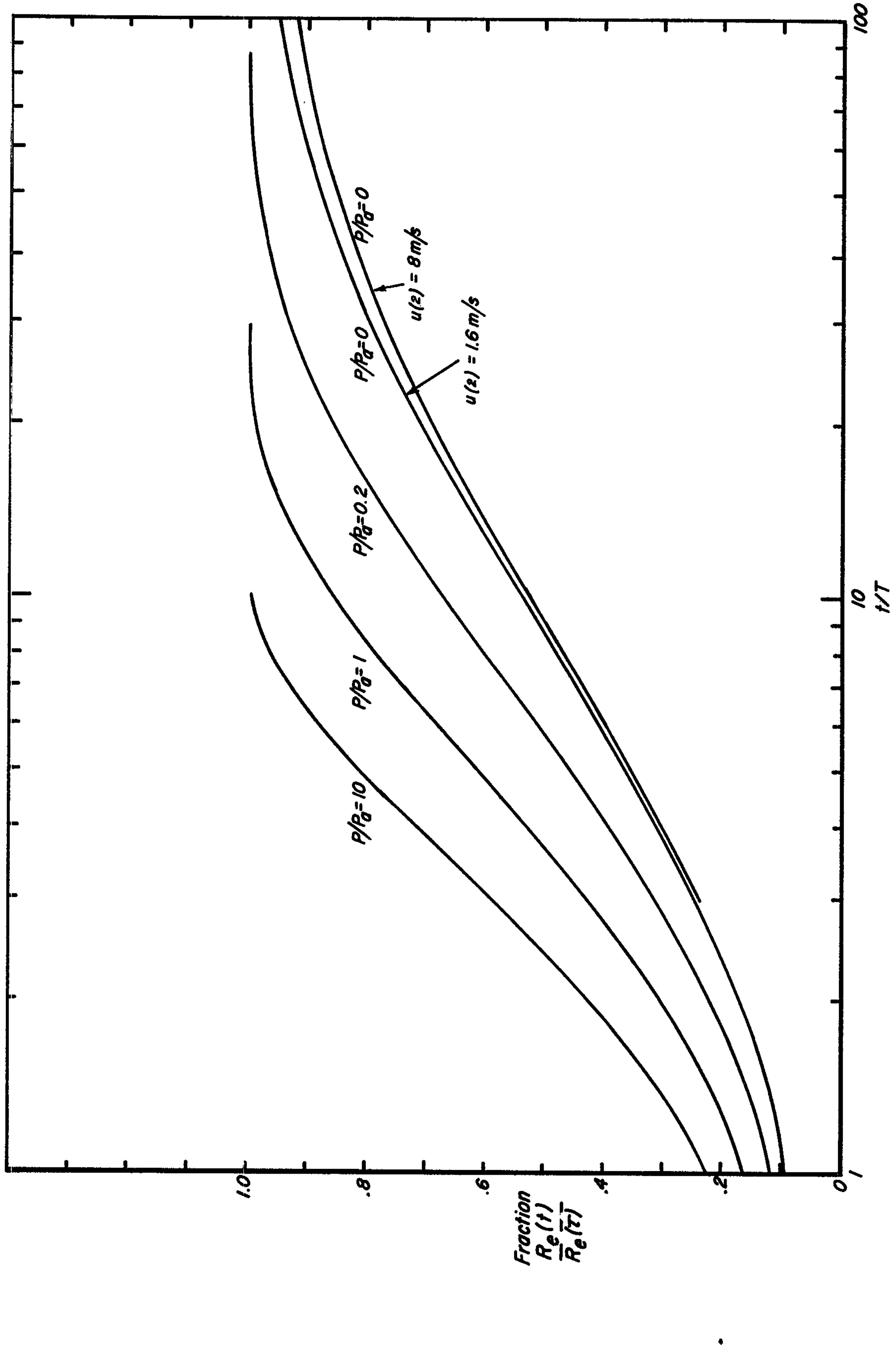

FIG. 8 FRACTION OF TOTAL OF LIQUID EVAPORATED v. VARIOUS VALUES OF P/P_a

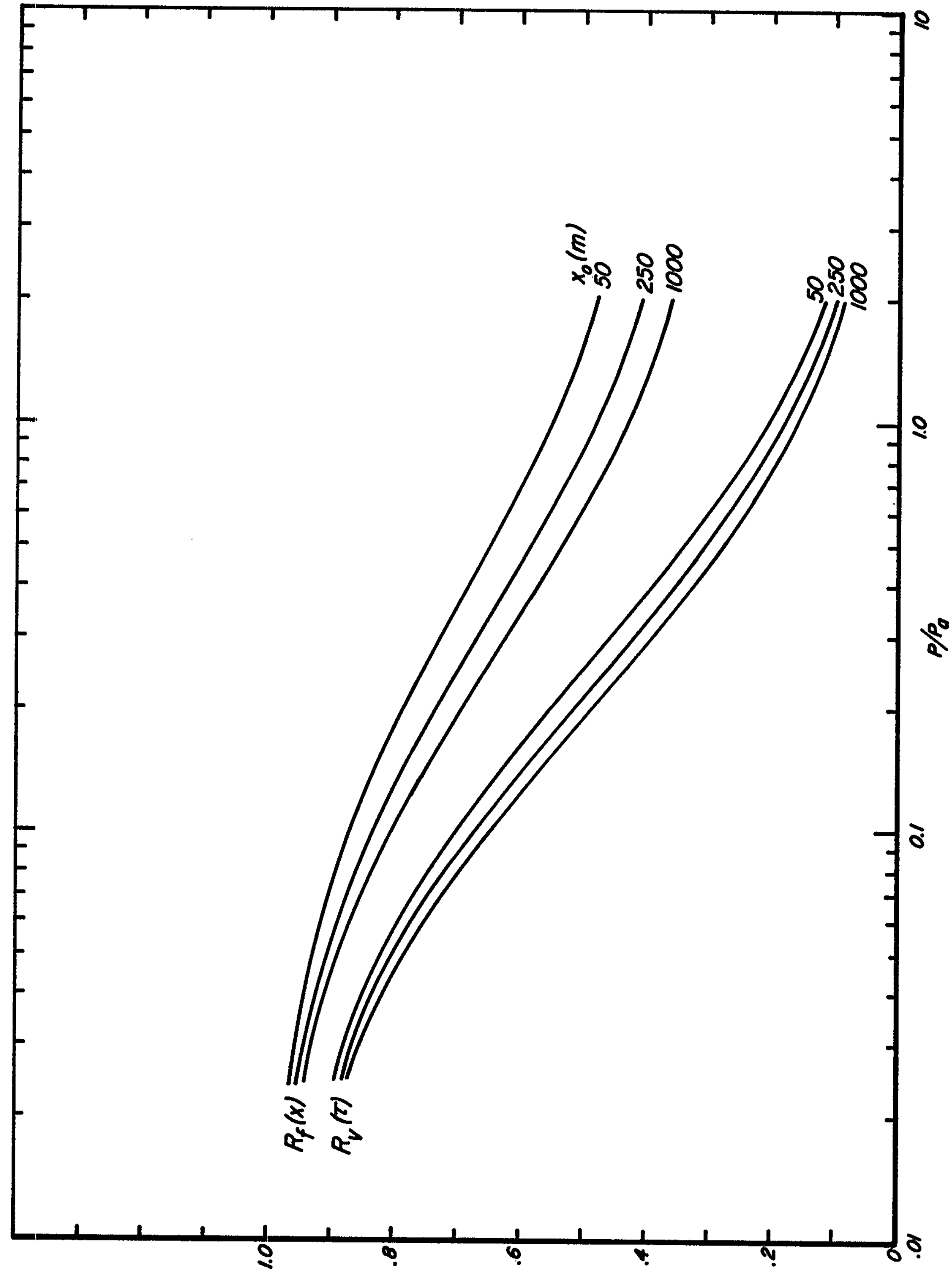

FIG. 9 $R_f(x)$ AND $R_v(\tau)$ v. P/P_a ON THE CONTAMINATED AREA, CATEGORY D.

TABLE 2

CARD NO.		CARD FORMAT	REMARKS
1	P_a(PA),P,p(M),S,S_1(S1),A (AA), SCAN, CHEKK, IREFL, IWRFL	6F10.0,4I2	The symbols in the brackets refer to the Fortran notation of the parameter. The use of the four integer inputs is described in the body of the Appendix.
2	JX	I2	No. of Δx_i to be read in max JX=2.
3	(XINCM(I),DELX(I),I=1,JX)	8F10.0	XINCM(I) = max downwind distance Δx_i is to be used to.
4	Z_2(Z2),H(HIGH),$\Delta \ell$(DELL)	3F10.0	
5	X_o(EDGE),ST0C,X0,N,NSTEP		The last four parameters are used for restarting the program. Their mode of use is described in the body of the Appendix.
6	NUM0X,N0VES	2I2	No. of downwind positions to be typed out, max 20, No. of vertical intervals to be typed out.
7	(X0UT(I), I=1,NUM0X)	8F10.0	Identification of required output position.
8a	(STATZ(I),ENDZ(I), Z0UIN(I),I=1,N0VES)	3F10.0	Description of required output intervals. Start position,end, and increment size. Max. size of output array is 25.
9	(HEAD(I), I=1,80)	80A1	Any alphanumeric heading information.

is stored on disk, ST0C is stored at the first position on the subfile and therefore when X0 is used as a starting position on a subsequent run, a parity check is carried out. If the stored ST0C and X0 are not the same, the run will be terminated with an error message.

Another feature of the retrieval of information from the disk store is the use of N and NSTEP. N defines the size of the concentration profile which is to be retrieved, max N=200, and NSTEP refers to whether all N elements are required, or only every NSTEPth one. N and NSTEP was used extensively in the development of the model but now are only of limited use. If N and NSTEP are left blank, then they are set at N=200 and NSTEP=1.

OUTPUT

The form of the output is controlled by cards 6-9. X0UT(I) is the array of downwind positions for which a normalized profiles of concentrations are to be typed out. Card 8 describes the degree of resolution in the vertical profile required. The values of concentration typed out are interpolations, with the aid of Bessel's formula, of those values calculated. A common output grid used by the authors for studies of small source areas is given in Table 3 below.

TABLE 3

SAMPLE OUTPUT GRID

CARD	STATZ (m)	ENDZ (m)	Z0UIN (m)
8a	0.0	1.0	0.1
8b	1.0	10.0	1.0
8c	10.0	50.0	10.0

Card 9 provides the user with 80 characters of descriptive heading information. This information is alphanumeric in nature.

A blank card will terminate a given series of runs. Consecutive run information is input sequentually.

COMPUTER PROGRAMS

The structure of the main line program is given in block diagram form in Fig. 1. The purpose of each of the six subroutines is given in this diagram. A listing of the fortran program in its present form along with a sample output is also included in this Appendix.

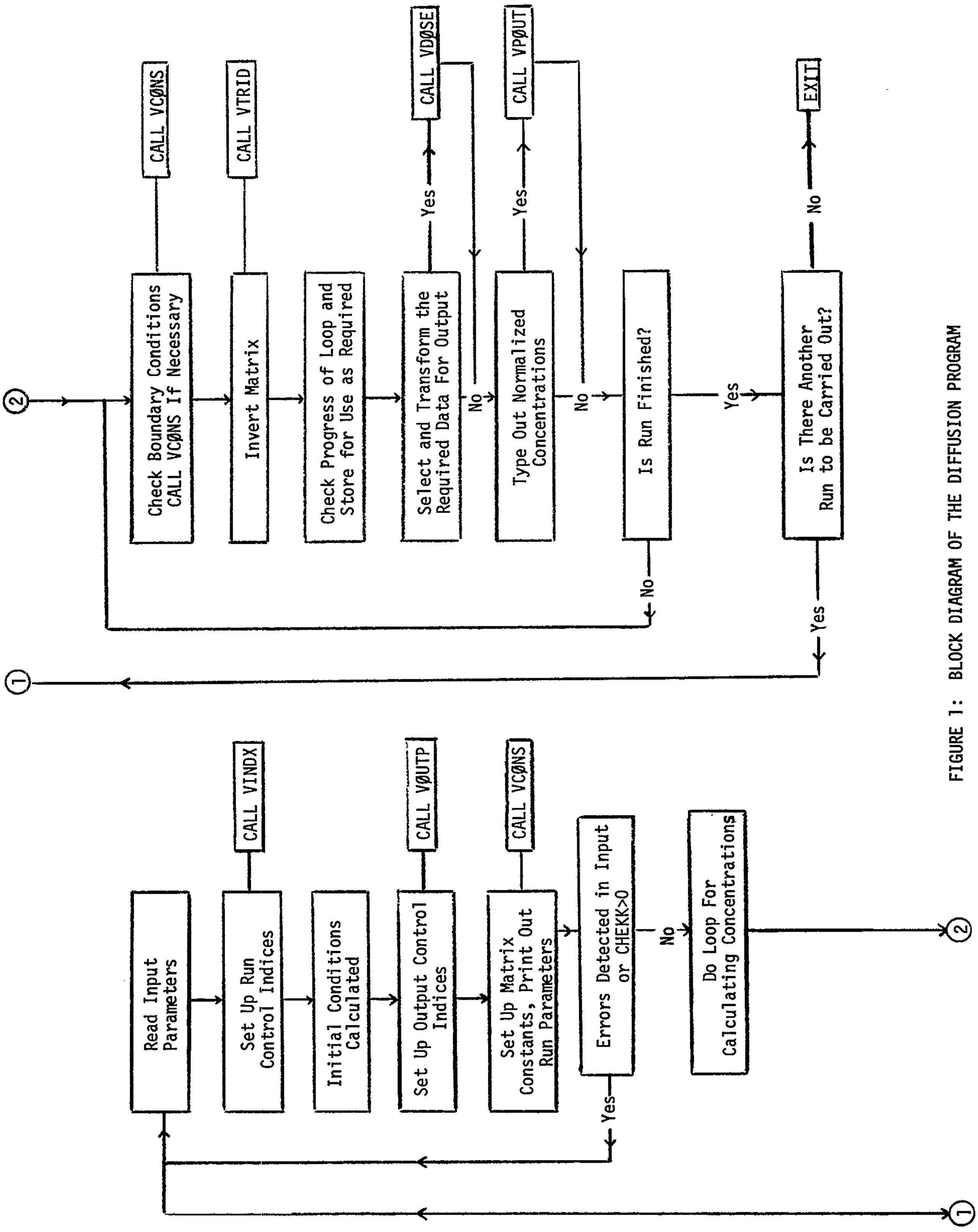

FIGURE 1: BLOCK DIAGRAM OF THE DIFFUSION PROGRAM

PROGRAM LISTING

```
      SUBROUTINE VOUTP(ZZ,Z2,DELL,ID,RD,K,XOUT,NXOUT,NUMOX,DELX,XINCM,NI
     1NX,XO,JX,SCAN,NEROR)
C
C     SUBROUTINE TO SET UP PRINT-OUT CONTROLS
      INTEGER SCAN
      DIMENSION XOUT(1),STATZ(25),ENDZ(25),ZOUIN(25),ZZ(1),ID(1),RD(1)
      DIMENSION XINCM(2),NXOUT(1),NINX(2),DELX(2)
      READ(2,101) NUMOX,NOVES
      READ(2,102) (XOUT(I),I=1,NUMOX)
      READ(2,103) (STATZ(I),ENDZ(I),ZOUIN(I),I=1,NOVES)
C
C     Z OUTPUT ARRAY SET UP
      K=1
      DO 1 J=1,NOVES
      IF(K-1) 2,2,3
    3 IF(IFIX(10.0*(STATZ(J)+0.005))-IFIX(10.0*(ZZ(K)+0.005))) 2,5,6
    6 K=K+1
    2 ZZ(K)=STATZ(J)
    5 DO 7 I=1,25
      K=K+1
      ZZ(K)=ZZ(K-1) + ZOUIN(J)
      IF(IFIX(10.*(ZZ(K)+0.005))-IFIX(10.*(ZZ(K-1)+0.005))) 10,10,8
    8 IF(IFIX(10.*(ZZ(K)+0.005))-IFIX(10.*(ENDZ(J)+0.005))) 7,1,1
    7 CONTINUE
      GO TO 9
   10 K=K-1
    1 CONTINUE
    9 IF(K-25) 11,11,12
   12 WRITE(3,104)
      NEROR=1
   11 DO 15 I=1,K
      RD(I)=1.0 + ALOG((ZZ(I)+DELL)/DELL)/ALOG((Z2+DELL)/DELL)
      ID(I)=IFIX(RD(I))
      RD(I)=RD(I)-ID(I)
   15 CONTINUE
C
C     X OUTPUT CONTROL INDICES ARE SET UP
      DO 13 I=1,NUMOX
      XOUT(I)=XOUT(I)-XO
   13 CONTINUE
      IF(NUMOX-20) 19,19,20
   20 WRITE(3,105)
      NEROR=1
   19 IF(XOUT(NUMOX)-XINCM(JX)) 21,21,22
   22 WRITE(3,106)
      NEROR=1
   21 DO 23 I=1,NUMOX
      IF(XOUT(I)-XINCM(1)) 24,24,25
   24 NXOUT(I)=IFIX(XOUT(I)/DELX(1) + 0.001)
      GO TO 23
   25 NXOUT(I)=NINX(1) + IFIX((XOUT(I)-XINCM(1))/DELX(2) + 0.001)
   23 CONTINUE
      DO 26 I=1,K
      ZZ(I)=ZZ(I) + 0.0001
   26 CONTINUE
```

```
      DO 27 I=1,NUMOX
      XOUT(I)=XOUT(I) + 0.0001
   27 CONTINUE
C
      IF(SCAN-1) 28,29,29
   29 WRITE(3,107) NUMOX
      WRITE(3,108)
      WRITE(3,109) (XOUT(I),NXOUT(I),I=1,NUMOX)
      WRITE(3,110) K
      WRITE(3,111)
      WRITE(3,112) (STATZ(I),ENDZ(I),ZOUIN(I),I=1,NOVES)
      WRITE(3,113)
      WRITE(3,114) (ZZ(I),ID(I),RD(I),I=1,K)
  101 FORMAT(2I2)
  102 FORMAT(8F10.0)
  103 FORMAT(3F10.0)
  104 FORMAT(10X,'YOU ARE ASKING FOR MORE THAN 25 VERTICAL POSITIONS TO
     1BE TYPED OUT,PROGRAM STOPPED')
  105 FORMAT(10X,'YOU ARE ASKING FOR MORE THAN 20 DOWNWIND POSITIONS TO
     1BE TYPED OUT,PROGRAM STOPPED')
  106 FORMAT(10X,'YOU ARE ASKING FOR A DOWNWIND POSITION TO BE TYPED OUT
     1 THAT HAS NOT BEEN CALCULATED, PROGRAM STOPPED')
  107 FORMAT(1H1,/,50X,'OUTPUT CONTROLS',//,36X,'NUMBER OF DOWNWIND POSI
     1TIONS TYPED OUT = ',I2,/)
  108 FORMAT(40X,'X (METERS)  STEPS   X (METERS)  STEP',/)
  109 FORMAT(39X,F8.2,4X,I5,4X,F8.2,4X,I5)
  110 FORMAT(/,36X,'NUMBER OF VERTICAL POSITIONS TYPED OUT = ',I2,/)
  111 FORMAT(40X,'Z OUTPUT CONTROLS',//,42X,'START',11X,'END',9X,'INCREM
     1ENT',/)
  112 FORMAT(40X,F7.2,8X,F7.2,8X,F7.2)
  113 FORMAT(/,19X,3(7X,'Z',7X,'ID   THETA'))
  114 FORMAT(20X,F9.2,I7,F9.4,F9.2,I7,F9.4,F9.2,I7,F9.4)
   28 RETURN
      END
```

```
      SUBROUTINE VINDX(XINCM,DELX,Z2,DELL,HIGH,EDGE,STOC,XO,N,NSTEP,NINX
     1,NE,NX,NSTOC,JX,SCAN,NEROR)
      INTEGER SCAN
      DIMENSION XINCM(2),DELX(2),NINX(2)
C
C     SUBROUTINE TO SET UP AREA CONTROL INDICES
      READ(2,101) JX
      READ(2,102) (XINCM(I),DELX(I),I=1,JX)
      READ(2,102) Z2,HIGH,DELL
      READ(2,103) EDGE,STOC,XO,N,NSTEP
      NEROR=0
      STOC=STOC - XO
      EDGE=EDGE - XO
      DO 1 I=1,JX
      XINCM(I)=XINCM(I)- XO
    1 CONTINUE
      NINX(1)=IFIX(XINCM(1)/DELX(1) + 0.001)
      NX=NINX(1)
      NSTOC=IFIX(STOC/DELX(1) + 0.001)
      NE=IFIX(EDGE/DELX(1) + 0.001)
      IF(JX-1) 2,2,3
    3 NINX(2)=IFIX((XINCM(2)-XINCM(1))/DELX(2) + 0.001)
      NX=NINX(1) + NINX(2)
      IF(STOC - XINCM(1)) 4,4,5
    5 NSTOC=NINX(1) + IFIX((STOC-XINCM(1))/DELX(2) + 0.001)
    4 IF(EDGE - XINCM(1)) 6,6,7
    7 NE=NINX(1) + IFIX((EDGE-XINCM(1))/DELX(2) + 0.001)
    6 IF(XINCM(1)-XINCM(2)) 8,8,9
    8 IF(STOC-XINCM(2)) 10,10,9
   10 IF(EDGE-XINCM(2)) 2,2,9
    9 WRITE(3,104)
      NEROR=1
    2 STOC=STOC + XO
      IF(SCAN-1) 11,12,12
   12 WRITE(3,105)
      WRITE(3,106) Z2,DELL
      WRITE(3,107) (XINCM(I),DELX(I),NINX(I),I=1,JX)
      WRITE(3,108) NX
      WRITE(3,109) EDGE,NE
  101 FORMAT(I2)
  102 FORMAT(8F10.0)
  103 FORMAT(3F10.0,2I3)
  104 FORMAT(10X,'ERROR DETECTED IN THE INPUT DIMESIONS OF THE LAYOUT,
     1PROGRAM STOPPED')
  105 FORMAT(1H1,53X,'CONTROL INDICES',//)
  106 FORMAT(36X,'Z CONTROLS',/,41X,'Z(2) =',F6.4,/,41X,'DELL =',F6.4,/)
  107 FORMAT(36X,'X CONTROLS',/,41X,'DISTANCE(METERS) INCREMENT(METERS)
     1  STEPS',//,2(44X,F8.2,11X,F7.3,8X,I4,/))
  108 FORMAT(78X,I4,/)
  109 FORMAT(36X,'EDGE OF CONTAMINATION',/,41X,'DISTANCE(METERS)',7X,'ST
     1EPS',//,43X,F8.2,13X,I4)
   11 RETURN
      END
```

```
      SUBROUTINE VCONS(NZ,Z,A,PSI,Z2,HIGH,DELL,S,S1,P,PA,AA,M,L,DELX,XO,
     1JX,XINCM,XI1,EDGE,SCAN)
C
C     SUBROUTINE TO CALCULATE MATRIX CONSTANTS AND OUTPUT PARAMETERS
      REAL M,NU
      INTEGER SCAN
      DIMENSION Z(1),A(1),DELZ(200),HEAD(80),XINCM(2),DELX(2)
      Z(1)=0.0
      NZ=IFIX(1.0 + ALOG((HIGH+DELL)/DELL)/ALOG((Z2+DELL)/DELL)) + 1
      NU=(Z2+DELL)/DELL
      IF(NZ-200) 1,1,2
    2 NZ=200
    1 A(1)=1.0 + ALOG(NU)*PSI*PA/AA
      XI1=ALOG(NU)*PA/AA
      DO 3 I=2,NZ
      RI=FLOAT(I)
      DELZ(I)=(NU**(RI-2.))*Z2
      Z(I)=Z(I-1) +DELZ(I)
      A(I)=2.0 + (DELL**(M+1.))*(NU**(RI-3./2.))*(NU-1.)*((NU**(RI-1.)-1
     1.)**M)*ALOG(NU**2.)/((2.**M)*AA*DELX(L))
    3 CONTINUE
C
      IF(ABS(Z(NZ)-HIGH)-ABS(Z(NZ-1)-HIGH)) 4,4,5
    5 NZ=NZ-1
    4 A(NZ)=A(NZ)-1.0
      GO TO (6,7),L
    6 READ(2,101) (HEAD(I),I=1,80)
      WRITE(3,102)
      WRITE(3,103) (HEAD(I),I=1,80)
      WRITE(3,104) PA
      WRITE(3,105) P
      WRITE(3,106) M
      WRITE(3,107) S
      WRITE(3,108) S1
      WRITE(3,109) AA
      XEDGE=XINCM(JX) + XO
      EDGOT=EDGE + XO
      WRITE(3,110) XEDGE,HIGH,EDGOT
      WRITE(3,111) Z2,Z(NZ),NZ,DELL
      WRITE(3,112) (DELX(I),I=1,JX)
    7 IF(SCAN-3) 8,8,9
    9 II=NZ-1
      DELZ(1)=0.0
      WRITE(3,113)
      WRITE(3,114)
      DO 10 I=1,II,2
      J=I+1
      WRITE(3,115)  I,Z(I),DELZ(I),A(I),J,Z(J),DELZ(J),A(J)
   10 CONTINUE
    8 RETURN
  101 FORMAT(80A1)
  102 FORMAT(1H1,32X,'A MATHEMATICAL MODEL DESIGNED TO DESCRIBE THE DOWN
     1WIND',/,28X,'TRAVEL AND VERTICAL PROFILE OF VAPOUR FROM A CONTAMIN
     2ATED AREA',//)
```

```
103 FORMAT(20X,80A1,/)
104 FORMAT(52X,'INPUT PARAMETERS',///,32X,'PA= ',F7.5,4X,'(AIR PERMEAB
   1ILITY)')
105 FORMAT(32X,'P = ',F7.5,4X,'(PLANT PERMEABILITY)')
106 FORMAT(32X,'M= ',F5.2,7X,'(WIND PROFILE PARAMETER)')
107 FORMAT(32X,'S = ',F5.3,6X,'(TOTAL SPECIFIC AREA)')
108 FORMAT(32X,'S1 = ',F6.3,4X,'(LIQUID SPECIFIC AREA)')
109 FORMAT(32X,'AA= ',F6.4,5X,'(VON KARMANS CONSTANT/10)')
110 FORMAT(//,44X,'DIMENSIONS OF CONTAMINATED AREA',//,32X,'XDOWN = ',
   1F7.1,1X,'MAXIMUM DOWNWIND DISTANCE CONSIDERED',/,32X,'ZLID = ',F6.
   21,3X,'MAXIMUM HEIGHT CONSIDERED-INPUT',/,32X,'EDGE = ',F6.1,3X,'DO
   3WNWIND DIMENSION OF CONTAMINATION',/)
111 FORMAT(45X,'VERTICAL AND HORIZONTAL CONTROLS',/,32X,'VERTICAL',//,
   132X,'Z2 = ',F7.4,/,32X,'Z(NZ) =',F6.1,/,32X,'NZ = ',I3,/,32X,'DELL
   2 = ',F6.4,/)
112 FORMAT(32X,'HORIZONTAL ',2(3X,F6.3))
113 FORMAT(1H1,42X,'VERTICAL ARRAYS AND MATRIX CONSTANTS',/)
114 FORMAT(7X,'I',15X,'Z',11X,'DELZ',13X,'A',14X,'I',15X,'Z',11X,'DELZ
   1',13X,'A',/)
115 FORMAT(5X,I3,11X,F8.3,6X,F8.3,7X,F8.3,9X,I3,11X,F8.3,6X,F8.3,7X,F8
   1.3)
    END
```

```
      SUBROUTINE VTRID(CV,A,S1,SOURC,PSI,J,N,NE,NZ,XI1,SCAN)
C
C     SUBROUTINE TO INVERT TRIDIAGONAL MATRIX AND CALCULATE CONCENTRATIONS
      INTEGER SCAN
      DIMENSION CV(2),A(1),D(200),W(200),G(200),Q(200)
      D(1)=CV(2)-(1.+XI1*PSI)*CV(1)+XI1*S1*SOURC
      II=NZ-1
      DO 1 I=2,II
      D(I)=CV(I-1)-(4.0-A(I))*CV(I) + CV(I+1)
    1 CONTINUE
      D(NZ) = CV(NZ-1) - (2.0-A(NZ))*CV(NZ)
      IF(J-1) 8,8,3
    8 IF(N) 2,2,3
    3 IF(J-(NE+1)) 4,2,2
    4 D(1)=D(1) + XI1*S1*SOURC
    2 W(1)=A(1)
      G(1)=D(1)/W(1)
C
      DO 5 I=2,NZ
      Q(I-1)=-1.0/W(I-1)
      W(I)= A(I) + 1.0*Q(I-1)
      G(I)= (D(I) + 1.0*G(I-1))/W(I)
    5 CONTINUE
      CV(NZ)=G(NZ)
      DO 6 I=1,II
      L=NZ-I
      CV(L)=G(L) - Q(L)*CV(L+1)
    6 CONTINUE
C
      IF(SCAN-4)  7,9,7
    9 WRITE(3,101) J,CV(1),CV(2),SOURC,D(1),G(1),Q(1)
      WRITE(3,102) (CV(I),I=1,NZ)
  102 FORMAT(7E17.6)
  101 FORMAT(10X,3X,I3,4X,6E15.6)
    7 RETURN
      END
```

```
      SUBROUTINE VDOSE(DOSE,ID,RD,INN,J1,CV,NZ,ZZ,Z)
C
C     SUBROUTINE TO CALCULATE INTERPOLATION VALUES FOR CONCENTRATION
      DIMENSION  DOSE(25,4),ID(1),RD(1),CV(1),ZZ(1),Z(1)
      DO 1 I=1,INN
      IRI=ID(I)
      IF(IRI-(NZ-2)) 2,2,3
    3 IF(RD(I)-0.5) 6,7,7
    6 IF(IRI-NZ) 8,8,9
    9 IRI=NZ
      GO TO 8
    7 IF(IRI+1-NZ) 10,10,9
   10 IRI=IRI+1
    8 ZZ(I)=Z(IRI)
      DOSE(I,J1)=CV(IRI)
      GO TO 11
    2 DO12F=CV(IRI+1)-CV(IRI)
      D2OF=DO12F-(CV(IRI)-CV(IRI-1))
      D2P1F=(CV(IRI+2)-CV(IRI+1))-DO12F
      D312F=D2P1F-D2OF
      B2=RD(I)*(RD(I)-1.)/4.0
      B3=RD(I)*(RD(I)-0.5)*(RD(I)-1.)/6.0
      DOSE(I,J1)=(CV(IRI)+CV(IRI+1))/2.0 + (RD(I)-0.5)*DO12F + B2*(D2OF+
     1 D2P1F) + B3*D312F
   11 IF(DOSE(I,J1))  5,1,1
    5 DOSE(I,J1)=0.0
    1 CONTINUE
    4 RETURN
      END
```

```
      SUBROUTINE VPOUT(J1,J2,DOSE,ZZ,INN,XOUT,N,XO,VAPOT,VAPIN)
C
C     OUTPUT SUBROUTINE
      DIMENSION XOUT(1),ZZ(1),DOSE(25,4),VAPOT(1),VAPIN(1)
      K1=J2-J1+1
      K2=J2
      WRITE(3,101)
      IF(N) 1,1,2
    2 DO 3 I=K1,K2
      XOUT(I)=XOUT(I)+XO
    3 CONTINUE
    1 WRITE(3,102) (XOUT(I),I=K1,K2)
      WRITE(3,103)
      DO 4 I=1,INN
      WRITE(3,104) ZZ(I),(DOSE(I,J),J=1,J1)
    4 CONTINUE
      WRITE(3,105) (VAPOT(I),I=K1,K2)
      WRITE(3,106) (VAPIN(I),I=K1,K2)
C
  101 FORMAT(1H1,48X,'NORMALIZED CONCENTRATIONS')
  102 FORMAT(//,4(22X,'X'),//,2X,4(15X,F8.2))
  103 FORMAT(/,4X,'VERTICAL GRID',4(10X,'CONCENTRATION'),/,9X,'Z(I)',16X
     1,4('C(I)/C(0)',14X))
  104 FORMAT(7X,F6.2,4X,4(10X,F13.6))
  105 FORMAT(/,6X,'VAPOUR OFF',1X,4(10X,F13.6))
  106 FORMAT(/,2X,'VAPOUR RETURNED',4(10X,F13.6))
C
      RETURN
      END
```

```
C     MAIN LINE PROGRAM FOR SOLUTION OF DIFFUSION PROBLEM
C
      INTEGER SCAN,CHEKK
      REAL M
      DEFINE FILE 1 (2020,2,U,ITRK)
      DIMENSION XINCM(2),DELX(2),NINX(2),XOUT(20),NXOUT(20)
      DIMENSION ZZ(25),ID(25),RD(25),DOSE(25,4)
      DIMENSION Z(200),CV(200),A(200),VAPOT(20),VAPIN(20)
C
C     INPUT PARAMETERS
   20 READ(2,101) PA,P,M,S,S1,AA,SCAN,CHEKK,IREFL,IWRFL
      IF(PA) 1,1,2
    1 CALL EXIT
C
C     SET UP RUNNING CONTROL INDICES
    2 CALL VINDX(XINCM,DELX,Z2,DELL,HIGH,EDGE,STOC,XO,N,NSTEP,NINX,NE,NX
     1 ,NSTOC,JX,SCAN,NEROR)
C
C     INITIAL CONDITIONS
      DO 3 I=1,200
      CV(I)=0.0
    3 CONTINUE
      IF(CHEKK) 4,4,5
    4 IF(XO) 5,5,6
    6 IF(N) 7,7,8
    7 N=200
    8 IF(NSTEP) 9,9,10
    9 NSTEP=1
   10 JMAX=N/NSTEP
      IST=1 + (IREFL-1)*202
      READ(1'IST) XOST
      READ(1'IST+1) Z22
      IF(IFIX(ABS(XOST-XO))) 11,12,11
   12 IF(IFIX(10000.*ABS(Z2-Z22))) 11,13,11
   11 WRITE(3,102)
      WRITE(3,103) IST,XOST,XO,Z22,Z2
      CHEKK=1
      SCAN=2
   13 I=IST + 2
      DO 14 J=1,JMAX
      READ(1'I) CV(J)
      I=I+NSTEP
   14 CONTINUE
    5 TVAOF=0.0
      VAREA=0.0
      PSI= (PA*S1 + P*S)/(PA+P)
      SOURC=1.0
      L=1
      J1=1
      J2=1
C
C     SET UP OUTPUT CONTROL INDICES
      CALL VOUTP(ZZ,Z2,DELL,ID,RD,INN,XOUT,NXOUT,NUMOX,DELX,XINCM,NINX,X
     10,JX,SCAN,NEROR)
```

```
C
C     SET UP Z AND MATRIX COEFFICIENTS, PRINT OUT PARAMETERS
      CALL VCONS(NZ,Z,A,PSI,Z2,HIGH,DELL,S,S1,P,PA,AA,M,L,DELX,XO,JX,XIN
     1CM,XI1,EDGE,SCAN)
      IF(XO) 15,15,16
   16 WRITE(3,104) XO
   15 IF(SCAN-2) 17,18,18
   18 WRITE(3,105)
      WRITE(3,106) (Z(I),CV(I),I=1,NZ)
   17 IF(CHEKK) 19,19,20
   19 IF(NEROR) 21,21,20
C
C     DO LOOP FOR CALCULATING CONCENTRATIONS
   21 DO 22 J=1,NX
C
C     CHECK BOUNDARY CONDITIONS
      IF(J-(NINX(1)+1)) 23,24,23
   24 L=L+1
      CALL VCONS(NZ,Z,A,PSI,Z2,HIGH,DELL,S,S1,P,PA,AA,M,L,DELX,XO,JX,XIN
     1CM,XI1,EDGE,SCAN)
   23 IF(J-(NE+2)) 25,26,27
   25 IF(J-(NE+1)) 27,28,27
   28 A(1)=1.0 + ALOG((Z2+DELL)/DELL)*P*S*PA/(AA*(P+PA))
      GO TO 27
   26 SOURC=0.0
      PSI=(P*S)/(P + PA)
C
C     INVERT MATRIX
   27 CALL VTRID(CV,A,S1,SOURC,PSI,J,N,NE,NZ,XI1,SCAN)
      IF(J-(NE+1)) 29,30,29
   30 S1=0.0
   29 TVAOF=TVAOF + (1.0-CV(1))*PA*S1*DELX(L)
      VAREA=VAREA + DELX(L)*(CV(1)*PA*P)*(S-S1)/(P+PA)
C
C     CHECK PROGRESS OF LOOP AND STORE FOR USE AS REQUIRED
      IF(J-NSTOC) 31,32,31
   32 IST=3+(IWRFL-1)*202
      WRITE(1'IST-2) STOC
      WRITE(1'IST-1) Z2
      WRITE(1'IST) (CV(I),I=1,NZ)
   31 IF(J2-NUMOX) 33,33,22
   33 IF(J-NXOUT(J2)) 22,34,34
C
C     SELECT AND TRANSFORM THE REQUIRED DATA FOR OUTPUT
   34 VAPOT(J2)=TVAOF
      VAPIN(J2)=VAREA
      CALL VDOSE(DOSE,ID,RD,INN,J1,CV,NZ,ZZ,Z)
      IF(J1-4) 35,36,36
   35 IF(J2-NUMOX) 37,36,36
C
C     TYPE OUT NORMALIZED CONCENTRATIONS
   36 CALL VPOUT(J1,J2,DOSE,ZZ,INN,XOUT,N,XO,VAPOT,VAPIN)
      J1=0
   37 J1=J1+1
      J2=J2+1
   22 CONTINUE
      GO TO 20
```

```
C
  101 FORMAT(6F10.0,4I2)
  102 FORMAT(1H1,36X,'RESTARTING AT THE WRONG POSITION, RUN TERMINATED',
     1/)
  103 FORMAT(36X,'FILE START POSITION NO.',I7,/,36X,'STORED START POSITI
     1ON',F10.2,/,36X,'INPUT START POSITION',F11.2,//,36X,'STORED Z2 INC
     2REMENT SIZE',F7.4,/,36X,'INPUT Z2  INCREMENT SIZE',F7.4,/)
  104 FORMAT(/,45X,'RUN RESTARTED AT X = ',F7.2)
  105 FORMAT(1H1,51X,'INITIAL CONDITIONS',//)
  106 FORMAT(6(F7.2,F13.6))
      END
```

```
                                  NORMALIZED CONCENTRATIONS

                     X                  X                  X                  X

                   20.00              30.00              40.00              50.00

  VERTICAL GRID   CONCENTRATION      CONCENTRATION      CONCENTRATION      CONCENTRATION
      Z(I)          C(I)/C(0)          C(I)/C(0)          C(I)/C(0)          C(I)/C(0)
      0.00            0.092052           0.018775           0.009233           0.006150
      0.10            0.052591           0.025278           0.012694           0.008506
      0.20            0.038663           0.025645           0.013493           0.009155
      0.30            0.030323           0.024568           0.013649           0.009401
      0.40            0.024540           0.022924           0.013498           0.009451
      0.50            0.020235           0.021067           0.013170           0.009386
      0.60            0.016893           0.019180           0.012734           0.009245
      0.70            0.014226           0.017355           0.012230           0.009052
      0.80            0.012059           0.015641           0.011684           0.008821
      0.90            0.010272           0.014062           0.011116           0.008566
      1.00            0.008784           0.012626           0.010540           0.008291
      2.00            0.002042           0.004318           0.005530           0.005400
      3.00            0.000511           0.001548           0.002644           0.003178
      4.00            0.000131           0.000570           0.001227           0.001779
      5.00            0.000035           0.000213           0.000564           0.000967
      6.00            0.000009           0.000082           0.000261           0.000518
      7.00            0.000002           0.000030           0.000120           0.000277
      8.00            0.000001           0.000013           0.000057           0.000147
      9.00            0.000000           0.000004           0.000026           0.000078
     10.00            0.000000           0.000001           0.000012           0.000042
     20.00            0.000000           0.000000           0.000000           0.000000
     30.00            0.000000           0.000000           0.000000           0.000000
     40.00            0.000000           0.000000           0.000000           0.000000
     50.00            0.000000           0.000000           0.000000           0.000000

    VAPOUR OFF        0.036725           0.045793           0.045793           0.045793

 VAPOUR RETURNED      0.014734           0.020398           0.021663           0.022405
```

```
    A MATHEMATICAL MODEL DESIGNED TO DESCRIBE THE DOWNWIND
 TRAVEL AND VERTICAL PROFILE OF VAPOUR FROM A CONTAMINATED AREA

                  EXAMPLE RUN-DIFFUSION PROGRAM

                         INPUT PARAMETERS

      PA= 0.01000     (AIR PERMEABILITY)
      P = 0.01000     (PLANT PERMEABILITY)
      M=  0.23        (WIND PROFILE PARAMETER)
      S = 2.000       (TOTAL SPECIFIC AREA)
      S1 =  0.200     (LIQUID SPECIFIC AREA)
      AA= 0.0400      (VON KARMANS CONSTANT/10)


                  DIMENSIONS OF CONTAMINATED AREA

      XDOWN =     50.0 MAXIMUM DOWNWIND DISTANCE CONSIDERED
      ZLID =   500.0   MAXIMUM HEIGHT CONSIDERED-INPUT
      EDGE =    25.0   DOWNWIND DIMENSION OF CONTAMINATION

                  VERTICAL AND HORIZONTAL CONTROLS
      VERTICAL

      Z2 =  0.0075
      Z(NZ) = 534.2
      NZ =  39
      DELL = 0.0250

      HORIZONTAL     0.500
```

```
     A MATHEMATICAL MODEL DESIGNED TO DESCRIBE THE DOWNWIND
TRAVEL AND VERTICAL PROFILE OF VAPOUR FROM A CONTAMINATED AREA


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0202 403/04

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1. ORIGINATING ACTIVITY
0204a
Defence Research Establishment Suffield,
0204b Ralston ALTA (CAN)

2a. DOCUMENT SECURITY CLASSIFICATION
UNCLASSIFIED

2b. GROUP

3. DOCUMENT TITLE
04a A MATHEMATICAL MODEL FOR PREDICTING VAPOUR DOSAGES ON AND DOWNWIND OF CONTAMINATED AREAS OF GRASSLAND (U)

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)
06a Technical Paper

5. AUTHOR(S) (Last name, first name, middle initial)
1101 1102
Monaghan, J. and McPherson, W.R.

6. DOCUMENT DATE
4C September 1971

7a. TOTAL NO. OF PAGES
0901 30 58

7b. NO. OF REFS
0902 6

8a. PROJECT OR GRANT NO.
35 D- 20-20-32

9a. ORIGINATOR'S DOCUMENT NUMBER(S)
0203
Suffield Technical Paper No. 386

8b. CONTRACT NO.

9b. OTHER DOCUMENT NO.(S) (Any other numbers that may be assigned this document)

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DSIS
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1. Predictive Model
2. Vapour Dosage
3. Contaminated Terrain
4. Evaporation
5. Liquid Absorption
6. Vapour Absorption
7. Vapour Diffusion
8. Rough Surface
9. Computer Program

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3. DOCUMENT TITLE

A MATHEMATICAL MODEL FOR PREDICTING VAPOUR DOSAGES ON AND DOWNWIND OF CONTAMINATED AREAS OF GRASSLAND (U)

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Monaghan, J. and McPherson, W.R.

6. DOCUMENT DATE September 1971	7a. TOTAL NO. OF PAGES 30	7b. NO. OF REFS 6

8a. PROJECT OR GRANT NO. 20-20-32	9a. ORIGINATOR'S DOCUMENT NUMBER(S) Suffield Technical Paper No. 386
8b. CONTRACT NO.	9b. OTHER DOCUMENT NO.(S) (Any other numbers that may be assigned this document)

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