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Presented in Partial Fulfillment of the Requirements for
the Degree Doctor of Philosophy in the Graduate
School of The Ohio State University

By

Iqbal S. Rai, B.A., B.Sc. (Civil Engineering),
M.E. (Structural Engineering)

* * * * *

The Ohio State University

1975

Reading Committee:
Charles A. Moore
Ranbir S. Sandhu
Charles Saltzer
Keith W. Bedford
Robert M. Sykes

Approved By

Adviser
Department of Civil Engineering
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VITA

January 29, 1936 Born, Majali Kalan (Punjab), India

1956 B.A., Government College, Ludhiana (Punjab), India

1960 B.Sc. (Civil Engineering), G.N. Engineering College, Ludhiana (Punjab), India

1960-1971 Lecturer/Asst. Prof./Assoc. Prof., G.N. Engineering College, Ludhiana (Punjab), India

1966 M.E. (Structural Engineering), University of Roorkee, Roorkee (U.P.), India

1971-1975 Graduate Research Assoc., Civil Engineering Dept., Ohio State University, Columbus, Ohio

PUBLICATIONS


FIELDS OF STUDY

Major Field: Civil Engineering

Studies in Structures: Professors R.S. Sandhu and Morris Ojalvo


Studies in Mathematics: Professors Henry D. Colson and Charles Saltzer

Studies in Computer Science: Professor Charles Saltzer
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<td>gas component A, concentration of $\text{H}_2\text{CO}_3$, operator or surface area</td>
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<td>$A_1$</td>
<td>initial equilibrium concentration of $[\text{H}_2\text{CO}_3]$</td>
<td></td>
</tr>
<tr>
<td>$A_2$</td>
<td>final equilibrium concentration of $[\text{H}_2\text{CO}_3]$</td>
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<td>change in concentration of $[\text{H}_2\text{CO}_3]$ due to solution of $\text{CO}_2(g)$</td>
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<td>${a_m(\vec{x})}$</td>
<td>row vector of spatial derivatives of interpolation functions</td>
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<td>B</td>
<td>concentration of $[\text{HCO}_3^-]$ ions</td>
<td></td>
</tr>
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<td>$[B]$</td>
<td>the derived matrix defined by Eq. (161)</td>
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<td>$B_i$</td>
<td>initial equilibrium concentration of $[\text{HCO}_3^-]$ ions</td>
<td></td>
</tr>
<tr>
<td>$B_2$</td>
<td>final equilibrium concentration of $[\text{HCO}_3^-]$ ions</td>
<td></td>
</tr>
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<td>$B_n$</td>
<td>operator defined on the boundary $S_n$</td>
<td></td>
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<tr>
<td>$\Delta B$</td>
<td>change in concentration of $[\text{HCO}_3^-]$ or $[\text{H}^+]$ ions due to ionization of $[\text{H}_2\text{CO}_3]$</td>
<td></td>
</tr>
<tr>
<td>${b_m(\vec{x})}$</td>
<td>row vector of interpolation functions</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>concentration of $[\text{CO}_3^-]$ ions, or total concentration of gas mixture</td>
<td></td>
</tr>
<tr>
<td>$C_{Ki}$</td>
<td>mass transfer coefficient at surface i</td>
<td></td>
</tr>
<tr>
<td>$\bar{C}$</td>
<td>a variation in concentration</td>
<td></td>
</tr>
<tr>
<td>$C_A$</td>
<td>concentration of gas A</td>
<td></td>
</tr>
<tr>
<td>$\bar{C}_A$</td>
<td>mean concentration of gas A over time $\Delta t$</td>
<td></td>
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<tr>
<td>$\dot{C}_A$</td>
<td>rate of change of concentration of gas A with time</td>
<td></td>
</tr>
<tr>
<td>$\bar{\dot{C}}_A$</td>
<td>mean rate of change of concentration of gas A over time $\Delta t$</td>
<td></td>
</tr>
<tr>
<td>$C_a$</td>
<td>set of unknown concentrations</td>
<td></td>
</tr>
<tr>
<td>$C_b$</td>
<td>set of known or prescribed concentrations</td>
<td></td>
</tr>
<tr>
<td>$C_e, C_a$</td>
<td>concentration outside the boundary</td>
<td></td>
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</table>
concentration on the boundary

initial concentration of $[\text{CO}_3^2]$ ions

final concentration of $[\text{CO}_3^2]$ ions

change in concentration of $[\text{CO}_3^2]$ ions due to ionization of $[\text{HCO}_3^-]$,

column vector of nodal point concentrations at time $t$

effective diffusion coefficient defined by Eq. (17), or concentration of $[\text{Ca}^{++}]$ ions

bulk diffusion coefficient for gas A in gas B

pressure independent diffusion coefficient defined by Eq. (3)

Knudsen diffusion coefficient for gas A

maximum value of effective diffusion coefficient

effective diffusion coefficient for element $m$

Gateaux differential defined by Eq. (125)

nodal point values of effective diffusion coefficient

difference in effective diffusion coefficients at nodes $i + 1$ and $i - 1$

initial equilibrium concentration of $[\text{Ca}^{++}]$ ions

final equilibrium concentration of $[\text{Ca}^{++}]$ ions

change in concentration of $[\text{Ca}^{++}]$ ions due to ionization of $\text{CaCO}_3(S)$

differential operator of order $\leq \alpha$

depth of fill

depth of impervious boundary

depth of vent

accumulating capacity matrix

accumulating capacity matrix for element $m$
total discretization error

field or function

flow vector

$\varepsilon V(r)$ void fraction in pores of radius $r - \Delta r$ to $r + \Delta r$

gravitational constant

$\varepsilon_n$ flow vector on boundary $n$

concentration of $[H^+]$ ions

initial concentration of $[H^+]$ ions

final concentration of $[H^+]$ ions

$H^m$ Sobolev space of $m$ times differentiable functions

$H^m_0$ Sobolev space of $m$ times differentiable functions with compact support

coefficient of mass transfer across the boundary layer

coefficient of mass transfer across the boundary layer of element $m$

indices used to denote coordinate axes

if and only if

Jacobian matrix

flow or diffusivity matrix

Henry's law constant for $CO_2$

flow or diffusivity matrix for element $m$

solid solution equilibrium constant for $CaCO_3$

equilibrium constant (ion product) for water

first acidity constant

second acidity constant

diffusivity matrix due to surface convection for element $m$

Knudsen diffusion parameter
k order of interpolation functions

f^m length of element m

M total number of elements in the system

M_α molecular weight of gas α

m the order of differential operator

N_A flux of gas A relative to a fixed point

N_A rate of change of flux of gas A

n number of gas moles, or normal to a surface

Δn change in number of gas moles

OH concentration of [OH^-] ions

OH_I initial concentration of [OH^-] ions

OH_E final concentration of [OH^-] ions

P total pressure, partial pressure of CO_2(g) or matrix defined in Eq. (157)

P_i initial equilibrium partial pressure of CO_2(g)

P_f final equilibrium partial pressure of CO_2(g)

ΔP change in partial pressure of CO_2(g)

Q_α_i rate of flux of gas α in direction i

q flux across the boundary

R gas constant or bounded closed region in three dimensional Euclidian space

R^n bounded closed region in n-dimensional Euclidian space

R_α mole fraction of gas A lost due to chemical reaction

r pore radius or radial coordinate of a point

r_f radial distance of fill boundary from its axis

r_i radial distance of node i from fill axis

r_max maximum pore radius
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<td>$r_{\text{min}}$</td>
<td>minimum pore radius</td>
</tr>
<tr>
<td>$r_s$</td>
<td>radial distance of soil boundary from fill axis</td>
</tr>
<tr>
<td>$r_v$</td>
<td>radial distance of vent from fill axis</td>
</tr>
<tr>
<td>$\mathbf{r}$</td>
<td>vector of nodal point values of radial distance of nodes of an element from fill axis</td>
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<td>$S$</td>
<td>degree of saturation (percent)</td>
</tr>
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<td>$S_A$</td>
<td>mole fraction of gas A lost due to surface convection</td>
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<tr>
<td>$S_h$</td>
<td>Sobolev space with support over h</td>
</tr>
<tr>
<td>$S_m$</td>
<td>surface of element m</td>
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<tr>
<td>$T$</td>
<td>temperature (K)</td>
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<td>$\Delta T$</td>
<td>time increment</td>
</tr>
<tr>
<td>$t$</td>
<td>time</td>
</tr>
<tr>
<td>$t_0$</td>
<td>time of decomposition</td>
</tr>
<tr>
<td>$U$</td>
<td>function satisfying Eq. (186)</td>
</tr>
<tr>
<td>$u$</td>
<td>unknown concentrations</td>
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<tr>
<td>$V$</td>
<td>Hilbert space</td>
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<tr>
<td>$V_G$</td>
<td>gas space volume</td>
</tr>
<tr>
<td>$V_W$</td>
<td>water space volume</td>
</tr>
<tr>
<td>$V_m$</td>
<td>volume of element m</td>
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<tr>
<td>$v, v_{i,j,k}$</td>
<td>approximation to mole fraction $X_A$ at the beginning of a time increment at mesh point $i, j, k$</td>
</tr>
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<td>$v^*$</td>
<td>finite difference solution for $v$ implicit in $r$ direction only</td>
</tr>
<tr>
<td>$v^{**}$</td>
<td>finite difference solution for $v$ implicit in $z$ direction only</td>
</tr>
<tr>
<td>$v^{***}$</td>
<td>finite difference solution for $v$ implicit in $\theta$ direction only</td>
</tr>
<tr>
<td>$v_A$</td>
<td>molar velocity of gas A</td>
</tr>
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</table>
Δw  change in concentration of [H⁺] ions due to ionization of water

x, y, z  coordinate axes

X  set of coordinates of a point

XA  mole fraction of gas A

X₀  mole fraction at the fill boundary during decomposition period

Xₐ  mole fraction of gas outside the soil boundary

{X}  solution vector defined in Section 1.1.2.2

{Xₖ}  k-th approximation to the solution vector {X}

ΔX  spatial increment in x direction

Δz  spatial increment in z direction

α, β  indices denoting gas components

γ  parameter used in Eq. (125)

δ  first order difference operator

δ²  second order difference operator

ε  porosity of soil, belongs to

η  ordinate in a transformed element

θ  angular coordinates of a point

Δθ  angular increment

Δθᵢ  (i - 1)Δθ

λ  parameter ΔT/(ΔX)²

λₙ  Lagrange multiplier for the terms for boundary n

ζ  abscissa in transformed element or time parameter

Σ r_{max}  summation over the pore size distribution

r = r_{min}

σ  semidiscrete approximation error
τ  tortuosity factor
τ̅  temporal discretization error
φ  null set
{φ}  set of interpolation functions
Ω  a bounded domain in n-dimensional Euclidian space \( \mathbb{R}^n \)
\( \Omega^m \)  domain of element \( m \)
\( \partial \Omega \)  boundary of region \( \Omega \)
\( \partial \Omega^m \)  boundary of region \( \Omega^m \)
\( \nabla \)  divergence or gradient operator
\( \nabla^2 \)  Laplacian operator
\( \langle \cdot, \cdot \rangle \)  inner product symbol
\( \| \cdot \| \)  norm of a function
| |  determinant
[ ]  matrix
{ }  column vector
( )  row vector
•*•  convolution product
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CHAPTER I

INTRODUCTION

The objective of this research is to study the flow of gases generated by decomposition of sanitary landfills. Equations describing the flow mechanisms have been presented for a multicomponent flow; however, analyses has been carried out for diffusion of a single component A through another component B, under uniform total pressure. Computer codes have been developed for the following cases:

a. Flow from a straight trench-type fill using a finite difference algorithm.

b. Flow from a fill approximated by a cylinder (Finite difference program).

c. Flow from an axisymmetric fill with pipe vents in the adjoining soil (Finite difference program).

d. Cases a and b using finite element formulation.

In cases a, b and d, surface convection and the chain of chemical reactions generated by a change of concentration of carbon dioxide have also been considered.

1.1 SUMMARY OF EQUATIONS DESCRIBING GAS FLOW IN POROUS MEDIA

1.1.1 Equations for Diffusional Flow in Nonreactive Media

Diffusional flow through porous media has been modelled by a number of investigators, e.g., Scott and Dullien (1962), and Rothfeld (1963). The combined bulk and Knudsen flow in the free pores leads to the following relation

\[ - \frac{P}{RT} \nabla x_a = \frac{\bar{N}_a}{D_{Ka}} + \sum_{\beta=1}^{n} \frac{x_{\beta Na} - x_{aNa}}{D_{a\beta}} \]  \( (1) \)

where

\[ P = \text{pressure (atm)} \]
\[ R = \text{gas constant (cm}^3 \text{ atm/gmole K)} \]
\[ T = \text{temperature (K)} \]
\[ X_\alpha = \frac{C_\alpha}{C} = \text{mole fraction of gas } \alpha \]
\[ N_\alpha = C_\alpha v_\alpha = \text{flux of gas } \alpha \text{ relative to a fixed point} \]
\[ D_{K\alpha} = \text{Knudsen diffusion coefficient for gas } \alpha \]
\[ D_{\alpha\beta} = \text{bulk diffusion coefficient for gas } \alpha \text{ in gas } \beta \]
\[ C_\alpha = \text{concentration of gas } \alpha \text{ (gmole} \cdot \text{cm}^{-3}) \]
\[ C = \sum C_\alpha = \text{total gas concentration (gmole} \cdot \text{cm}^{-3}) \]
\[ v_\alpha = \text{molar velocity of gas } \alpha \]

Satterfield and Cadle (1968a and 1968b) have suggested that flow under a total pressure gradient can be treated in the same manner as the flow under a partial pressure gradient; the only change being that the total pressure is a function of space. They have further pointed out that equation (1) can be applied to any single pore size. In the case of porous medium, the situation is very complex and they proposed a compromise model. The mass flux is predicted by applying the relevant equation to each pore (which is assumed to be circular and uniform along its length) and summing up the individual contributions over the whole pore size distribution. It is further assumed that on any cross section perpendicular to the direction of mass transport the concentration is uniform and independent of pore size. The deficiency between the transport mechanism and the pore structure is recognized by introducing an adjustable parameter, \( \tau \), called the tortuosity factor. The Knudsen diffusion coefficient \( D_{K\alpha} \) is expressed as the product \( K_{\alpha}r \) in order to isolate the invariant terms from pore radius. Satterfield and Cadle wrote their equation for a binary system. Moore and Alzaydi (1975), extended this concept to the multicomponent diffusion. Introducing the effect of tortuosity and pore size distribution, equation (1) may be written as

\[
- \frac{P}{RT} \sum_{r=r_{\min}}^{r_{\max}} v_{X_\alpha} = \tau \sum_{r=r_{\min}}^{r_{\max}} \sum_{\alpha} \frac{N_\alpha}{K_{\alpha}r} + \sum_{\beta=1}^{n} \frac{X_\alpha N_\beta - X_\beta N_\alpha}{D_{\alpha\beta} f_\nu(r)}
\]

where

\[ \sum_{r} = \text{a sum over the pore size distribution curve for the porous medium} \]
\[ \sum_{\beta} = \text{sum over the components of the mixture, } \beta \neq \alpha \]
\[ f_\nu(r) = \text{the volumetric fraction of the pores with radius between } r - \Delta r \text{ and } r + \Delta r \]
\( N_a \) = flux of gas \( a \) relative to a fixed point, \( \text{g mole/cm}^2 \cdot \text{s} \)
\( \tau \) = tortuosity factor
\( K_a \) = Knudsen diffusion parameter
\[ = 9.7 \times 10^{-5} \sqrt{T/M_a} \text{ cm}^2/\text{s} \cdot \text{Å} \]
\( r \) = pore radius (Å)
\( M_a \) = molecular weight of component \( a \)
\( X_a \) = mole fraction of gas \( a \)

For a mean pore radius \( r \), porosity \( \epsilon \) and uniform total pressure

Equation (2) reduces to

\[ - \frac{\epsilon}{\tau} \nabla N_a = \frac{N_a}{K_a r} + N_a \sum_{\beta} \frac{RT}{D_{a\beta}} C_{\beta} - \frac{C_a}{D_{a\beta}} \sum_{\beta} \frac{RT}{D_{a\beta}} N_{\beta} \tag{3} \]

where

\[ \overline{D_{a\beta}} = \frac{PD_{a\beta}}{r} \]

Using the continuity equation

\[ \dot{C}_a = \frac{\partial C_a}{\partial t} = -\nabla N_a \tag{4} \]

and the divergence of equation (3) gives

\[ - \frac{\epsilon}{\tau} \nabla^2 C_a = - \frac{1}{K_a r} \dot{C}_a + N_a \sum_{\beta} \frac{RT}{D_{a\beta}} \nabla C_{\beta} - \dot{C}_a \sum_{\beta} \frac{RT}{D_{a\beta}} C_{\beta} \]

\[ + C_a \sum_{\beta} \frac{RT}{D_{a\beta}} \dot{C}_{\beta} - \nabla C_a \sum_{\beta} \frac{RT}{D_{a\beta}} N_{\beta} \tag{5} \]

Equation (5) may be rewritten as

\[ K_a \epsilon \frac{1}{r} \nabla^2 C_a - \dot{C}_a = K_a \frac{RT}{P} \sum_{\beta=1}^{n} \frac{(C_{\beta} \dot{C}_a - C_a \dot{C}_{\beta} - \dot{N}_a \nabla C_{\beta} + \dot{N}_\beta \nabla C_a)}{D_{a\beta}} \tag{6} \]

Using Latin letters \( i, j, \ldots \) to denote the Cartesian axes, equation (6) may be written as

\[ E{(a)}_i C_{a,i} - G{(a)}_a \dot{C}_a + H{(a)}_a C_a - g{(a)} + h{(a)} = 0 \text{ on } V \tag{7} \]

with boundary conditions

\[ n_i E{(a)}_i C_{a,i} - Q_{a,i} n_i + n_i g{(a)} = 0 \text{ on } S \tag{8} \]
where

\[ E(a) = K_a \frac{e^{x}}{s} \]

\[ G(a) = 1 + \frac{K(a) rRT}{p} D_{\alpha\beta} c_{\beta} \]

\[ H(a) = K(a) \frac{rRT}{p} D_{\alpha\beta} c_{\beta} \]

\[ g(a) = K(a) \frac{rRT}{p} D_{\alpha\beta} c_{\beta} c(a) \]

\[ h(a) = K(a) \frac{rRT}{p} D_{\alpha\beta} c_{\beta} n(a) \]

\[ G = H = g = h = 0 \quad \text{for} \quad \alpha = \beta \]

\[ Q_{ait} = \text{rate of flux of gas} \ \alpha \ \text{in direction} \ i \ (\text{gmole/s}) \]

\[ \bar{c}_{\beta} = \text{mean concentration of component} \ \beta \]

\[ \ddot{c}_{\beta} = \text{mean rate of change of concentration of component} \ \beta \]

Defining

\[ \dot{Q}_{ait} = \int_{0}^{t} Q_{ait}(\vec{x}, \tau) d\tau , \quad (9) \]

then

\[ \dot{Q}_{ait} = Q_{ait} \]

hence, boundary conditions (8) can be written as

\[ n_{i}(E(a)c_{\alpha}, - \dot{Q}_{ait}) = 0 \quad (10) \]

Eliminating \( N_{\beta} \) from equations (3) and (5) gives

\[ N_{a} = \frac{\frac{\varepsilon}{\tau} (\nabla c_{\alpha} \cdot \nabla c_{\alpha} - c_{\alpha} \nabla c_{\alpha}) + \frac{C_{a} \dot{c}_{\alpha}}{K_{a} r} + \sum_{d} \frac{C_{a} rRT}{D_{a\beta} p} (\dot{c}_{a} c_{\beta} - c_{a} \dot{c}_{\beta})}{- \frac{1}{K_{a} r} \nabla c_{a} + \sum_{d} \frac{RT}{D_{a\beta} p} (c_{a} \nabla c_{\beta} - c_{\beta} \nabla c_{a})} \quad (11) \]

Equations (7), (10) and (11) describe the mechanism of multicomponent diffusion. This is a complicated system of equations; coupled as well as nonlinear. In the following chapters diffusion of only two
components is presented. If \( \alpha \) and \( \beta \) are the two components, equation (3) reduces to

\[
- \frac{\epsilon}{\tau} \nabla C_\alpha = \frac{N_\alpha}{K_\alpha r} + \frac{N_\alpha \chi_\beta - N_\beta \chi_\alpha}{D_{\alpha \beta}/P}
\]  

(12)

Similarly, for component \( \beta \)

\[
- \frac{\epsilon}{\tau} \nabla C_\beta = \frac{N_\beta}{K_\beta r} + \frac{N_\beta \chi_\alpha - N_\alpha \chi_\beta}{D_{\alpha \beta}/P}
\]  

(13)

Adding equations (12) and (13) gives

\[
\frac{N_\alpha}{K_\alpha} + \frac{N_\beta}{K_\beta} = 0
\]

or

\[
\frac{N_\alpha}{N_\beta} = - \frac{K_\alpha}{K_\beta} = - \sqrt{\frac{M_\beta}{M_\alpha}}
\]  

(14)

Note that \( \nabla C_\alpha = - \nabla C_\beta \) for constant total pressure.

Substituting equation (14) into equation (12) and applying the continuity equation (4) gives

\[
\dot{C}_\alpha = \nabla \left( \frac{\frac{D_{\alpha \beta}}{P}}{1 - (1 - \sqrt{\frac{M_\alpha}{M_\beta}}) \chi_\alpha + \frac{D_{\alpha \beta}}{P D_{\alpha \beta}}} \nabla C_\alpha \right)
\]  

(15)

or

\[
\dot{C}_\alpha = \nabla(D \nabla C_\alpha)
\]  

(16)

where

\[
D = \sum_{r = r_{\text{min}}}^{r_{\text{max}}} \frac{f_v(r) \frac{D_{\alpha \beta}}{P}}{1 - (1 - \sqrt{\frac{M_\alpha}{M_\beta}}) \chi_\alpha + \frac{D_{\alpha \beta}}{P D_{\alpha \beta}}}
\]  

(17)

Equation (16) is the standard nonlinear diffusion equation wherein the diffusion coefficient \( D \) is a function of the mole fraction \( \chi_\alpha \) of component \( \alpha \), the pore size distribution, the bulk diffusion coefficient, the Knudsen diffusion coefficient, the total pressure \( P \) and the molecular weights of components as given by equation (17). The maximum variation in \( D \) over the whole range of possible \( \chi_\alpha \) is approximately 10%. Thus, within a time increment \( \Delta t \), this variation may be even less than 0.01%. The problem is thus only mildly nonlinear and has been solved by using the diffusion coefficient based on the concentration at a mesh point in
the beginning of a time increment and treating it constant over the interval.

1.1.2 Equations for Chemical Reactions Which Occur Between the Gas and Other Phases of the System

Carbon dioxide reacts with water to form $H_2CO_3$, which subsequently reacts with Ca and changes the alkalinity, pH value and hardness of soil water. The effect of the changed concentration at the end of a time increment perturbs the chemical equilibrium of the system. The reactions involved occur quickly, taking only a few seconds to attain the new equilibrium state. Thus, there is an immediate reduction in the mole fraction of $CO_2$. To quantify the influence of such reactions on the flow rates of the gas and the changes in the ground water quality, the chemical reactions and the corresponding equilibrium constants must be known.

1.1.2.1 Equilibrium Species and Constants for Carbon Dioxide in Water—

The reaction sequence involves carbon dioxide gas dissolving in water, subsequent reaction with water to form carbonic acid, release of hydrogen to form bicarbonate, and further release of hydrogen to form carbonate which combines with Ca$^{++}$ to give Ca$CO_3$:

$$
CO_2(g) \rightarrow CO_2(aq) \rightarrow H_2CO_3 \rightarrow HCO_3^- \rightarrow CO_3^{2-} \rightarrow CaCO_3
$$

At the same time hydrolysis of water gives $H_2O \rightarrow H^+ + OH^-$. The equilibrium constants are

$$K_H = \frac{[CO_2(aq)]}{[CO_2(g)]}$$  \hspace{1cm} (18a)

$$K = \frac{[H_2CO_3]}{[CO_2(aq)]}$$  \hspace{1cm} (18b)

$$K_1 = \frac{[H^+][HCO_3^-]}{[H_2CO_3]}$$  \hspace{1cm} (18c)

$$K_2 = \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]}$$  \hspace{1cm} (18d)

$$K_s = [Ca^{++}][CO_3^{2-}]$$  \hspace{1cm} (18e)

and

$$K_w = [H^+][OH^-]$$  \hspace{1cm} (18f)
Normally, however, only the overall equilibrium for \( \text{CO}_2(\text{g}) \rightarrow \text{H}_2\text{CO}_3 \) is reported since \( \text{CO}_2(\text{aq}) \) cannot be measured separately from \( \text{H}_2\text{CO}_3 \).

Therefore, five equilibria are considered:

\[
K_H = K_{\text{H}+}\text{K} = \frac{[\text{H}_2\text{CO}_3]}{\text{CO}_2(\text{g})} = \frac{A}{P} \tag{19a}
\]

\[
K_1 = \frac{[\text{H}^+][\text{HCO}_3^{-}]}{[\text{H}_2\text{CO}_3]} = \frac{\text{H}B}{\text{A}} \tag{19b}
\]

\[
K_2 = \frac{[\text{H}^+][\text{CO}_3^{2-}]}{[\text{HCO}_3^{-}]} = \frac{\text{HC}}{\text{B}} \tag{19c}
\]

\[
K_s = [\text{Ca}^{+2}][\text{CO}_3^{2-}] = D.C \tag{19d}
\]

\[
K_w = [\text{H}^+][\text{OH}^-] = \text{H.OH} \tag{19e}
\]

where

\[
A = \text{concentration of } \text{H}_2\text{CO}_3 \text{ (mole/\ell)}
\]

\[
B = \text{concentration of } \text{HCO}_3^{-} \text{ (mole/\ell)}
\]

\[
C = \text{concentration of } \text{CO}_3^{2-} \text{ (mole/\ell)}
\]

\[
H = \text{concentration of } \text{H}^+ \text{ (mole/\ell)}
\]

\[
\text{OH} = \text{concentration of } \text{OH}^- \text{ (mole/\ell)}
\]

\[
D = \text{concentration of } \text{Ca}^{+2} \text{ (mole/\ell)}
\]

\[
P = \text{concentration of } \text{CO}_2(\text{g}) \text{ partial pressure (atm)}
\]

Typical equilibrium constants are given below.

| Table 1. Equilibrium constants for chemical reactions |
|------------------------------------------|--------|--------|--------|--------|--------|
| Temperature (°C)                       | 5      | 10     | 15     | 20     | 25     |
| \( K_H \times 10^2 \)                  | 6.456  | 5.370  | 4.786  | 3.890  | 3.388  |
| \( K_1 \times 10^7 \)                  | 3.041  | 3.436  | 3.811  | 4.159  | 4.446  |
| \( K_2 \times 10^{11} \)               | 2.649  | 3.236  | 3.715  | 4.198  | 4.688  |
| \( K_s \times 10^3 \)                  | 8.128  | 7.079  | 6.026  | 5.248  | 4.571  |
| \( K_w \times 10^{14} \)               | 0.1846 | 0.2920 | 0.4505 | 0.6809 | 1.008  |

(after Stumm and Morgan, 1970)

When treating soil water, the chemical species are determined as:

\[ H = 10^{-\text{pH}} \text{ (mole/\ell)} \]
Thus, the total hardness and pH values of the soil water give D and H.

By using the equilibrium constants, C, B, OH, A and P are obtained in succession. Thus, the initial concentrations in the soil water are completely determined.

To treat displacement of initial equilibrium, consider a right-cylindrical pore with an annular water film.

Let

\[ V_G = \text{gas space volume (l)} \]
\[ V_W = \text{water space volume (l)} \]

The ideal gas law gives

\[ n = \frac{PV_G}{RT} \] (20)

where

\[ n = \text{number of gas moles} \]
\[ P = \text{partial pressure of gas (atm)} \]
\[ R = 0.08205 \ (\ell \ \text{atm/\text{K mole}}) \]
\[ T = \text{temperature (K)} \]

If \( \Delta n \) moles of gas dissolve, the partial pressure drops through \( \Delta P \) such that

\[ 
\Delta n = \frac{\Delta P}{RT} V_G
\] (21)

The dissolving of \( \text{CO}_2 \) in water increases the concentration of \( \text{H}_2\text{CO}_3 \) by

\[ 
\Delta A = \frac{\Delta n}{V_L} = \frac{\Delta P}{RTV_W} V_G \ (\text{mole/\ell})
\] (22)

The partial pressure drop of \( \text{CO}_2(g) \) and increase in concentration of \( \text{H}_2\text{CO}_3 \) may be written as

\[
\text{CO}_2(g) \quad \overset{-\Delta P}{\longrightarrow} \quad \text{H}_2\text{CO}_3 \quad +\Delta A
\]
Other reactions are:

1) ionization of H$_2$CO$_3$:

\[
\text{H}_2\text{CO}_3 \rightarrow \text{H}^+ + \text{HCO}_3^- \\
-\Delta B + \Delta B + \Delta B
\]

2) ionization of HCO$_3$:

\[
\text{HCO}_3^- \rightarrow \text{H}^+ + \text{CO}_3^2- \\
-\Delta C + \Delta C + \Delta C
\]

3) ionization of H$_2$O:

\[
\text{H}_2\text{O} \rightarrow \text{H}^+ + \text{OH}^- \\
-\Delta \omega + \Delta \omega + \Delta \omega
\]

4) ionization of CaCO$_3$(S):

\[
\text{CaCO}_3(\text{S}) \rightarrow \text{Ca}^{++} + \text{CO}_3^2- \\
-\Delta D + \Delta D + \Delta D
\]

1.1.2.2 Equations Describing Equilibrium Processes for Carbon Dioxide in Water—

Let $P_1$ be the initial equilibrium partial pressure of CO$_2$(g)

$A_1$ be the initial equilibrium concentration of [H$_2$CO$_3$]

$B_1$ be the initial equilibrium concentration of [HCO$_3$]

$C_1$ be the initial equilibrium concentration of [CO$_3$]

$D_1$ be the initial equilibrium concentration of [Ca$^{++}$]

$H_1$ be the initial equilibrium concentration of [H$^+$]

OH$^-_1$ be the initial equilibrium concentration of [OH$^-$]

The introduction of additional CO$_2$(g) increases the partial pressure of CO$_2$ to $P'$. This forces the system to re-equilibrate with the pore water to yield a new set of equilibrium concentrations as follows:

<table>
<thead>
<tr>
<th>Component</th>
<th>New Equilibrium Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2$(g)</td>
<td>$P_2 = P' - \Delta P$</td>
</tr>
<tr>
<td>H$_2$CO$_3$</td>
<td>$A_2 = A_1 + \Delta A - \Delta B$</td>
</tr>
<tr>
<td>HCO$_3$</td>
<td>$B_2 = B_1 + \Delta B - \Delta C$</td>
</tr>
<tr>
<td>CO$_3$</td>
<td>$C_2 = C_1 + \Delta C + \Delta D$</td>
</tr>
<tr>
<td>OH$^-$</td>
<td>$\text{OH}_2 = \text{OH}_1 + \Delta \omega$</td>
</tr>
<tr>
<td>H$^+$</td>
<td>$H_2 = H_1 + \Delta B + \Delta C + \Delta \omega$</td>
</tr>
<tr>
<td>Ca$^{++}$</td>
<td>$D_2 = D_1 + \Delta D$</td>
</tr>
</tbody>
</table>

Let $S$ be the degree of saturation, then $\frac{V_G}{V_W} = \frac{100 - S}{S}$ and the equilibrium displacement equations can be written as
The set of simultaneous equations (23a) through (23f) on simplification gives

\[ \Delta P = \frac{\text{RTS}}{100 - S} \Delta A \]  

(24a)

\[ \Delta A = \frac{K^{'P'} - B_1 H_1}{K^{'T} \frac{\text{RTS}}{100 - S} + 1} + \frac{K_1 K^{'} P' - B_1 H_1}{K^{'T} \frac{\text{RTS}}{100 - S} + 1} - \Delta B^2 - \Delta C^2 - \Delta B C - \Delta C = 0 \]  

(24c)

\[ (K_2 - C_1)\Delta B - (K_2 + H_1 + C_1)\Delta C - H_1 \Delta D - C_1 \Delta \omega \]  

\[ - \Delta C \Delta B - \Delta C^2 - \Delta C = - \Delta B \Delta D - \Delta C \Delta D - \Delta D \Delta \omega = 0 \]  

(24d)

\[ D_1 \Delta C + \Delta D(C_1 + D_1) + \Delta C \Delta D + \Delta D^2 = 0 \]  

(24e)

\[ \Delta B \Delta H_1 + \Delta C \Delta H_1 + \Delta \omega (H_1 + \Delta H_1) + \Delta \omega \Delta B + \Delta \omega \Delta C + \Delta \omega^2 = 0 \]  

(24f)

The set of equations (24a) through (24f) consists of six simultaneous equations in terms of concentration changes of various components of the system. The first two of these simultaneous equations are linear;
whereas the last four are nonlinear. A Newton-Raphson method may be used to solve these four nonlinear equations, (Henrici, 1964):

Let \( \{X\} = \begin{bmatrix} \Delta B \\ \Delta C \\ \Delta D \\ \Delta \omega \end{bmatrix} \) be the solution to equations (24c) through (24f) and \( \{X_k\} \) be a good approximation to \( X \). For each function, \( f_i \), Taylor's theorem for \( n \) variables gives,

\[
0 = f_i(X) = f_i(X_k) + \sum_{j=1}^{n} (X_j - X_{jk}) \left( \frac{\partial f_i}{\partial x_j} \right)_{x=x_k} + O \left[ \sum_{j=1}^{n} (X_j - X_{jk})^2 \right] \tag{25}
\]

Hence, if second order terms are neglected, \( X_{k+1} \) will be a better approximation than \( X_k \); where \( X_{k+1} \) is given by

\[
\sum_{j=1}^{n} (x_{j,k+1} - x_{jk}) \left( \frac{\partial f_i}{\partial x_j} \right)_{x=x_k} = -f_i(x_k) \quad x = 1, \ldots, n \tag{26}
\]

Let

\[
\frac{K_1}{RTS} - \frac{K_1 - H_1 - B_1 - C_2}{100 - S + 1} = C_3
\]

\[
H_1 - B_1 = C_3
\]

\[
\frac{K_1K_H'P' - B_1H_1}{K_H'RTS + 1} = C_4
\]

\[
K_2 - C_1 = C_5
\]

\[
K_2 + H_1 + C_1 = C_6
\]

\[
C_1 + D_1 = C_7
\]

\[
H_1 + OH_1 = C_8
\]

Then equations (24c) through (24f) can be written as:

\[
0 = f_1 = C_2\Delta B - C_3\Delta C - B_1\Delta \omega + C_4 - \Delta B^2 + \Delta C^2 - \Delta B\omega + \Delta C\omega \tag{27a}
\]

\[
0 = f_2 = C_5\Delta B - C_6\Delta C - H_1\Delta D - C_1\Delta \omega - \Delta C\Delta B - \Delta C^2 - \Delta C\omega
- \Delta B\Delta D - \Delta C\Delta D - \Delta D\Delta \omega \tag{27b}
\]
\[ 0 = f_3 = D_2 \Delta C + C_7 \Delta D + \Delta C \Delta D + \Delta D^2 \]  
\[ (27c) \]
\[ 0 = f_4 = O_2 B \Delta B + O_1 A C + C_8 \Delta \omega + \Delta \omega \Delta B + \Delta \omega \Delta C + \Delta \omega^2 \]  
\[ (27d) \]

Let

\[
A = \begin{bmatrix}
\frac{\partial f_1}{\partial \Delta B} & \frac{\partial f_1}{\partial \Delta C} & \frac{\partial f_1}{\partial \Delta D} & \frac{\partial f_1}{\partial \Delta \omega} \\
\frac{\partial f_2}{\partial \Delta B} & \frac{\partial f_2}{\partial \Delta C} & \frac{\partial f_2}{\partial \Delta D} & \frac{\partial f_2}{\partial \Delta \omega} \\
\frac{\partial f_3}{\partial \Delta B} & \frac{\partial f_3}{\partial \Delta C} & \frac{\partial f_3}{\partial \Delta D} & \frac{\partial f_3}{\partial \Delta \omega} \\
\frac{\partial f_4}{\partial \Delta B} & \frac{\partial f_4}{\partial \Delta C} & \frac{\partial f_4}{\partial \Delta D} & \frac{\partial f_4}{\partial \Delta \omega}
\end{bmatrix}
\]

\[ (28) \]

or

\[
A = \begin{bmatrix}
C_2 - 2 \Delta B - \Delta \omega & -C_3 + 2 \Delta C + \Delta \omega & 0 & -B_1 - \Delta \omega + \Delta C \\
C_5 - \Delta C - \Delta D & -C_6 - \Delta B - 2 \Delta C - \Delta \omega - \Delta D & -H_1 - \Delta B - \Delta C - \Delta \omega & -C_1 - \Delta C - \Delta D \\
0 & D_1 + \Delta D & C_7 + \Delta C + 2 \Delta D & 0 \\
O_1 + \Delta \omega & O_1 + \Delta \omega & 0 & C_8 + \Delta B + \Delta C + 2 \Delta \omega
\end{bmatrix}
\]

\[ (29) \]

Let the first estimate be \( \{x_0\} = \begin{bmatrix} \Delta B \\ \Delta C \\ \Delta D \\ \Delta \omega \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \)
then

\[
-[f(x_0)] = -\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} = \begin{bmatrix} -C_4 \\ 0 \\ 0 \\ 0 \end{bmatrix}
\]

\[ (30) \]

and

\[
[A](\delta x_0) = -[f(x_0)]
\]

\[ (31) \]

Solve for \( \delta x_0 \), and then the better approximation \( x_1 = x_0 + \delta x_0 \)

Similarly

\[
[A](\delta x_1) = -[f(x_1)]
\]

gives

\[ x_2 = x_1 + \delta x_1 \]
The sequence \((X_0, X_1, X_2, \cdots)\) converges to the correct solution and within two or three iterations a reasonably accurate result is obtained. The equations (24a) and (24b) are now solved by direct substitution. Thus, the equilibrium concentrations at a mesh point are updated. This procedure is adopted for each of the mesh points at the end of each time increment.

1.2 GEOMETRIC CONDITIONS FOR SIMULATING SANITARY LANDFILLS

For this solution the geometry of the landfill is approximated by a cylindrical volume which is circular in plan and of radius \(r_f\), and which is of depth, \(d_f\), as shown in Figure 1. The soil surrounding the landfill extends radially to a distance \(r_s\), at which point a boundary which may be specified as having either a prescribed gas concentration or a prescribed convection rate is encountered. The soil extends to a depth \(d_s\), at which an impervious boundary is encountered. The ground surface may have either a prescribed gas concentration or a prescribed convection. In addition, vents penetrating to a depth \(d_v\) may be placed at a radial distance \(r_v\). These vents must be equally spaced around a circle at radius \(r_v\); however, the frequency of spacing may attain any value. Continuous spacing allows approximating a partially penetrating ditch. In the finite element code (Section 5) it is possible to specify the concentration, or convection at any arbitrary point or at any arbitrary surface, respectively. The convection is generated by the effect of wind as described in Section 1.3.2.

The gas concentration is specified at the landfill-soil boundary for a period designated as \(t_0\), during which decomposition occurs. After this time the landfill-soil interface is assumed impervious.

1.3 EQUATIONS DESCRIBING BOUNDARY CONDITIONS

As discussed in Section 1.2, several physical conditions may exist at the boundary. These conditions can be classified into two categories, viz., prescribed concentrations and prescribed convections.

1.3.1 Prescribed Concentrations

Prescribed concentration means that the mole fraction of the gas component under consideration at a given time and coordinate is known (e.g., the concentration on the soil-landfill boundary should be prescribed during the period of decomposition, or in case of a radial boundary far away from the fill, the concentration of methane may be assumed to be zero) whereas the concentration of \(\text{CO}_2\) depends on pH value and hardness of the subsoil water.
Fig. 1 - Delineation of solution geometry and boundary condition types.

Note: Numbers refer to boundary condition types in section (1.3.3)
1.3.2 Boundary with Prescribed Convective Flow

A boundary along which the mass flow is prescribed will be defined as a prescribed convective flow boundary. If the flow across this boundary is zero it is called an impervious boundary (e.g., interface between subsoil water and the soil, axis of the axisymmetrical case, a plane passing through the trench of a trench-type fill). In general, a surface may neither be completely impervious nor may it be possible to prescribe the concentration at the surface arbitrarily. The mass transfer on such a surface is related to the difference in gas concentrations at the surface and in the outside atmosphere and the surface transfer coefficient. No work seems to have been done in evaluating the transfer coefficient from the surface. The transfer phenomenon is analogous to surface evaporation. The transfer coefficient for surface convection may be taken as a fraction of mass transfer coefficients for evaporation. These vary with wind velocity as follows (Brutsaert and Yu, 1967):

<table>
<thead>
<tr>
<th>Average Wind Velocity 3m Above Ground Surface (mph)</th>
<th>Mass Transfer Coefficient x 10^5 (gmole/cm^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.5950</td>
</tr>
<tr>
<td>1</td>
<td>2.0721</td>
</tr>
<tr>
<td>2</td>
<td>2.5492</td>
</tr>
<tr>
<td>3</td>
<td>3.0263</td>
</tr>
<tr>
<td>4</td>
<td>3.5034</td>
</tr>
<tr>
<td>5</td>
<td>3.9805</td>
</tr>
<tr>
<td>6</td>
<td>4.4576</td>
</tr>
<tr>
<td>7</td>
<td>4.9347</td>
</tr>
<tr>
<td>8</td>
<td>5.4118</td>
</tr>
<tr>
<td>9</td>
<td>5.8889</td>
</tr>
<tr>
<td>10</td>
<td>6.3660</td>
</tr>
<tr>
<td>15</td>
<td>8.7515</td>
</tr>
<tr>
<td>20</td>
<td>11.1370</td>
</tr>
<tr>
<td>25</td>
<td>13.5225</td>
</tr>
<tr>
<td>30</td>
<td>15.9080</td>
</tr>
</tbody>
</table>

The mass entering the surface through an area A is given by

\[ S_A = C_K A (X_a - X_o) \]  \hspace{1cm} (32)

where

- \( S_A \) = mass entering the surface
- \( X_a \) = mole fraction of gas outside the soil boundary
- \( X_o \) = mole fraction of gas on the soil boundary

and

\( C_K \) = mass transfer coefficient
A mass balance in the outside half-element gives

\[
C_K A(x_a - x_o) - D_{AB} \frac{A(x_o - x_1)}{\Delta x} = \frac{A}{2} \frac{\Delta x}{\Delta t} (x_{1/4, n+1} - x_{1/4, n-1})
\]  

(33)

Assuming \(x_{1/4} = x_o\) (Geankoplis, 1972), equation (33) reduces to

\[
2CK \frac{(x_{g, n+1} - x_{o, n+1})}{\Delta x} - \frac{2D_{AB}(x_{o, n+1} - x_{1, n+1})}{\Delta x^2} = \frac{x_{o, n+1} - x_0}{\Delta T}
\]  

(34)

For a three-dimensional case, equation (34) reduces to

\[
\frac{\partial x_A}{\partial t} = \nabla \cdot (D\nabla x_A) + S_A
\]

where

\[
S_A = \sum_i 2C_{Ki}(x_{ai} - x_{oi})
\]  

(35)

\(x_{ai}\) = mole fraction outside the boundary \(i\)
\(x_{oi}\) = mole fraction on the boundary \(i\)

and

\(C_{Ki}\) = surface transfer coefficient for the boundary \(i\)

In the axisymmetric case we have to consider the increasing surface area on the boundary \(r = r_s\) due to an increase in radial distance.

Surface area of an element at \(r_s = (i - 1)\Delta r\Delta z\)

Volume of the element before this surface = \((2i - 3) \frac{\Delta r^2 \Delta x}{2}\)

This changes the convective term corresponding to the boundary \(r = r_s\) and the corresponding equation then becomes

\[
\frac{\partial c}{\partial t} = \nabla \cdot (D\nabla c) + 2CK_1 \left( \frac{C_{a1} - C_{o1}}{\Delta z} \right) + 2CK_2 \left( \frac{C_{a2} - C_{o2}}{\Delta r} \right) \frac{2i - 2}{2i - 3}
\]  

(36)

The convective term \(2CK_1 \frac{C_{a1} - C_{o1}}{\Delta z}\) applies to all points on the surface and the term \(2CK_2 \left( \frac{C_{a2} - C_{o2}}{\Delta r} \right) \frac{2i - 2}{2i - 3}\) applies to points on the boundary \(r = r_s\). Both terms together apply only to the edge \(z = 0, r = r_s\).
1.3.3 Mathematical Representation

In this section the boundary conditions described above have been represented mathematically. The condition numbers refer to the boundaries shown in Figure 1.

Condition of Axisymmetry (Condition #1)

\[
\frac{\partial x_A}{\partial r} = 0 \quad \text{for} \quad r = 0 , \quad d_f < z \leq d_s
\]  

(37)

In this case the Laplacian operator with respect to \( r \) becomes

\[
\nabla^2 = 2 \frac{\partial^2}{\partial r^2}
\]  

(38)

Condition of Impervious Base of Soil (Condition #2)

\[
\frac{\partial x_A}{\partial z} = 0 \quad \text{for} \quad z = d_s
\]  

(39)

Condition of Constant Gas Concentration Along Base of Landfill for Times During Decomposition (Condition #3)

\[
x_A = x_0 \quad \text{for} \quad z = d_f , \quad r \leq r_f , \quad t \leq t_0 .
\]  

(40)

Condition of Imperviousness Along Base of Landfill for Times After Decomposition (Condition #4)

\[
\frac{\partial x_A}{\partial z} = 0 \quad \text{for} \quad z = d_f , \quad r \leq r_f , \quad t > t_0 .
\]  

(41)

Condition of Constant Gas Concentration Along Radial Boundary of Landfill for Times During Decomposition (Condition #5)

\[
x_A = x_0 \quad \text{for} \quad r = r_f , \quad z \leq d_f , \quad t \leq t_0 .
\]  

(42)

Condition of Imperviousness Along Radial Boundary of Landfill for Times After Decomposition (Condition #6)

\[
\frac{\partial x_A}{\partial r} = 0 \quad \text{for} \quad r = r_f , \quad z \leq d_f , \quad t > t_0 .
\]  

(43)

Condition of Prescribed Concentration at Radial Soil Boundary (Condition #7)

\[
x_A = \text{const.} \quad \text{for} \quad r = r_s , \quad z \leq d_s .
\]  

(44)
Convective Flow at Radial Soil Boundary (Condition #8)

\[ 2CK_2 \frac{\partial x_A}{\partial r} = S_A \text{ for } r = r_s , \ z \leq d_s . \]  

(45)

Condition of Prescribed Concentration at Ground Surface (Condition #9)

\[ x_A = \text{const. for } r > r_f , \ z = 0 . \]  

(46)

Convective Flow at Ground Surface (Condition #10)

\[ 2CK_1 \frac{\partial x_A}{\partial z} = S_A \text{ for } r > r_f , \ z = 0 . \]  

(47)

Condition of No Circumferential Flow at Radial Line Through Vent (Condition #11)

\[ \frac{\partial x_A}{\partial \theta} = 0 \text{ for } \theta = 0 , \ r_f < r \leq r_s . \]  

(48)

Condition of No Circumferential Flow at Radial Line at Mid-point Between Vent Pairs (Condition #12)

\[ \frac{\partial x_A}{\partial \theta} = 0 \text{ for } \theta = \Delta \theta_v/2 . \]  

(49)

Condition of Perviousness at Vents (Condition #13)

\[ x_A = 0 \text{ for } r = r_v , \ z \leq d_v . \]  

(50)
CHAPTER II

FINITE DIFFERENCE FORMULATION

The partial differential equation (16) can be solved analytically if the diffusion coefficient is constant and the boundary conditions are constant with time. However, when the effective diffusion coefficient is a function of concentration itself or the boundary conditions are not constant with time and/or the initial conditions are not constant with position, analytical solutions are virtually impossible. In such cases we have to resort to numerical methods. The finite difference method has been successfully used for the solution of heat conduction and molecular mass transport equations, which are often called parabolic partial differential equations.

Finite difference methods have been used extensively for the solution of initial-value and boundary value problems. They have been classified into explicit and implicit techniques. Explicit methods put a restriction on the time increment for reasons of stability of the solution. Also they make use of forward differences in the time domain and central differences in space. Thus the discretization errors are of the order of $O(\Delta t)$ and $O(\Delta x)^2$.

These objections are avoided in the implicit methods (Crank-Nicolson, 1947). These methods are unconditionally stable; however, their use requires the solution of a large number of simultaneous linear algebraic equations at each step. These equations, obtained by finite difference approximation, have a banded structure and may be solved by Gaussian elimination, but this process is time consuming. Iterative methods are somewhat better, but with a large system of equations their convergence becomes slow and the saving in computer time is doubtful.

The alternating direction implicit method (ADI method) suggested by Peaceman and Rachford (1955) and further developed by Brian (1961), Douglas and Gunn (1964) and Brakat and Clark (1966) among others, overcomes both of the above disadvantages. It is unconditionally stable and requires less computational time. Therefore, the ADI method has been used for the solution of the problem using finite difference procedures. This solution procedure uses a system of equations with tridiagonal coefficient matrix. Essentially, the principle is to employ three difference equations which are used in turn over successive time-steps, each of duration $\Delta t/2$. The first equation is implicit only in the $r$-direction, the second is implicit only in the $z$-direction and the third is implicit in the $\theta$-direction.
2.1 FINITE DIFFERENCE ALGORITHMS
FOR INTERIOR POINTS

Following the method developed by Brian (1961) the finite difference analog for an alternating direction implicit solution to a multidimensional axisymmetric problem involving equations of the type of equation (16) is given by

\[
\frac{v^*-v}{\Delta t/2} = D\frac{\delta_r^2 v^*}{r} + \frac{D}{r} \delta_r v^* + \frac{D}{r^2} \delta_\theta^2 v + D\delta_z^2 v + \delta_r D \cdot \delta_r v^* + \frac{1}{r^2} \delta_\theta D \cdot \delta_\theta v \\
+ \delta_z D \cdot \delta_z v - R_A + S_A
\]

where

\[
v = v_{i,j,k} = \text{approximation to } x_A \text{ at the present at point } i, j, k
\]
\[v^* = v^*_{i,j,k} = \text{approximation to } x_A \text{ at intermediate time } \Delta t/2 \text{ at point } i, j, k
\]
\[D = \text{diffusion coefficient given by equation (17)}
\]
\[\Delta t = \text{time increment}
\]
\[r = \text{radial distance from symmetry axis}
\]
\[\theta = \text{angle to radial line delineating symmetrical wedge}
\]
\[z = \text{depth from ground surface}
\]
\[R_A = \text{mole fraction lost in chemical reaction}
\]
\[S_A = \text{mole fraction lost due to convection at boundaries } r = r_s \text{ and/or } z = 0
\]

with differential operators, \( \delta \), given by

\[
\delta_{x^f_l} = \frac{f_{l+1} - f_{l-1}}{2\Delta x}
\]
\[
\delta_{x^2f_l} = \frac{f_{l-1} - 2f_l + f_{l+1}}{(2\Delta x)^2}
\]

where

\[f = v, v^*, \text{ or } D
\]
\[l = i, j, \text{ or } k
\]
\[x = r, \theta, \text{ or } z
\]
\[\Delta x = \Delta r, x\Delta \theta, \text{ or } \Delta z
\]
Equations similar to equation (51) may be written for intermediate times while stepping in each coordinate direction individually and assuming constancy in the other coordinate directions:

\[ v^* \] implies solution incrementing in \( v \) direction
\[ v^{**} \] implies solution incrementing in \( z \) direction
\[ v^{***} \] implies solution incrementing in \( \theta \) direction

In the case of a trench-type fill, equation (51) changes to

\[
\frac{v^* - v}{\Delta t/2} = D_s x v^* + D_s z v^* + \delta x D_s x v^* + \delta z D_s z v^* - R_A + S_A
\]  

This requires only a small change in the algorithm, i.e., all terms containing \( r \) in the denominator have to be dropped.

2.1.1 Discretization of Algorithms for Interior Points

Evaluating the differentials in terms of the values of the functions at adjoining grid points by central differences and substituting into equation (51) with rearrangement gives

\[
\left( \frac{D_i}{4} - \frac{2i-3}{2i-2} D_i, j, k \right) v^*_{i-1,j,k} + \left( \frac{2}{\lambda} + 2D_i, j, k \right) v^*_{i,j,k} \\
- \left( \frac{Di'}{4} + \frac{2i-1}{2i-2} D_i, j, k \right) v^*_{i+1,j,k} = \left( D_i, j, k - \frac{D_i}{4} \right) v_{i,j,k-1} \\
+ \left( \frac{2}{\lambda} - 2D_i, j, k \right) v_{i,j,k} + \left( \frac{Di'}{4} + D_i, j, k \right) v_{i,j,k+1} - 2D_i, j, k \frac{v_{i,j,k}}{\Delta \theta_i^2}
\]  

\[
\left( \frac{D_i'}{4} - D_i, j, k \right) v^{**}_{i,j-1,k} + \left( \frac{2}{\lambda} + 2D_i, j, k \right) v^{**}_{i,j,k} \\
- \left( \frac{D_i'}{4} + D_i, j, k \right) v^{**}_{i,j+1,k} = \left( \frac{D_i'}{4} + \frac{2i-1}{2i-2} D_i, j, k \right) v^{**}_{i,j,k+1} \\
+ \left( \frac{2}{\lambda} - 2D_i, j, k \right) v^{**}_{i,j,k} + \left( \frac{D_i'}{4} + D_i, j, k \right) v^{**}_{i,j,k-1} - 2D_i, j, k \frac{v^{**}_{i,j,k}}{\Delta \theta_i^2}
\]  

\[
\left( \frac{D_i'}{4} - \frac{2i-3}{2i-2} D_i, j, k \right) v^{***}_{i-1,j,k} + \left( \frac{2}{\lambda} + 2D_i, j, k \right) v^{***}_{i,j,k} \\
- \left( \frac{D_i'}{4} + \frac{2i-1}{2i-2} D_i, j, k \right) v^{***}_{i+1,j,k} = \left( D_i, j, k - \frac{D_i}{4} \right) v^{***}_{i,j,k+1} \\
+ \left( \frac{2}{\lambda} - 2D_i, j, k \right) v^{***}_{i,j,k} + \left( \frac{D_i'}{4} + D_i, j, k \right) v^{***}_{i,j,k-1} - 2D_i, j, k \frac{v^{***}_{i,j,k}}{\Delta \theta_i^2}
\]  

(55)
and

\[
\left( \frac{D_i^k}{4} - D_{i,j,k} \right) \frac{v_{i,j,k}^{**}}{\Delta \theta_i^2} + \left( \frac{2}{\lambda} + \frac{D_{i,j,k}}{2} \right) v_{i,j,k}^{**} - \left( \frac{D_i^k}{4} + D_{i,j,k} \right) v_{i,j,k+1}^{**} = \left( 2i - \frac{3}{2} D_{i,j,k} - \frac{D_i^k}{4} \right) v_{i-1,j,k}^{**} - 2D_{i,j,k} v_{i,j,k}^{**} + \\
+ \left( \frac{2i - 1}{2i - 2} D_{i,j,k} + \frac{D_i^k}{4} \right) v_{i+1,j,k}^{**} + \left( D_{i,j,k} - \frac{D_j^k}{4} \right) v_{i,j-1,k}^{**} + \\
+ \left( \frac{2}{\lambda} - 2D_{i,j,k} \right) v_{i,j,k}^{**} + \left( D_{i,j,k} + \frac{D_j^k}{4} \right) v_{i,j+1,k}^{**}
\]

(57)

where

\[
\Delta \theta_i = (i - 1) \Delta \theta
\]

(58)

\[
D_i^k = D_{i+1,j,k} - D_{i-1,j,k}
\]

(59)

\[
D_j^k = D_{i,j+1,k} - D_{i,j-1,k}
\]

(60)

\[
D_k = D_{i,j,k+1} - D_{i,j,k-1}
\]

(61)

\[
\lambda = \frac{\Delta t}{(\Delta x)^2} = \frac{\Delta t}{(\Delta \theta)^2}
\]

(62)

**NOTE:** In the development of these equations the reaction term, \( R_A \), need not be included. For the axisymmetric code simply omit the \( k \) subscript, the derivatives with respect to \( \theta \), and equation (57).

### 2.2 FINITE DIFFERENCE ALGORITHMS FOR BOUNDARIES

The finite difference algorithms for the boundary conditions described in Section 1.3.3 are:

**Condition #1**

To avoid singularity, the boundary must be artificially placed one grid point beyond \( r = 0 \) and the boundary \( r = \Delta r \) treated as impervious boundary. Therefore equation (51) becomes

\[
\frac{v_{i,j,k}^* - v}{\Delta t/2} = D_{i,j,k} v_{i,j,k}^* + \frac{D}{\Delta x} \frac{\partial v}{\partial x} + D_{i,j,k} \frac{\partial^2 v}{\partial \theta^2} + \frac{1}{\Delta x^2} \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial \theta^2} + \frac{\partial^2 v}{\partial x^2} \frac{\partial v}{\partial x} + \frac{1}{\Delta x^2} \frac{\partial^2 v}{\partial x^2} \frac{\partial v}{\partial x} \]

(63)

**Condition #2**

In equation (51)

\[
\frac{\partial v}{\partial \theta} = 0
\]

(64)
Condition #3

\[ \nu = \nu_0 \quad (65) \]

Condition #4

In equation (51)

\[ \delta_z \nu = 0 \quad (66) \]

Condition #5

\[ \nu = \nu_0 \quad (67) \]

Condition #6

In equation (51)

\[ \delta_r \nu = 0 \quad (68) \]

Condition #7

\[ \nu = \text{const.} \quad (69) \]

Condition #8

In equation (51)

\[ S_A = 2CK_2(v_{a2} - v_0)/\Delta r \]

where \( v_{a2} \) = mole fraction of gas in the soil beyond the radial boundary.

Condition #9

\[ \nu = \text{const.} \quad (70) \]

Condition #10

In equation (51)

\[ S_A = 2CK_1(v_{a1} - v_0)/\Delta z \]

where \( v_{a1} \) = mole fraction of gas outside the fill above the ground surface.

Condition #11

In equation (51)

\[ \delta_\theta \nu = 0 \quad (71) \]
Condition #12

In equation (51)

$$\delta_g v = 0.$$  \hfill (72)

Condition #13

$$v = 0.$$  \hfill (73)

2.2.1 Discretization of Algorithms for Boundaries

Along boundaries and at intersections of boundaries, equations (55) through (57) must be altered. For economy, two computer codes were prepared. In Code I, vents were not allowed so that the problem degenerates to two spatial dimensions, r and z. In Code II, vents were included and the solution involves all three spatial coordinates, r, z and $\theta$.

2.2.1.1 Discretization for Code I--

The following equations hold for the boundaries delineated in Figure 2. The numbers shown in Figure 2 correspond to equation numbers given below. Note that at the intersection of two or more boundaries, the equation holds only at a single point. Subscripts are omitted on $D$ and $v$ unless different from i and/or j.

Condition #1 along $d_f < z < d_s$, $r = 0$

$$\left(\frac{2}{\lambda} + 4D\right) v^* - 4Dv^*_{i+1} = \left( D - \frac{D^i}{4} \right) v_{j-1} + \left( \frac{2}{\lambda} - 2D \right) v + \left( D + \frac{D^i}{4} \right) v_{j+1}$$  \hfill (74a)

and

$$\left( \frac{D^i}{4} - D \right) v_{j-1}^{**} + \left( \frac{2}{\lambda} + 2D \right) v^{**} - \left( \frac{D^i}{4} + D \right) v_{j+1}^{**} = \left( \frac{2}{\lambda} - 4D \right) v^* + 4Dv^*_{i+1}$$  \hfill (74b)

Conditions #1 and #2 at $r = 0$ and $z = d_s$

$$\left( \frac{2}{\lambda} + 4D \right) v^* - 4Dv^*_{i+1} = 2Dv_{j-1} + \left( \frac{2}{\lambda} - 2D \right) v$$  \hfill (75a)

and

$$-2Dv_{j-1}^{**} + \left( \frac{2}{\lambda} + 2D \right) v^{**} = \left( \frac{2}{\lambda} - 4D \right) v^* + 4Dv^*_{i+1}$$  \hfill (75b)
Fig. 2 - Delineation of boundary equation numbers for axisymmetric problem.

Condition #2 along $z = d_s, 0 < r < r_s$

\[
\left( \frac{D_i'}{4} - \frac{2i - 3}{21 - 2} D \right) v_{i-1}^* + \left( \frac{2}{\lambda} + 2D \right) v^* - \left( \frac{D_i'}{4} + \frac{2i - 1}{21 - 2} D \right) v_{i+1}^* = 2Dv_{j-1} + \left( \frac{2}{\lambda} - 2D \right) v
\]  

(76a)

and

\[
-2Dv_{j-1}^* + \frac{2}{\lambda} + 2D \quad v^{**} = \left( - \frac{D_i'}{4} + \frac{2i - 3}{21 - 2} D \right) v_{i-1}^*
\]

\[
+ \left( \frac{2}{\lambda} - 2D \right) v^* + \left( \frac{D_i'}{4} + \frac{2i - 1}{21 - 2} D \right) v_{i+1}^*
\]

(76b)
Conditions #2 and #8 at \( r = r_s, \ z = d_s \)
\[
-(\frac{1-2}{1-1} D + D_{i-1}) v_{i-1}^* + \left(\frac{2}{\lambda} + \frac{1-2}{1-1} D + D_{i-1} + 2CK_2 \frac{2i-2}{2i-3} \Delta r\right) v^*
\]
\[
= 2D v_{j-1} + \left(\frac{2}{\lambda} - 2D\right) v + 2CK_2 v_{d2} \Delta r \frac{2i-2}{2i-3}
\]
and
\[
-2D v_{j-1}^{**} + \left(\frac{2}{\lambda} + 2D\right) v^{**} = \left(D_{i-1} + \frac{1-2}{1-1} D\right) v_{i-1}^* + \left(\frac{2}{\lambda} - D_{i-1} - \frac{i-2}{1-3} D\right)
\]
\[
- 2CK_2 \frac{2i-2}{2i-3} \Delta r v^* + 2CK_2 \frac{2i-2}{2i-3} \Delta r v_{d2}
\]

Condition #8 along \( r = r_s, 0 < z < d_s \)
\[
-(\frac{1-2}{1-1} D + D_{i-1}) v_{i-1}^* + \left(\frac{2}{\lambda} + \frac{1-2}{1-1} D + D_{i-1} + 2CK_2 \frac{2i-2}{2i-3} \Delta r\right) v^*
\]
\[
= \left(D - \frac{D_i}{4}\right) v_{j-1} + \left(\frac{2}{\lambda} - 2D\right) v + \left(D + \frac{D_i}{4}\right) v_{j+1}
\]
\[
+ 2CK_2 v_{d2} \Delta r \frac{2i-2}{2i-3}
\]
and
\[
\left(D_i - D\right) v_{j-1}^{**} + \left(\frac{2}{\lambda} + 2D\right) v^{**} - \left(D + \frac{D_i}{4}\right) v_{j+1}^{**}
\]
\[
= \left(D_{i-1} + \frac{1-2}{1-1} D\right) v_{i-1}^* + \left(\frac{2}{\lambda} - D_{i-1} - \frac{i-2}{1-1} D - 2CK_2 \frac{2i-2}{2i-3} \Delta r\right) v^*
\]
\[
+ 2CK_2 \frac{2i-2}{2i-3} \Delta r v_{d2}
\]

Condition #10 along \( r_j < r < r_s, z = 0, t > t_0 \)
\[
\left(D_i - \frac{2i-3}{2i-2} D\right) v_{i-1}^* + \left(\frac{2}{\lambda} + 2D\right) v^* - \left(D_i + \frac{2i-1}{2i-2} D\right) v_{i+1}^*
\]
\[
= \left(\frac{2}{\lambda} - D - D_{j+1} - 2CK_1 \Delta z\right) v + \left(D + D_{j+1}\right) v_{j+1}
\]
\[
+ 2CK_1 v_{d1} \Delta z
\]
and

$$\left( \frac{2}{\lambda} + D + D_{j+1} + 2CK_1\Delta z \right) v^{**} - (D + D_{j+1})v^{**}_{j+1}$$

$$= \left( - \frac{D_{j+1}}{4} + \frac{2i - 3}{2i - 2} D \right) v^{**}_{j-1} + \left( \frac{2}{\lambda} - 2D \right) v^* + \left( \frac{D_{j+1}}{4} + \frac{2i - 1}{2i - 2} D \right) v^{**}_{j+1}$$

$$+ 2CK_1v_{a1}\Delta z$$

(79b)

Condition #4 along $0 < r < r_f$, $z = d_f$, $t > t_0$

$$\left( \frac{D_{j+1}}{4} - \frac{2i - 3}{2i - 2} D \right) v^{**}_{j-1} + \left( \frac{2}{\lambda} + 2D \right) v^* - \left( \frac{D_{j+1}}{4} + \frac{2i - 1}{2i - 2} D \right) v^{**}_{j+1}$$

$$= \left( \frac{2}{\lambda} - 2D \right) v^* + 2D v_{j+1}$$

(80a)

and

$$\left( \frac{2}{\lambda} + 2D \right) v^{**} - 2D v^{**}_{j+1} = \left( - \frac{D_{j+1}}{4} + \frac{2i - 3}{2i - 2} D \right) v^{**}_{j-1}$$

$$+ \left( \frac{2}{\lambda} - 2D \right) v^* + \left( \frac{D_{j+1}}{4} + \frac{2i - 1}{2i - 2} D \right) v^{**}_{j+1}$$

(80b)

Conditions #6 and #10 at $r = r_s$, $z = 0$, $t > 0$

$$-\left( \frac{i - 2}{i - 1} D + D_{i-1} \right) v^{**}_{i-1} + \left( \frac{2}{\lambda} + \frac{i - 2}{i - 1} D + D_{i-1} + 2CK_2 \frac{2i - 2}{2i - 3} \Delta r \right) v^*$$

$$= \left( \frac{2}{\lambda} - D - D_{j+1} - 2CK_1\Delta z \right) v + (D + D_{j+1})v_{j+1}$$

$$+ 2CK_1v_{a1}\Delta z + 2CK_2v_{a2}\Delta r$$

(81a)

and

$$\left( \frac{2}{\lambda} + D + D_{j+1} + 2CK_1\Delta z \right) v^{**} - (D + D_{j+1})v^{**}_{j+1}$$

$$= \left( D_{i-1} + \frac{i - 2}{i - 1} D \right) v^{**}_{i-1} + \left( \frac{2}{\lambda} - D_{i-1} - \frac{i - 2}{i - 1} D - 2CK_2 \frac{2i - 2}{2i - 3} \Delta r \right) v^*$$

$$+ 2CK_2 \frac{2i - 2}{2i - 3} v_{a2}\Delta r + 2CK_1v_{a1}\Delta z$$

(81b)

Condition #6 along $r = r_f$, $0 < z \leq d_f$, $t > t_0$

$$\left( \frac{2}{\lambda} + 2D \right) v^* - 2D v^{**}_{j+1} = \left( D - \frac{D_{j+1}}{4} \right) v_{j-1} + \left( \frac{2}{\lambda} - 2D \right) v + (D + \frac{D_{j+1}}{4}) v_{j+1}$$

(82a)
\[
\left(\frac{D_j^i}{4} - D\right) v_{j-1}^{**} + \left(\frac{2}{\lambda} + 2D\right) v^{**} - \left(D + \frac{D_j^i}{4}\right) v_{j+1}^{**} = 2D v_{j+1}^* + \left(\frac{2}{\lambda} - 2D\right) v^*
\]

Condition #4 and #6 at \( r = r_f, z = 0, t > t_0 \)

\[
\left(\frac{2}{\lambda} + 2D\right) v^* - 2D v_{i+1}^* = \left(\frac{2}{\lambda} - D - D_{j+1} - 2C_k\lambda z\right) v + (D + D_{j+1})v_{j+1}
\]

\[
+ 2C_k\lambda z v_{a1}
\]

(83a)

\[
\left(\frac{2}{\lambda} + D + D_{j+1} + 2C_k\lambda z\right) v^{**} - (D + D_{j+1})v_{j+1}^{**} = 2D v_{i+1}^* + \left(\frac{2}{\lambda} - 2D\right) v^* + 2C_k\lambda v_{a1}\lambda z
\]

(83b)

Condition #4 and #1 at \( r = 0, z = d_f, t > t_0 \)

\[
\left(\frac{2}{\lambda} + 4D\right) v^* - 4D v_{i+1}^* = 2D v_{j+1}^* + \left(\frac{2}{\lambda} - 2D\right) v
\]

(84a)

\[
-2D v_{j+1}^{**} + \left(\frac{2}{\lambda} + 2D\right) v^{**} = \left(\frac{2}{\lambda} - 4D\right) v^* + 4D v_{i+1}^*
\]

(84b)

2.2.1.2 Discretization for Code II--

The following equations hold for the boundaries delineated in Figure 3. The numbers shown in Figure 3 correspond to equation numbers given below. Note that at the intersection of two or more boundaries, the equation holds only at a single point.

Subscripts are omitted on \( D \) and \( v \) unless different from \( i, j, \) and/or \( k \).

Condition #1 along \( r = 0, d_f < z < d_s \)

\[
\left(\frac{2}{\lambda} + 4D\right) v^* - 4D v_{i+1}^* = \left(\frac{D}{4} - D_{j+1}\right) v_{j-1} + \left(\frac{2}{\lambda} - 2D\right) v + (D + D_{j+1})v_{j+1}
\]

(85a)

\[
\left(\frac{D_j^i}{4} - D\right) v_{j-1}^{**} + \left(\frac{2}{\lambda} + 2D\right) v^{**} - \left(D_{j+1} + \frac{D_j^i}{4}\right) v_{j+1}^{**} = 4D v_{i+1}^* - 4D v^* + \frac{2}{\lambda} v
\]

(85b)

\[
\frac{2}{\lambda} v^{**} = 4D v_{i+1}^* - 4D v^* + \left(\frac{2}{\lambda} - 2D\right) v^{**} + (D - \frac{D_j^i}{4})v_{j-1}^{**} + (D + \frac{D_j^i}{4})v_{j+1}^{**}
\]

(85c)
Fig. 3 - Delineation of boundary equation numbers for three dimensional axisymmetric problem with partially penetrating vents.
Conditions #1, #2, #11 and #12 at \( r = 0, z = d_s \)
\[
\left( \frac{2}{\lambda} + 4D \right) v^* - 4D v^*_{j+1} = 2D v_{j-1} + \left( \frac{2}{\lambda} - 2D \right) v \quad (86a)
\]
\[-2D v^*_{j-1} + \left( \frac{2}{\lambda} + 2D \right) v^* = 4D v^*_{j+1} - 4D v^* + \frac{2}{\lambda} v \quad (86b)
\]
and
\[
\frac{2}{\lambda} v^{***} = 4D v^*_{j+1} - 4D v^* + 2D v^{**}_{j-1} + \left( \frac{2}{\lambda} - 2D \right) v^{**} \quad (86c)
\]

Conditions #2 and #11 along \( 0 < r < r_s, z = d_s, \theta = \theta_I \)
\[
\left( \frac{D_i}{4} - \frac{2i - 3}{2i - 2} D \right) v^*_{i-1} + \left( \frac{2}{\lambda} + 2D \right) v^* - \left( \frac{D_i}{4} + \frac{2i - 1}{2i - 2} D \right) v^*_{i+1} = 2D v_{j-1} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_i^2} \right) v + 2D \frac{v_{k+1}}{\Delta \theta_i^2} \quad (87a)
\]
\[-2D v^{**}_{j-1} + \left( \frac{2}{\lambda} + 2D \right) v^{**} = \left( \frac{2i - 3}{2i - 2} D - \frac{D_i}{4} \right) v^{**}_{i-1} - 2D v^* + \left( \frac{2i - 1}{2i - 2} D + \frac{D_i}{4} \right) v^{*+1}_{i+1} + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_i^2} \right) v + 2D \frac{v_{k+1}}{\Delta \theta_i^2} \quad (87b)
\]
and
\[
\left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_i^2} \right) v^{***} - \frac{2D}{\Delta \theta_i^2} v^{**}_{k+1} = \left( \frac{2i - 3}{2i - 2} D - \frac{D_i}{4} \right) v^{***}_{i-1} - 2D v^* + \left( \frac{2i - 1}{2i - 2} D + \frac{D_i}{4} \right) v^{*+1}_{i+1} + \left( \frac{2}{\lambda} - 2D \right) v^{**} \quad (87c)
\]

Conditions #2 and #12 along \( 0 < r < r_s, z = d_s, \theta = \theta_F \)
\[
\left( \frac{D_i}{4} - \frac{2i - 3}{2i - 2} D \right) v^*_{i-1} + \left( \frac{2}{\lambda} + 2D \right) v^* - \left( \frac{D_i}{4} + \frac{2i - 1}{2i - 2} D \right) v^*_{i+1} = 2D v_{j-1} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_i^2} \right) v + 2D \frac{v_{k-1}}{\Delta \theta_i^2} \quad (88a)
\]
\[-2D v^{**}_{j-1} + \left( \frac{2}{\lambda} + 2D \right) v^{**} = \left( \frac{2i - 3}{2i - 2} D - \frac{D_i}{4} \right) v^{**}_{i-1} - 2D v^* + \left( \frac{2i - 1}{2i - 2} D + \frac{D_i}{4} \right) v^{*+1}_{i+1} + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_i^2} \right) v + 2D \frac{v_{k-1}}{\Delta \theta_i^2} \quad (88b)
\]
and

\[
\frac{-2D}{\Delta \theta_1^2} v_{k-1}^{**} + \left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1^2} \right) v^{**} = \left( \frac{2i - 3}{2i - 2} D - \frac{D_i^I}{4} \right) v_{i-1}^{*} - 2D v^{*} + \left( \frac{2i - 1}{2i - 2} D + \frac{D_i^I}{4} \right) v_{i+1}^{*} + 2D v_{j-1}^{**} + \left( \frac{2}{\lambda} - 2D \right) v^{**}
\]

(88c)

Condition #2 on \(0 < r < r_s\), \(z = d_s\), \(\theta_I < \theta < \theta_F\)

\[
\left( \frac{D_i^I}{4} - \frac{2i - 3}{2i - 2} D \right) v_{i-1}^{*} + \left( \frac{2}{\lambda} + 2D \right) v^{*} - \left( \frac{D_i^I}{4} + \frac{2i - 1}{2i - 2} D \right) v_{i+1}^{*}
\]

\[
= 2D v_{j-1}^{*} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1^2} \right) v + \left( D - \frac{D_k^I}{4} \right) v_{k-1}^{*} + \left( D + \frac{D_k^I}{4} \right) v_{k+1}^{*} \]

(89a)

\[
-2D v_{j-1}^{**} + \left( \frac{2}{\lambda} + 2D \right) v^{**} = \left( \frac{2i - 3}{2i - 2} D - \frac{D_i^I}{4} \right) v_{i-1}^{*} + \left( \frac{2i - 1}{2i - 2} D + \frac{D_i^I}{4} \right) v_{i+1}^{*}
\]

\[-2D v^{*} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1^2} \right) v + \left( D - \frac{D_k^I}{4} \right) v_{k-1}^{*} + \left( D + \frac{D_k^I}{4} \right) v_{k+1}^{*} \]

(89b)

and

\[
\left( \frac{D_k^I}{4} - D \right) \frac{v_{k-1}^{**}}{\Delta \theta_1^2} + \left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1^2} \right) v^{**} - \left( \frac{D_k^I}{4} + D \right) \frac{v_{k+1}^{**}}{\Delta \theta_1^2}
\]

\[
= \left( \frac{2i - 3}{2i - 2} D - \frac{D_i^I}{4} \right) v_{i-1}^{*} - 2D v^{*} + \left( \frac{2i - 1}{2i - 2} D + \frac{D_i^I}{4} \right) v_{i+1}^{*}
\]

\[+ 2D v_{j-1}^{**} + \left( \frac{2}{\lambda} - 2D \right) v^{**} \]

(89c)

Conditions #2 and #3 along \(r = r_s\), \(z = d_s\), \(\theta_I < \theta < \theta_F\)

\[
-2D v_{i-1}^{*} + \left( \frac{2}{\lambda} + 2D \right) v^{*} = 2D v_{j-1}^{*} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1^2} \right) v + \left( D - \frac{D_k^I}{4} \right) v_{k-1}^{**} + \left( D + \frac{D_k^I}{4} \right) v_{k+1}^{**} \]

(90a)
\[-2D v_j^{**} + \left( \frac{2}{\lambda} + 2D \right) v^{**} = 2D v_{j-1}^* - 2D v^* + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_1^2} \right) v^* + \left( D - \frac{D_1^i}{4} \right) \frac{v_{k-1}}{\Delta \theta_1^2} + \left( D + \frac{D_1^i}{4} \right) \frac{v_{k+1}}{\Delta \theta_1^2} \] (90b)

and
\[
\left( \frac{D_1^i}{4} - D \right) \frac{v_{k-1}^{**}}{\Delta \theta_1^2} + \left( \frac{2}{\lambda} + 2D \right) v^{**} - \left( \frac{D_1^i}{4} + D \right) \frac{v_{k+1}^{**}}{\Delta \theta_1^2} = 2D v_{i-1}^* - 2D v^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + 2D v_{j-1}^* \] (90c)

**Condition #11** on \( 0 < r < r_s, 0 < z < d_s, \theta = \theta_T \)
\[
\left( \frac{D_1^i}{4} - \frac{2i - 3}{2i - 2} D \right) v_{i-1}^* + \left( \frac{2}{\lambda} + 2D \right) v^* - \left( \frac{D_1^i}{4} + \frac{2i - 1}{2i - 2} D \right) v_{i+1}^* = \left( D - \frac{D_1^i}{4} \right) v_{j-1} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1^2} \right) v + \left( D + \frac{D_1^i}{4} \right) v_{j+1} + \frac{2D}{\Delta \theta_1^2} v_{k+1} \] (91a)

\[
\left( \frac{D_1^i}{4} - D \right) v_{j-1}^{**} + \left( \frac{2}{\lambda} + 2D \right) v^{**} - \left( \frac{D_1^i}{4} + D \right) v_{j+1}^{**} = \left( \frac{2i - 3}{2i - 2} D - \frac{D_1^i}{4} \right) v_{i-1}^* - 2D v^* + \left( \frac{2i - 1}{2i - 2} D + \frac{D_1^i}{4} \right) v_{i+1}^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + \left( D + \frac{D_1^i}{4} \right) v_{j+1}^{**} \] (91b)

\[
\left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1^2} \right) v^{**} - \frac{2D}{\Delta \theta_1^2} v_{k+1}^{**} = \left( \frac{2i - 3}{2i - 2} D - \frac{D_1^i}{4} \right) v_{i-1}^* - 2D v^* + \left( \frac{2i - 1}{2i - 2} D + \frac{D_1^i}{4} \right) v_{i+1}^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + \left( D + \frac{D_1^i}{4} \right) v_{j+1}^{**} \] (91c)

**Condition #12** on \( 0 < r < r_s, 0 < z < d_s, \theta = \theta_F \)
\[
\left( \frac{D_1^i}{4} - \frac{2i - 3}{2i - 2} D \right) v_{i-1}^* + \left( \frac{2}{\lambda} + 2D \right) v^* - \left( \frac{D_1^i}{4} + \frac{2i - 1}{2i - 2} D \right) v_{i+1}^* = \left( D - \frac{D_1^i}{4} \right) v_{j-1} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1^2} \right) v + \left( D + \frac{D_1^i}{4} \right) v_{j+1} + \frac{2D}{\Delta \theta_1^2} v_{k+1} \] (92a)
\[
(D_{j}^{I} - D) v_{j-1}^{**} + \left(\frac{2}{\lambda} + 2D\right) v^{**} - \left(\frac{D_{j}^{I}}{4} + D\right) v_{j+1}^{**} = \left(\frac{2i - 3}{2i - 2} D - \frac{D_{j}^{I}}{4}\right) v_{i-1}^{*} - 2D v^{*} + \left(\frac{2i - 1}{2i - 2} D + \frac{D_{j}^{I}}{4}\right) v_{i+1}^{*} + \left(\frac{2}{\lambda} - \frac{2D}{\Delta \theta_{j}^{2}}\right) v + \frac{2D}{\Delta \theta_{j}^{2}} v_{k-1} \quad (92b)
\]

and
\[
- \frac{2D}{\Delta \theta_{j}^{2}} v_{k-1}^{**} + \left(\frac{2}{\lambda} + \frac{2D}{\Delta \theta_{j}^{2}}\right) v^{**} = \left(\frac{2i - 3}{2i - 2} D - \frac{D_{j}^{I}}{4}\right) v_{i+1}^{*} - 2D v^{*} + \left(\frac{2i - 1}{2i - 2} D + \frac{D_{j}^{I}}{4}\right) v_{i+1}^{*} + \left(\frac{2}{\lambda} - 2D\right) v^{**} + \left(D + \frac{D_{j}^{I}}{4}\right) v_{j+1}^{**} \quad (92c)
\]

Conditions #8 and #11 along \( r = r_{S}, 0 < z < d_{S}, \theta = \theta_{I} \)
\[
-2D v_{i-1}^{*} + \left(\frac{2}{\lambda} + 2D\right) v^{*} = \left(D - \frac{D_{j}^{I}}{4}\right) v_{j-1}^{*} + \left(\frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_{j}^{2}}\right) v + \left(D + \frac{D_{j}^{I}}{4}\right) v_{j+1}^{**} + \frac{2D}{\Delta \theta_{j}^{2}} v_{k+1} \quad (93a)
\]

\[
(D_{j}^{I} - D) v_{j-1}^{**} + \left(\frac{2}{\lambda} + 2D\right) v^{**} - \left(\frac{D_{j}^{I}}{4} + D\right) v_{j+1}^{**} = 2D v_{i-1}^{*} - 2D v^{*} + \left(\frac{2}{\lambda} - \frac{2D}{\Delta \theta_{j}^{2}}\right) v + \frac{2D}{\Delta \theta_{j}^{2}} v_{k+1} \quad (93b)
\]

\[
\left(\frac{2}{\lambda} + \frac{2D}{\Delta \theta_{j}^{2}}\right) v^{**} - \frac{2D}{\Delta \theta_{j}^{2}} v_{k+1}^{**} = 2D v_{i-1}^{*} - 2D v^{*} + \left(\frac{2}{\lambda} - 2D\right) v^{**} + \left(D - \frac{D_{j}^{I}}{4}\right) v_{j-1}^{**} + \left(D + \frac{D_{j}^{I}}{4}\right) v_{j+1}^{**} \quad (93c)
\]

Conditions #8 and #12 along \( r = r_{S}, 0 < z < d_{S}, \theta = \theta_{F} \)
\[
-2D v_{i-1}^{*} + \left(\frac{2}{\lambda} + 2D\right) v^{*} = \left(D - \frac{D_{j}^{I}}{4}\right) v_{j-1}^{*} + \left(\frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_{j}^{2}}\right) v + \left(D + \frac{D_{j}^{I}}{4}\right) v_{j+1}^{**} + \frac{2D}{\Delta \theta_{j}^{2}} v_{k-1} \quad (94a)
\]
\[
(D'_k - D) v^*_{j-1} + \left( \frac{2}{\lambda} + 2D \right) v^* - \left( \frac{D'_k}{4} + D \right) v^*_{j+1} = 2D v^*_{i-1} - 2D v^* + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta^2_1} \right) v + \frac{2D}{\Delta \theta^2_1} v_{k-1} \quad (94b)
\]

and
\[
- \frac{2D}{\Delta \theta^2_1} v^*_{k-1} + \left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta^2_1} \right) v^{**} = 2D v^*_{i-1} - 2D v^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + \left( D - \frac{D'_k}{4} \right) v^*_{j-1} + \left( D + \frac{D'_k}{4} \right) v^*_{j+1} \quad (94c)
\]

Conditions #8 and #10 along \( r = r_s, z = 0, < \theta < \theta_F \)
\[
-2D v^*_{i-1} + \left( \frac{2}{\lambda} + 2D \right) v^* = \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta^2_1} \right) v + 2D v^*_{j+1} + \left( D - \frac{D'_k}{4} \right) v_{k-1} + \left( D + \frac{D'_k}{4} \right) v_{k+1} \quad (95a)
\]

\[
\left( \frac{2}{\lambda} + 2D \right) v^{**} - 2D v^{**}_{j+1} = 2D v^*_{i-1} - 2D v^* + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta^2_1} \right) v + \left( D - \frac{D'_k}{4} \right) v_{k-1} + \left( D + \frac{D'_k}{4} \right) v_{k+1} \quad (95b)
\]

\[
\left( \frac{D'_k}{4} - D \right) \frac{v^{**}_{k-1}}{\Delta \theta^2_1} + \left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta^2_1} \right) v^{***} - \left( \frac{D'_k}{4} + D \right) \frac{v^{***}_{k+1}}{\Delta \theta^2_1} = 2D v^*_{i-1} - 2D v^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + 2D v^{**}_{j+1} \quad (95c)
\]

Conditions #8, #10 and #11 at \( r = r_s, z = 0, \theta = \theta_I \)
\[
-2D v^*_{i-1} + \left( \frac{2}{\lambda} + 2D \right) v^* = \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta^2_1} \right) v + 2D v^*_{j+1} + 2D \frac{v_{k+1}}{\Delta \theta^2_1} \quad (96a)
\]

\[
\left( \frac{2}{\lambda} + 2D \right) v^{**} - 2D v^{**}_{j+1} = 2D v^*_{i-1} - 2D v^* + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta^2_1} \right) v + 2D \frac{v_{k+1}}{\Delta \theta^2_1} \quad (96b)
\]

and
\[
\left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta^2_1} \right) v^{***} - \frac{2D}{\Delta \theta^2_1} v^{***}_{k+1} = 2D v^*_{i-1} - 2D v^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + 2D v^{**}_{j+1} \quad (96c)
\]
Conditions #8, #10 and #12 at \( r = r_s, z = 0, \theta = \theta_F \)

\[-2D v_{i-1}^* + \left( \frac{2}{\lambda} + 2D \right) v^* = \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_i^2} \right) v + 2D v_{j+1} + \frac{2D}{\Delta \theta_i^2} v_{k-1} \] ~ (97a)

\[\left( \frac{2}{\lambda} + 2D \right) v_{j+1}^{**} - 2D v_{j-1}^{**} = 2D v_{i-1}^* - 2D v^* + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_i^2} \right) v + \frac{2D}{\Delta \theta_i^2} v_{k-1} \] ~ (97b)

and

\[-\frac{2D}{\Delta \theta_i^2} v_{k-1}^{***} + \left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_i^2} \right) v^{***} = 2D v_{i-1}^* - 2D v^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + 2D v_{j+1}^{**} \] ~ (97c)

Conditions #2, #8 and #11 at \( r = r_s, z = d_s, \theta = \theta_I \)

\[-2D v_{i-1}^* + \left( \frac{2}{\lambda} + 2D \right) v^* = 2D v_{j-1} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_i^2} \right) v + 2D \frac{v_{k+1}}{\Delta \theta_i^2} \] ~ (98a)

\[-2D v_{j-1}^{**} + \left( \frac{2}{\lambda} + 2D \right) v^{**} = 2D v_{i-1}^* - 2D v^* + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_i^2} \right) v + 2D \frac{v_{k+1}}{\Delta \theta_i^2} \] ~ (98b)

and

\[\left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_i^2} \right) v^{***} - 2D \frac{v_{k+1}}{\Delta \theta_i^2} = 2D v_{i-1}^* - 2D v^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + 2D v_{j-1}^{**} \] ~ (98c)

Conditions #2, #8 and #12 at \( r = r_s, z = d_s, \theta = \theta_F \)

\[-2D v_{i-1}^* + \left( \frac{2}{\lambda} + 2D \right) v^* = 2D v_{j-1} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_i^2} \right) v + 2D \frac{v_{k+1}}{\Delta \theta_i^2} \] ~ (99a)

\[-2D v_{j-1}^{**} + \left( \frac{2}{\lambda} + 2D \right) v^{**} = 2D v_{i-1}^* - 2D v^* + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_i^2} \right) v + 2D \frac{v_{k+1}}{\Delta \theta_i^2} \] ~ (99b)

and

\[-2D \frac{v_{k+1}}{\Delta \theta_i^2} + \left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_i^2} \right) v^{***} = 2D v_{i-1}^* - 2D v^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + 2D v_{j-1}^{**} \] ~ (99c)

Condition #10 on \( r = r_s, 0 < z < d_s, \theta_I < \theta < \theta_F \)

\[-2D v_{i-1}^* + \left( \frac{2}{\lambda} + 2D \right) v^* = \left( D - \frac{D^i_j}{4} \right) v_{j-1} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_i^2} \right) v \]

\[+ \left( D + \frac{D^i_j}{4} \right) v_{j+1} + \left( D - \frac{D^i_k}{4} \right) \frac{v_{k-1}}{\Delta \theta_i^2} + \left( D + \frac{D^i_k}{4} \right) v_{k+1} \] ~ (100a)
\[
\left( \frac{D^i_j}{4} - D \right) v^*_{j-1} + \left( \frac{2}{\lambda} + 2D \right) v^{**} - \left( \frac{D^i_j}{4} + D \right) v^*_j + 2D v^*_j - 2D v^* + \left( \frac{2}{\lambda} - 2D \right) v^* + \left( D - \frac{D^i_j}{4} \right) \frac{v_{k-1}}{\Delta \theta^2_1} + \left( D + \frac{D^i_j}{4} \right) \frac{v_{k+1}}{\Delta \theta^2_1}
\]

and

\[
\left( \frac{D^i_k}{4} - D \right) \frac{v^{***}_{k-1}}{\Delta \theta^2_1} + \left( \frac{2}{\lambda} + 2D \right) v^{***} - \left( \frac{D^i_k}{4} + D \right) \frac{v^{***}_{k+1}}{\Delta \theta^2_1}
\]

\[
= 2D v^*_{j-1} - 2D v^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + \left( D - \frac{D^i_j}{4} \right) v^*_j + \left( D + \frac{D^i_j}{4} \right) v^*_j + \left( D - \frac{D^i_j}{4} \right) v^{**}_j + \left( D + \frac{D^i_j}{4} \right) v^{**}_j + \left( D - \frac{D^i_j}{4} \right) v^{***}_j + \left( D + \frac{D^i_j}{4} \right) v^{***}_j
\]

Conditions #10 and #12 along \( r_s < r < r_s, z = 0, \theta = \theta_F \) and

Conditions #4 and #4 along \( 0 < r < r_f, z = d_s, \theta = \theta_F, t > t_0 \)

\[
\left( \frac{D^i_j}{4} - \frac{21 - 3}{21 - 2} D \right) v^*_{j-1} + \left( \frac{2}{\lambda} + 2D \right) v^{**} - \left( \frac{D^i_j}{4} + \frac{21 - 1}{21 - 2} \right) v^*_j + \left( \frac{2}{\lambda} - 2D \right) v^{**}_j + \left( \frac{D^i_j}{4} + \frac{21 - 1}{21 - 2} D \right) v^*_j + \left( 2 \frac{2}{\lambda} - 2D \right) v^{**}_j + \left( \frac{D^i_j}{4} + \frac{21 - 1}{21 - 2} D \right) \frac{v_{k-1}}{\Delta \theta^2_1}
\]

and

\[
\left( \frac{2}{\lambda} + 2D \right) v^{**} - 2D v^{**}_j = \left( \frac{21 - 3}{21 - 2} D - \frac{D^i_j}{4} \right) v^*_j - 2D v^* + \left( \frac{D^i_j}{4} + \frac{21 - 1}{21 - 2} D \right) \frac{v_{k-1}}{\Delta \theta^2_1} + \left( 2 \frac{2}{\lambda} - 2D \right) \frac{v_{k-1}}{\Delta \theta^2_1}
\]

and

\[
- \frac{2D}{\Delta \theta^2_1} v^{***}_{k-1} + \left( \frac{2}{\lambda} + 2D \right) v^{***} = \left( \frac{21 - 3}{21 - 2} D - \frac{D^i_j}{4} \right) v^*_j - 2D v^* + \left( \frac{21 - 1}{21 - 2} D + \frac{D^i_j}{4} \right) \frac{v^{**}_{k+1}}{\Delta \theta^2_1} + \left( \frac{2}{\lambda} - 2D \right) v^{**}_j
\]

Conditions #10a and #12 along \( r_s < r < r_s, z = 0, \theta = \theta_F \), and

Conditions #4 along \( 0 < r < r_f, z = d_s, \theta = \theta_F, t > t_0 \)
Conditions #10 and #11 along $r_f < r < r_s$, $z = 0$, $\theta = \theta_1$ and
Conditions #4 and #11 along $0 < r < r_f$, $z = d_f$, $\theta = \theta_1$, $t > t_0$

\[
\left( \frac{D_i'}{4} - \frac{2i - 3}{21 - 2} D \right) v_{i-1}^* + \left( \frac{2}{\lambda} + 2D \right) v^* - \left( \frac{D_i'}{4} + \frac{2i - 1}{21 - 2} D \right) v_{i+1}^* \\
= \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1^2} \right) v + 2D v_{j+1} + \frac{2D}{\Delta \theta_1^2} v_{k+1} \\
(102a)
\]

\[
\left( \frac{2}{\lambda} + 2D \right) v^{**} - 2D v_{j+1}^{**} = \left( \frac{2i - 3}{21 - 2} D - \frac{D_i'}{4} \right) v_{i-1}^* - 2D v^* \\
+ \left( \frac{D_i'}{4} + \frac{2i - 1}{21 - 2} D \right) v_{i+1}^* + \left( \frac{2}{\lambda} - 2D \right) v + \frac{2D}{\Delta \theta_1^2} v_{k+1} \\
(102b)
\]

and

\[
\left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1^2} \right) v^{***} - \frac{2D}{\Delta \theta_1^2} v_{k+1}^{***} = \left( \frac{2i - 3}{21 - 2} D - \frac{D_i'}{4} \right) v_{i-1}^* - 2D v^* \\
+ \left( \frac{2i - 1}{21 - 2} D + \frac{D_i'}{4} \right) v_{i+1}^* + 2D v_{j+1}^{**} \\
+ \left( \frac{2}{\lambda} - 2D \right) v^{**} \\
(102c)
\]

Condition #10 on $r_f < r < r_s$, $z = 0$, $\theta_1 < \theta < \theta_f$ and
Condition #4 on $0 < r < r_f$, $z = d_f$, $\theta_1 < \theta < \theta_f$, $t > t_0$

\[
\left( \frac{D_i'}{4} - \frac{2i - 3}{21 - 2} D \right) v_{i-1}^* + \left( \frac{2}{\lambda} + 2D \right) v^* - \left( \frac{D_i'}{4} + \frac{2i - 1}{21 - 2} D \right) v_{i+1}^* \\
= \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1^2} \right) v + 2D v_{j+1} + \left( D - \frac{D_k'}{4} \right) v_{k-1} + \left( D + \frac{D_k'}{4} \right) v_{k+1} \\
(103a)
\]

\[
\left( \frac{2}{\lambda} + 2D \right) v^{**} - 2D v_{j+1}^{**} = \left( \frac{2i - 3}{21 - 2} D - \frac{D_i'}{4} \right) v_{i-1}^* + \left( \frac{2i - 1}{21 - 2} D + \frac{D_i'}{4} \right) v_{i+1}^* \\
- 2D v^* + \left( D - \frac{D_k'}{4} \right) v_{k-1} + \left( D + \frac{D_k'}{4} \right) v_{k+1} \\
+ \left( \frac{2}{\lambda} - 2D \right) v \\
(103b)
\]
and

\[
\left( \frac{D_k}{4} - D \right) \frac{v_{k-1}^{***}}{\Delta \theta_1^2} + \left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1^2} \right) v^{***} - \left( \frac{D_k}{4} + D \right) \frac{v_{k+1}^{***}}{\Delta \theta_1^2} = \left( \frac{2\lambda - 3}{21 - 2} \right) v_{k-1} - 2D v^* + \left( \frac{2\lambda - 1}{21 - 2} D + \frac{D_k}{4} \right) v_{k+1}
\]

\[+ 2D v_{j+1}^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} \quad (103c)\]

Conditions #6 and #10 along \( r = r_f, z = 0, \theta_1 < \theta < \theta_f, t > t_0 \) and

Conditions #4 and #6 along \( r = r_f, z = d_f, \theta_1 < \theta < \theta_f, t > t_0 \)

\[
\left( \frac{2}{\lambda} + 2D \right) v^* - 2D v_{i+1}^* = \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1^2} \right) v + 2D v_{j+1}^*
\]

\[+ \left( D - \frac{D_k}{4} \right) \frac{v_{k-1}}{\Delta \theta_1^2} + \left( D + \frac{D_k}{4} \right) \frac{v_{k+1}}{\Delta \theta_1^2} \quad (104a)\]

\[
\left( \frac{2}{\lambda} + 2D \right) v^{**} - 2D v_{j+1}^{**} = -2D v^* + 2D v_{i+1}^* + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_1^2} \right) v
\]

\[+ \left( D - \frac{D_k}{4} \right) \frac{v_{k-1}}{\Delta \theta_1^2} + \left( D + \frac{D_k}{4} \right) \frac{v_{k+1}}{\Delta \theta_1^2} \quad (104b)\]

and

\[
\left( \frac{D_k}{4} - D \right) \frac{v_{k-1}^{***}}{\Delta \theta_1^2} + \left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1^2} \right) v^{***} - \left( \frac{D_k}{4} + D \right) \frac{v_{k+1}^{***}}{\Delta \theta_1^2} = -2D v^* + 2D v_{i+1}^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + 2D v_{j+1}^{**} \quad (104c)\]

Conditions #6, #10 and #11 at \( r = r_f, z = 0, \theta = \theta_1, t > t_0 \) and

Conditions #4, #6 and #11 at \( r = r_f, z = d_f, \theta = \theta_1, t > t_0 \)

\[
\left( \frac{2}{\lambda} + 2D \right) v^* - 2D v_{i+1}^* = \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1^2} \right) v + 2D v_{j-1} + \frac{2D}{\Delta \theta_1^2} v_{k+1} \quad (105a)\]

\[
\left( \frac{2}{\lambda} + 2D \right) v^{**} - 2D v_{j-1}^{**} = -2D v^* + 2D v_{i+1}^* + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_1^2} \right) v + \frac{2D}{\Delta \theta_1^2} v_{k+1} \quad (105b)\]

and

\[
\left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1^2} \right) v^{***} - \frac{2D}{\Delta \theta_1^2} v_{k+1}^{***} = -2D v^* + 2D v_{i+1}^* + \left( \frac{2}{\lambda} - 2D \right) v^{**} + 2D v_{j-1}^{**} \quad (105c)\]
Conditions #6, #10 and #12 at \( r = r_f, z = 0, \theta = \theta_F, t > t_0 \) and

\[
\left( \frac{2}{\lambda} + 2D \right) v^* - 2D v^*_{i+1} = \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1} \right) v + 2D v_{j-1} + \frac{2D}{\Delta \theta_1} v_{k-1} \quad (106a)
\]

\[
\left( \frac{2}{\lambda} + 2D \right) v^{**} - 2D v^{**}_{j-1} = -2D v^* + 2D v^*_{i+1} + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_1} \right) v + \frac{2D}{\Delta \theta_1} v_{k-1} \quad (106b)
\]

and

\[
- \frac{2D}{\Delta \theta_1} v^{***}_{k-1} + \left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1} \right) v^{***} = -2D v^* + 2D v^*_{i+1} + \left( \frac{2}{\lambda} - 2D \right) v^{**} + 2D v^{**}_{j-1} \quad (106c)
\]

Conditions #4, #6 and #12 at \( r = r_f, z = d_f, \theta = \theta_F, t > t_0 \)

\[
\left( \frac{2}{\lambda} + 2D \right) v^* - 2D v^*_{i+1} = \left( D - \frac{D_j}{4} \right) v_{j-1} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1} \right) v + \left( D + \frac{D_j}{4} \right) v_{j+1} + \frac{2D}{\Delta \theta_1} v_{k+1} \quad (107a)
\]

\[
\left( D_j - D \right) v^{**}_{j-1} + \left( \frac{2}{\lambda} + 2D \right) v^{**} - \left( \frac{D_j}{4} + D \right) v^{**}_{j+1} = -2D v^* + 2D v^*_{i+1} + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_1} \right) v + \frac{2D}{\Delta \theta_1} v_{k+1} \quad (107b)
\]

and

\[
\left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1} \right) v^{***} - \frac{2D}{\Delta \theta_1} v^{***}_{k+1} = -2D v^* + 2D v^*_{i+1} + \left( \frac{2}{\lambda} - 2D \right) v^{**} + \frac{2D}{\Delta \theta_1} v_{j-1} + \frac{2D}{\Delta \theta_1} v_{j+1} \quad (107c)
\]

Conditions #6 and #11 along \( r = r_f, 0 < z < d_f, \theta = \theta_I, t > t_0 \)

\[
\left( \frac{2}{\lambda} + 2D \right) v^* - 2D v^*_{i+1} = \left( D - \frac{D_j}{4} \right) v_{j-1} + \left( \frac{2}{\lambda} - 2D - \frac{2D}{\Delta \theta_1} \right) v + \left( D + \frac{D_j}{4} \right) v_{j+1} + \frac{2D}{\Delta \theta_1} v_{k-1} \quad (108a)
\]

\[
\left( D_j - D \right) v^{**}_{j-1} + \left( \frac{2}{\lambda} + 2D \right) v^{**} - \left( \frac{D_j}{4} + D \right) v^{**}_{j+1} = -2D v^* + 2D v^*_{i+1} + \left( \frac{2}{\lambda} - \frac{2D}{\Delta \theta_1} \right) v + \frac{2D}{\Delta \theta_1} v_{k+1} \quad (107b)
\]

and

\[
\left( \frac{2}{\lambda} + \frac{2D}{\Delta \theta_1} \right) v^{***} - \frac{2D}{\Delta \theta_1} v^{***}_{k+1} = -2D v^* + 2D v^*_{i+1} + \left( \frac{2}{\lambda} - 2D \right) v^{**} + \frac{2D}{\Delta \theta_1} v_{j-1} + \frac{2D}{\Delta \theta_1} v_{j+1} \quad (107c)
\]
\((D_j^1 - D) v_{j-1}^{**} + \left(\frac{2}{\lambda} + 2D\right) v^{**} - (D_j^1 + D) v_{j+1}^{**}\)

\[= -2D v^* + 2D v_{i+1}^* + \left(\frac{2}{\lambda} - 2D \frac{\Delta \theta_1^2}{\Delta \theta_1^2}\right) v + \frac{2D}{\Delta \theta_1^2} v_{k-1} \quad (108b)\]

and

\[\left(\frac{2}{\lambda} + \frac{2D}{\Delta \theta_1^2}\right) v^{**} - \frac{2D}{\Delta \theta_1^2} v^{**} = -2D v^* + 2D v_{i+1}^* + \left(\frac{2}{\lambda} - 2D\right) v^{**}\]

\[+ \left(D - \frac{D_j^1}{4}\right) v_{j-1}^{**} + \left(D + \frac{D_j^1}{4}\right) v_{j+1}^{**} \quad (108c)\]

Condition #6 on \(r = r_f, 0 < z < d_f, \theta_I < \theta < \theta_F, t > t_0\)

\[\left(\frac{2}{\lambda} + 2D\right) v^* - 2D v_{i+1}^* = \left(D - \frac{D_j^1}{4}\right) v_{j-1} + \left(\frac{2}{\lambda} - 2D - 2D \frac{\Delta \theta_1^2}{\Delta \theta_1^2}\right) v + \left(D + \frac{D_j^1}{4}\right) v_{j+1}\]

\[+ \left(D - \frac{D_k^1}{4}\right) v_{k-1} + \left(D + \frac{D_k^1}{4}\right) v_{k+1} \quad (109a)\]

\[\left(D_j^1 - D\right) v_{j-1}^{**} + \left(\frac{2}{\lambda} + 2D\right) v^{**} - \left(D_j^1 + D\right) v_{j+1}^{**}\]

\[= -2D v^* + 2D v_{i+1}^* + \left(\frac{2}{\lambda} - 2D \frac{\Delta \theta_1^2}{\Delta \theta_1^2}\right) v\]

\[+ \left(D - \frac{D_j^1}{4}\right) v_{k-1}^{**} + \left(D + \frac{D_j^1}{4}\right) v_{k+1}^{**} \quad (109b)\]

and

\[\left(D_k^1 - D\right) v_{k-1}^{**} + \left(\frac{2}{\lambda} + 2D \frac{\Delta \theta_1^2}{\Delta \theta_1^2}\right) v^{**} - \left(D_j^1 + D\right) v_{k+1}^{**}\]

\[= -2D v^* + 2D v_{i+1}^* + \left(\frac{2}{\lambda} - 2D\right) v^{**}\]

\[+ \left(D - \frac{D_j^1}{4}\right) v_{j-1}^{**} + \left(D + \frac{D_j^1}{4}\right) v_{j+1}^{**} \quad (109c)\]

Conditions #1, #4, #11, and #12 at \(r = 0, z = d_f, \theta_I < \theta < \theta_F, t > t_0\)

\[\left(\frac{2}{\lambda} + 4D\right) v^* - 4D v_{i+1}^* = 2D v_{j+1} + \left(\frac{2}{\lambda} - 2D\right) v \quad (110a)\]

\[\left(\frac{2}{\lambda} + 2D\right) v^{**} - 2D v_{j+1}^{**} = 4D v_{i+1}^* - 4D v^* + \frac{2}{\lambda} v \quad (110b)\]
and

\[
\frac{2}{\lambda} v^{***} = 4D v^*_i + 4D v^*_j + 2D v^{**}_j + \left( \frac{2}{\lambda} - 2D \right) v^{**}
\]  

(110c)
CHAPTER III

SYNTHESIS OF FINITE DIFFERENCE COMPUTER CODES

For the problem of gas diffusion with boundary and initial conditions described in Chapter II, there is very little change in the effective diffusion coefficient $D$ at a mesh point over a time $\Delta T$. Thus, the value of $D$ based on the concentration at a mesh point in the beginning of a time interval may be assumed constant.

The problem could be solved by explicit techniques. It has been established (Carnahan, et al., 1969) that the results are stable provided that

$$\lambda = D\Delta T \left[ \left( \frac{1}{\Delta X} \right)^2 + \left( \frac{1}{\Delta Y} \right)^2 \right] \leq \frac{1}{2} \quad (111)$$

Furthermore, as time and space increments, $\Delta T$, $\Delta X$, $\Delta Y$ approach zero, the solution converges to the exact solution subject to condition (111). The restriction on $\Delta T$ introduces a very large number of time steps for analysis. Thus, explicit methods are not particularly attractive.

As discussed in Section 2, it is desirable to use the alternating direction implicit (ADI) method. It may be pointed out that although the ADI methods are unconditionally stable, the time increment cannot be taken arbitrarily large, particularly at small time levels, if the numerical technique is to satisfactorily approximate the solution of the differential equation. A solution will be obtained but it may not represent the actual physical problem. With large $\Delta T$ it was observed that the values of concentration at the second and third mesh points from the fill were oscillating around the true values, particularly during the initial stage of analysis. It was decided to begin with a small $\Delta T$. A $\Delta T$ giving a value of $\lambda < 1/4$ was observed to be quite adequate at small time levels. Use of this value retains reasonable numerical accuracy. The time increment is made larger as the calculations proceed to higher time levels. An arbitrary criterion for increasing the time increment was used. The time increment was doubled if the maximum difference between the concentration at the end of the whole time increment and at the end of the half-time increment at any point was less than 10% of the initial concentration in the fill. To reduce the approximation error, the time increment was limited to a maximum of $1.2(\Delta X)^2/D_{\text{max}}$. 

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3.1 LIST OF PRINCIPAL VARIABLES

MFIL = Number of mesh points up to end of fill \( (r = r_f) \)

NFIL = Number of mesh points over the depth of fill

MLAND = Number of mesh points up to the radial boundary \( (r = r_s) \)

NLAND = Number of mesh points over the depth of soil

MPIPE = Mesh point number at the location of the vent/trench

NPIPE = Number of mesh points over the depth of vent/trench

KPIPE = Number of mesh points in \( \theta \)-direction

NPIES = Total number of pipes along the circumference

IFROG = Code for using axisymmetric analysis program

\[
\begin{align*}
\text{IFROG} &= 0 \Rightarrow \text{Axisymmetric analysis program} \\
\text{IFROG} \neq 0 &\Rightarrow \text{Cartesian coordinates program}
\end{align*}
\]

NCASE = Code for selecting boundary conditions for code II

\[
\begin{align*}
\text{NCASE} &= 4 \Rightarrow \text{Prescribed concentration at surface} \\
& \quad \text{and at boundary } r = r_s \\
\text{NCASE} &= 5 \Rightarrow \text{Impervious top and prescribed concentration at } r = r_s \\
\text{NCASE} &= 6 \Rightarrow \text{Impervious at } r = r_s, \text{ prescribed concentration at top}
\end{align*}
\]

MTOT = Variable array size. Set MTOT = the dimension of array A in common block. In case the number of mesh points is increased the program capacity can be increased by changing cards 11 and 12 in the MAIN PROGRAM ROUTINE. This arrangement is called a dynamic storage capacity. Variable dimensions used in other subroutines are automatically set from the problem data.

TORT = Tortuosity (dimensionless)

BM = Molecular weight of gas B (g/mole)

AM = Molecular weight of gas A (g/mole)

PR = Total pressure of gas mixture (atmospheres)

TEMP = Temperature in the system (K)

DAB = Bulk diffusion coefficient of gas A through B (cm²·atm/s)
DX = Spatial mesh size (cm)

CO = Mole fraction of component A in the fill during decomposition

TMAX1 = Duration of decomposition (days)

CTOL = Termination mole fraction. Program execution is terminated when the concentration at the farthest point where it is greater than CTOL starts decreasing

CK1 = Convection coefficient for soil surface

CK2 = Surface convection coefficient for boundary \( r = r_s \)

CK3 = Surface convection coefficient for vent top

CK4 = Ratio of effective diffusion coefficient in vent to bulk diffusion coefficient

HRDO = Initial hardness in soil water (mg Ca/l)

PHO = Initial pH value of soil water

S = Degree of saturation (% age)

ALKO = Initial alkalinity

CCO = Initial concentration of CO2 in the soil

NRADII = Number of radii considered for soil

E = Porosity of soil

R = Pore radii of soil

FV = Volumetric fraction

IFREQ = Number of time increments between successive printouts

NSTEP = Maximum number of steps allowed before program termination

DTI = Initial increment of time (days)

TMAX2 = Maximum time allowed before program termination (days)

CDT = Check on opening of time step. Time step is doubled if change between concentrations CA and CSTAR is less than \((CDT \times CO)\) at all points

AK = Knudsen diffusion coefficient
EMDA = \frac{2}{\lambda} = 2(\Delta x)^2/\Delta T

KOUNT = A count on total number of time steps

ICOUNT = A count on number of time steps since last printout

TAU = A count on time

RTS = RT \frac{S}{100 - S} where R = 0.08205, T = temperature (K)

AK1 = K_1, First acidity constant

AK2 = K_2, Second acidity constant

HK = \text{K}_H^*, Henry's law constant for CO₂

SK = \text{K}_S, Solid solution equilibrium constant for CaCO₃

WK = \text{K}_W, Equilibrium constant (ion product) for water

CA = Array of mole fractions \(X_A\) at each grid point

CSTAR = Array of mole fractions \(X^*_A\) at each grid point

DSTAR = Array of mole fraction \(X^{**}_A\) at each grid point

D = Nodal point values of effective diffusion coefficients

A = Array of coefficients on lower codiagonal of coefficient matrix

B = Array of coefficients on the diagonal of coefficient matrix

C = Array of coefficients on upper codiagonal of coefficient matrix

F = Vector containing values on the right hand side of equation

CPRIM = Temporary array used to store mole fractions computed by TRIDAG

BETA = Temporary array used in subroutine TRIDAG

GAMMA = Temporary array used in subroutine TRIDAG

X = Distance along the radius or along depth of soil

ALK = Mesh point values of alkalinity

PH = Mesh point pH values
HRD = Mesh point values of hardness
IC02 = Code for considering chemical reaction
   IC02 = 0  ⇒  No CO2 reaction is considered
   IC02 ≠ 0  ⇒  Chemical reaction is considered
ITOP = Code for specified concentration on top boundary
   ITOP = 0  ⇒  Concentration at top does not change with time
   ITOP ≠ 0  ⇒  Concentration at top is not prescribed
IEND = Code for specified concentration at the boundary r = rs
   IEND = 0  ⇒  Concentration at r = rs does not change with time
   IEND ≠ 0  ⇒  Concentration at r = rs is not prescribed

3.2 CODE I - AXISYMMETRIC

Code I has the capability of solving both the axisymmetric and rectangular cartesian coordinate cases. In general, the axisymmetric code is used, but in cases where the fill is large with a straight boundary and the region of interest is the area close to the fill, a rectangular region approximates the geometry better and gives an upper bound solution for outward excursion of gas. The program has a capacity of handling ten different pore radii; however, more pore radii can be treated by simply increasing the size of the array R and FV in the dimension statement in subroutine SOLV. In the beginning of each time step the effective diffusion coefficient is evaluated at all the mesh points and the maximum allowable ∆T is evaluated depending upon the maximum value of D. The mole fractions in the beginning of each time step are stored in array CA. To solve for mole fractions, CSTAR, the coefficients of the matrix are set for each row. The set of simultaneous equations so obtained for a particular row is solved using a tridiagonal equation solver; and the values of the mole fraction at the end of half time increment, obtained by sweeping over the system radially, are stored in the array CSTAR. Then the sweep in the vertical direction is carried out by solving the set of simultaneous equations for each column of mesh points at a time. This gives the concentrations at the end of the whole time increment. An arbitrary criterion based on limiting the change of mole fraction within a time interval has been found very useful. If the difference between mole fraction at the end of whole time increment and the half time increment is less than 10% of the initial mole fraction, the time step ∆T is doubled subject to a maximum ∆T of 1.2(∆X)²/D_max. Mole fractions are printed out after every IFREQ steps.
After the decomposition time TMAX1, the soil-fill boundary is assumed to be impervious, and a search is made at the end of each step to note the time at which the CTOL (5%) mole fraction point stops moving further. At this stage a detailed printout is obtained for mole fraction around the 5% point.

In the case of diffusion of CO₂ through partially saturated soil, the solution of CO₂ in water generates a chain of reactions (Section 1.1.2). The change of hardness, alkalinity and pH values of water are evaluated by solving a set of simultaneous equations. The details of setting up these equations is given in Section 1.1.2.2. If ICO₂ equals zero, the program does not take into consideration any chemical reaction or solution processes.

At the end of each time increment the CO₂ concentration is evaluated at all mesh points. Any change in concentration affects the chemical equilibrium of the system. A part of the change in mole fraction at a point goes into the solution, thus reducing the mole fraction of CO₂ which would have been there in the absence of chemical reaction. It also decreases the pH value at that point and changes the hardness and alkalinity of water. Thus, the concentrations used during the next time interval will be those obtained after chemical equilibrium. The rate of chemical reaction is very fast when compared to the diffusion process and has been considered as an instantaneous process. The hardness, alkalinity and pH values are printed along with mole fractions. The program is terminated when the mole fraction stops dropping at the farthest point where it reaches the termination mole fraction CTOL as in the case of methane.
3.2.1. **Flow Chart for Code I**

The flow chart given below gives a detail of the execution of Code I.

```
MAIN PROGRAM

START

MFIL, NFIL, MLAND, NLAND,
IPROG, MPIPE, NPIPE, ICO2,
ITOP, IEND, HED

SET UP DUMMY DIMENSIONS
& ARRAYS

CALL SOLVE:
(for setting up coefficients
and printing results)

STOP
```
SUBROUTINE SOLV

ENTER

TORT,BM,AM,PR,TEMP,DAB,DX,CO,TMAX1,
CTOL,CK1,CK2,CK3,CK4,HRDO,PHO,S,
NRADII,Ri,FV1,IFREQ,NSTEP,DTI,TMAX2,CDT,
NCO,TIM1,CPO1

RTS = 0.02205*TEMP
AK1 = 4.446x10^-7
AK2 = 4.688x10^-11
HK = 3.388x10^-2
SK = 4.571x10^-9
WK = 1.0x10^-14
D1 = HRDOx10^-5

B1 = (10^-PH+2.0xD1xWK/H1)/(1.0+2.0xAK2/H1)
ALK0 = B1/2x10^-5
CCO = H1xB1/(AK1xHK)
CK1 = 2.0*AX*CK1
CK2 = 2.0*AX*CK2
CK3 = 2.0*AX*CK3
BAN = 1.0-AM/BM

AK = 9.7x10^-5*TEMP/AM
DKR = DAB/(AKxREQ)

DMAX = \sum_{E=DAB}^{TORT}(1-BAN*CO+DKR)
DTMAX = 1.2*DX*DX/DMAX

INITIALIZE CA_{ij},C^*_{ij},HRD_{ij},PH_{ij},ALK_{ij},X_{ij}
TAU = 0.0,KOUNT = 0,ICOUNT = 0
TAU, KOUNT

FIND DMIN, DMAX, DTMAX

TAU, DTAU, DTMAX, DMIN, DMAX, KOUNT

X1,i, Xj,j, CAi,j

ICO2 = 0

TDAYS, KOUNT, X1,i, Xj,j, ALK1,j, PH1,j, HRD1,j

FIND DMIN, DMAX, DTMAX
TAU < TMAX

LOCATE IMAX where C > 5%
JMAX, CMAX

IMAX, JMAX, CMAX

I2 = C

IMAX > IOLD or for same IMAX and IOLD
CMAX > COLD

IMAX, JMAX, CMAX, TAU, KCONT
i, X_i, CA_{i,j} and CA_{i,j} detailed around (IMAX, JMAX)

IOLD = IMAX
JOLD = JMAX
COLD = CMAX

CDT < MAX |C^*_i,j - CA_{i,j}|

DTAU = 2.0*DTAU
IF (DTAU > DTMAX) DTAU = DTMAX

TAU = TAU + DTAU
KOUNT = KOUNT + 1
ICOUNT = ICOUNT + 1

CALL CFIL(TAU, CO)
Calculation of $C^*$

1. **TAU > TMAX2** or **KOUNT > NSTEP**
   - Calculate $D_{ij}$
   - $j = 1, 2, \ldots, NLAND$

2. **MIN = 1**
   - **MAX = MLAND**

3. **i = 1, 2, \ldots, MLAND**

4. **MFIL**
   - **NFIL**
     - **i < MFIL** and **j < NFIL**
       - **TAU > TMAX1**
         - **MIN = MFIL**
       - **F**
     - **NFIL = NLAND**
       - **i < MFIL**
         - **F**
     - **T**
       - **MIN = MFIL**
     - **F**
   - **T**
     - **F**
   - **F**

5. **CALCULATE COEFFICIENTS $A_i, B_i, C_i$, AND VECTOR $F_i$**

6. **MODIFY FOR PRESCRIBED CONCENTRATIONS**
   - CALL TRIDAG TO GET THE SOLUTION FOR CONCENTRATION $C_{ij}^*$
CALCULATE COEFFICIENTS $A_j, B_j, C_j$ AND VECTOR $F_j$

MODIFY FOR PRESCRIBED CONCENTRATIONS
CALL TRIDAG TO GET THE SOLUTION FOR CONCENTRATIONS $C_{ij}$ AT THE END OF WHOLE TIME INCREMENT
\[ \text{CHEK} = \max_{i,j} |c_{i,j} - c_{i,j}^*| \]

- If \( \text{ICO2} = 0 \), call SOLUTE.

- If \( \text{ICOUNT} = \text{IFREQ} \) or \( \text{TAU} = \text{TMAX1} \), go to 2.

- Otherwise, go to 16.
SUBROUTINE CFIL

8

ENTER

INTERPOLATE CONCENTRATION ON FILL BOUNDARY AT TIME OF ANALYSIS FROM CONCENTRATION HISTORY

RETURN
SUBROUTINE SOLUTE

ENTER

\[ \text{II} = 1, 2, \ldots, \text{NUMNP} \]

15

\[ \text{KKK} = 1 \]

\[ \text{PH} = \text{HP} (\text{II}) \]

\[ \text{ALK} = \text{AKL} (\text{II}) \times 10^{-5} \]

\[ \text{CFA} = \text{CA} (\text{II}) \]

\[ \text{HRD} = \text{HDR} (\text{II}) \times 10^{-5} \]

\[ \text{DCO} = 0 \]

10

\[ \text{KKK} = 21 \]

\[ \text{DCO} = (\text{CO} - \text{C0}) / 20 \]

\[ \text{CFA} = \text{C0} \]

\[ \text{PH} = \text{PHO} \]

\[ \text{ALK} = \text{ALKO} \times 10^{-5} \]

\[ \text{HRD} = \text{HRDO} \times 10^{-5} \]

T

F

KOUNT = 0

10

RETURN

[Flowchart showing the process of initializing, setting up nonlinear equations, solving for variables, updating values, and returning.]
3.2.2 Listing for Code I

Code I consists of five routines including the MAIN program, subroutine SOLV, subroutine TRIDAG, subroutine CFIL and subroutine SOLUTE. The following pages give the program listing. Note that in case of two-dimensional Cartesian coordinates, variables FIIM and FIIP involving the variations in the circumference with radius are set equal to 1.0 because of constant thickness of elements.
PROGRAM DIFFUSION WITH SOLUTION OF CD-2
PROGRAM FINITE DIFFERENCE PROGRAM FOR DIFFUSION PROBLEM
PROGRAMMED BY I.S. RAITH, OHIO STATE UNIVERSITY
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONE/MFIL,NFIL,MLAND,NLAND,MM,IPROG,MPipe,NPipe,KOUNT
1,ICO2,MLCO2,NLCO2,MMCO2,ITOP,IEND
COMMON/TWO/AK1,AK2,SK,WK,HK,C0,CC0,PHD,ALKO,PROD
COMMON/THREE/CFO(20),TIM(20),NCO
DIMENSION HED(16)
COMMON A (6000)
Mtot=60cc

CALL ERRSET (206, 256, -1, 1)

READ (5, 50) MFIL,NFIL,MLAND,NLAND,IPROG,MPipe,NPipe,ICO2,ITOP,IEND
IF(MFIL.EQ.0) GO TO 40
FL=MLAND-1
FF=MFIL-1
R1=FL/FF
FL=NLAND-1
FF=NFIL-1
R2=FL/FF
READ (5, 60) MED
WRITE (6, 80) MED, R1, R2
WRITE (6, 70) MFIL,NFIL,MLAND,NLAND,MPipe,NPipe
MN=MLAND*NLAND
MM=MLAND
IF(NLANP.GT.MM) MM=NLAND
MLCO2=MLAND
NLCO2=NLAND
MMCO2=MN
IF(ICO2.NE.0) GO TO 20
MLCO2=1
NLCO2=1
MMCO2=1

20 M1=1
M2=M1+MN
M3=M2+MN
M4=M3+MN
M5=M4+MM
M6=M5+MM
M7=M6+MM
M8=M7+MM
M9=M8+MM
M10=M9+MM
M11=M10+MM
M12=M11+MLAND
M13=M12+MMCO2
M14=M13+MNC02
M15=M14+MNC02
IF(M15 .LT. MTOT) GO TO 30
JJ=M15-MTOT-1
WRITE (6,90) JJ
GO TO 40

CALL SOLV (A(M1),A(M2),A(M3),A(M4),A(M5),A(M6),A(M7),A(M8),A(M9),A(M10),A(M11),A(M12),A(M13),A(M14))

GO TO 10
STOP

FORMAT (1015)
FORMAT (18A4)
FORMAT (110)
END
SUBROUTINE SOLV (CA, CSTAR, D, A, B, C, F, CPRIM, ETA, GAMMA, X, ALK, PH, HRP)

IMPLICIT REAL*8 (A-H, O-Z)

COMMON/ONE/ MFIL, NFIL, MLAND, NLAND, MM, IPRG, NPIPE, NPIPE, KOUT
1, JCO2, MLCO2, NLC02, NCO2, ITOP, IEND

COMMON/TWO/AK1, AK2, SK, WK, CK, C0, CCO, PH0, ALKO, HRPO

COMMON/THREE/CFO(20), TIM(20), NCO

DIMENSION CA(MLAND, NLAND), CSTAR(MLAND, NLAND), DMLAND, NLAND), AM(NM),
1, B(MM), C(MM), F(MM), CPRIM(MM), ETA(MM), GAMMA(MM), X(NLAND),
2, ALK(MLCO2, NLC02), PH(MLCO2, NLC02), HRP(MLCO2, NLC02)

DIMENSION R(10), FV(10)

DATA STAR/IH* /

KSTOP = 0
MLAND1 = MLAND - 1
MFIL1 = MFIL + 1
NFIL1 = NFIL + 1
MFL = MFIL1
MFIL2 = MFIL12
IF(MFIL1, GT. MLAND) MFIL2 = MLAND
KFIL = NFIL
MPIP1 = MPIPE - 5
MPIP2 = MPIPE + 5
IF(MPIP1, LT, 1) MPIP1 = 1
IF(MPIP2, GT, MLAND) MPIP2 = MLAND
I2 = 0

*** READ MATERIAL PROPERTIES, MESH SIZE AND INITIAL CONCENTRATION

READ (5,860) TORT, BM, AM, PR, TEMP, DAB, DX, CO, Tmax, C0, Ck1, Ck2, Ck3, C
1, K4, HRPO, PH0, S
READ (5,870) NRADI
READ (5,880) (R(I), FV(I), I=1, NRADI)
READ (5,890) IFREQ, NSTEP, DT, Tmax, C0
READ (5,830) NCO, (TIM(I), CFO(I), I=1, NC0)

E = 0.
DO 10 I = 1, NRADI

10 E = E + FV(I)

WRITE (6,900) E, TORT, BM, AM, PR, TEMP, DAB, DX, Tmax, CO, C0, Ck1, Ck2, Ck3, C
13, K4, HRPO, PH0, S
WRITE (6,930) (I, R(I), FV(I), I=1, NRADI)
WRITE (6,840) (TIM(I), CFO(I), I=1, NC0)
C01 = Ck1 * DX ^ 2.0
C02 = Ck2 * DX ^ 2.0
C03 = Ck3 * DX ^ 2.0
C04 = Ck4 * DAB
C05 = E / TORT * DAB * 1.5
FACTOR = 8.4400.000
BAN = 1.0 - DSORT(AM/RM)
AK = 9.7D- 05 * DSQRT(TEMP/AM)
COMAX = 0.00
DO 20 I=1,NC0
IF(CF0(I),GT,COMAX) COMAX=CF0(I)
20 CONTINUE
DMAX=0.DO
DMIN=0.DO
DO 30 K=1,NNMAX
RFO=R(K)
E=FV(K)*(100.-5)/100.
ETPD=EV(ITEMAX/DOMAX)
DKR=DAE/(AK*REP)
DMAX=DMAX+ETPD/(1.DO+RAN*COMAX+DKR)
DMIN=DMIN+ETPD/(1.DO+DKR)
DMAX=1.2*DX*DX/(DMAX*FACTOR)
NMAX=DTSAMAX
DMIN=NTMAX
WRITE (6,940) IFREQ,NSF,STEP,DTI,MAX2,DTMAX
D TAU=DTI
MOUT=(MLAND-2)/12+1
NOUT=(NLAND-2)/12+1
NSTA=(MFIL-1)*9/MOUT+1
IF(IPROG.NE.0) GO TO 40
FP=4.000
WRITE (6,950)
GO TO 50
40 FP=2.000
FII=1.000
FIIIM=1.000
WRITE (6,960)
C
C
50 TAU=0.DO
CDT=CDT+C0
KOUNT=0
COUNT=0
MFII=MFII+1
NFII=NFII+1
CO=CF0(I)
IF(ICO.PE.0) GO TO 60
C0=0.DO
WRITE (6,1080)
GO TO 90
60 WRITE (6,1070)
TPH=10.DO**((-PHO)
RTS=0.08205*TEMP*6/(100.-S)
AK1=4.4460-07
AK2=4.6800-11
HK=3.3FND-02
SK=4.5710-09
WK=1.00D-14
H1=THV
D1=HRDO*1.0D-5
B1=(H1+2.0*HI-WK/H1)/(1.0+2.0*AK2/H1)
ALK0=81/2.0D -0.5
CC0=H1*B)/AK1*HK)

*** SET INITIAL CONDITIONS ............................

DO 70 I=1,MLAND
DO 70 J=1,NLAND
ALK(I,J)=ALK0
PH(I,J)=PHG
70 HRD(I,J)=HRDO

CALL SOLUTE (CA,PH,ALK,HRD,RTS,TAU,TMAX1)
DO 80 I=1,MFILE
DO 80 J=1,NFILE
PH(I,J)=PHG
ALK(I,J)=ALK0
HRD(I,J)=HRDO
80 DO 100 I=1 ,MLAND
X(I)=(I-1)*DX
DO 100 J=1,NLAND
CSTAR(I,J)=CC0
100 CA(I,J)=C0
DO 110 I=1,MFILE
DO 110 J=1,NFILE
CSTAR(I,J)=C0
110 CA(I,J)=C0
WRITE (6,910) TAU,KOUNT
GO TO 140
120 WRITE (6,910) TAU,KOUNT
WRITE (6,980) (X(I),I=MP1,MP2)
WRITE (6,970) (I,I=MP1,MP2)
DO 130 J=1,NLAND
WRITE (6,990) X(J),(CA(I,J),I=MP1,MP2)
WRITE (6,1050) J
130 CONTINUE
WRITE (6,920) TAU,DTAU,DTMAX,DMIN,DMAX,KOUNT
140 WRITE (6,980) (X(I),I=1,MLAND,MOUT)
WRITE (6,970) (I,I=1,MLAND,MOUT)
DO 150 J=1,NLAND,MOUT
WRITE (6,990) X(J),(CA(I,J),I=1,MLAND,MOUT)
WRITE (6,1050) J
IF(J.LE.NFILE) WRITE (6,1060) (STAR,I=1,NSTAR)
150 CONTINUE
IF(ICO2.EQ.0) GO TO 190
WRITE (6,1020) TAU,KOUNT
WRITE (6,980) (X(I),I=1,MLAND,MOUT)
WRITE (6,970) (I,I=1,MLAND,MOUT)
DO 160 J=1,NLAND,MOUT

WRITE (6,990) X(J), (ALK(I,J), I=1,MLAND,MOUT)
WRITE (6,1050) J
IF(J.LE.NFIL) WRITE (6,1060) (STAR, I=1,NSTAR)

CONTINUE
WRITE (6,1030) TAU,KOUNT
WRITE (6,980) (X(I), I=1,MLAND,MOUT)
DO 170 J=1,NLAND,NOUT
WRITE (6,990) X(J), (PH(I,J), I=1,MLAND,MOUT)
WRITE (6,1050) J
IF(J.LE.NFIL) WRITE (6,1060) (STAR, I=1,NSTAR)

CONTINUE
WRITE (6,1040) TAU,KOUNT
WRITE (6,980) (X(I), I=1,MLAND,MOUT)
DO 180 J=1,NLAND,NOUT
WRITE (6,990) X(J), (HR(I,J), I=1,MLAND,MOUT)
WRITE (6,1050) J
IF(J.LE.NFIL) WRITE (6,1060) (STAR, I=1,NSTAR)

CONTINUE
IF(KSTOP.EQ.1) GO TO 250
IF(KOUNT.EQ.0) GO TO 290
IF(CHFkle.LT.DTAU) DTAU=2.0*DTAU
IF(DTAU.GT.DTMAX) DTAU=DTMAX
IF(TAU.GT.TMAX1) GO TO 220
TCHEK=TKMAX-TAU
IF(TCHEK.LT.DTAU) DTAU=TCHEK
IF(DABS(TAU-TMAX1).LT.DTI) DTAU=DTI
GO TO 290

IHAX=1
CHAX=0.DO
DO 240 J=1,KFIL
IHAX=1
DO 230 I=1,MLAND
CIVAL=CIJ
IF(CI.J.LT.CTOL.0R.IHAX.GT.I) GO TO 230
IHAX=I
JHAX=J
CHAX=CIJ
CONTINUE
IF(IHAX.LT.IHAX) GO TO 240
IF(IHAVX.EQ.IHAX.AND.CHAX.GT.CHAX) GO TO 240
CHAX=CHAX
JHAX=JHAX
IHAX=IHAX
CONTINUE
IF(IHAX.GT.IHAX) GO TO 270
IF(IHAX.GT.IHAX.EQ.0) GO TO 280
IF(IHAX.GT.IHAX.EQ.0) GO TO 270
IF(IMAX.FQ.JOLD.AND.JMAX.FQ.JOLD.AND.COLD.LT.CMAX) GO TO 270
IF(IMAX.FQ.JOLD.AND.JMAX.NE.JOLD) GO TO 270
WRITE (6,1010) IMAX,JMAX,CMAX,TAU
WRITE (6,910) TAU,KOUNT
KSTOP=1
GO TO 140
250 CONTINUE
I1=MAX0(1,IMAX-5)
I2=MIN0(MLAND,IMAX+5)
J1=MAX0(1, JMAX-3)
J2=MIN0(NLAND, JMAX+3)
WRITE (6,910) TAU,KOUNT
WRITE (6,980) (X(I),I=11,I2)
WRITE (6,970) (I, I=11,12)
260 CONTINUE...
DO 260 J=J1,J2
WRITE (6,990) X(J),(CA(I,J),I=11,12)
270 CONTINUE
280 I2=1
IOLD=IMAX
JOLD=JMAX
COLD=CMAX
C
290 TAU=TAU+DTAU
KOUNT=KOUNT+1
ICOUNT=ICOUNT+1
CALL CFIL (TAU,CO)
DO 300 I=1,MFLIL
DO 300 J=1,NFLIL
CSTART(I,J)=CO
300 C(A(I,J))=CO
C
... COMPUTE CONCENTRATIONS AT THE END OF HALF TIME INCREMENT
C
IF(TAU.GT.TMAX2.0.OR.KCOUNT.GT.NSTEP) GO TO 820
EMDA=2.0*DX*PX/(DTAU*FACTOR)
DO 310 I=1,MLAND
DO 310 J=1,NLAND
310 D(I,J)=0.D0
DO 320 K=1,NRADI
REQ=R(K)
E=FV(K)*(100.*S/100.*
ETPD=E*DAB/TORT
DKR=DAB/(AK*REQ)
DO 320 I=1,MLAND
DO 320 J=1,NLAND
320 D(I,J)=D(I,J)+ETPD/(1.DO-BAN*CA(I,J)+DKR)
DO 540 J=1,NLAND
IF(ITOP.EQ.0.AND.J.EQ.1) GO TO 540.
MIN=1
MAX=MLAND
DO 480 I=1,MLAND
IF(TAU.GT.TMAX) GO TO 330
IF(I.LE.MFIL.AND.J.LE.NFIL) GO TO 460
330 IF(I.LE.NFIL.AND.J.LE.NFIL) GO TO 470
IF(NFIL.EQ.NLAND.AND.I.LE.MFIL) GO TO 470
DIJ=D(I,J)
IF(CK4.LT.CK5) CK4=DIJ
FIJ=(EMDA-2.*DIJ)*CA(I,J)
IF(I.EQ.1) GO TO 470
IF(HFIL.EQ.NLAND.AND.J.EQ.NFIL) GO TO 450
IF(HFIL.EQ.NLAND.AND.I.EQ.MFIL) GO TO 450
IF(IPROG.NF.0) GO TO 340
FIJ=2*I-2
FIIP=(FIJ+1.)/FIJ
FIIM=(FIJ-1.)/FIJ
FIF=FIJ+2.0
FIM=FIJ-2.0
IF(J.EQ.NLAND) GO TO 440
340 DPRIM=(D(I+1,J)-D(I-1,J))/4.
A(I)=DPRI-M-DIJ*FIIM
B(I)=EMDA+2.*DIJ
C(I)=-DPRI-M-DIJ*FIIP
GO TO 430
350 IF(J.EQ.MPIPE.AND.J.LE.NPIPE) GO TO 360
DPRJR=(DIJ+DPRIVATE)*CA(I,J-1)+FIJ+(DIJ-DPRIVATE)*CA(I,J+1)
GO TO 430
360 IF(J.LT.NPIPE) F(I)=(EMDA-2.0*CK4)*CA(I,J)+CK4*(CA(I,J-1)+CA(I,J+1))
IF(J.EQ.NPIPE) F(I)=(EMDA-CK4-DIJ)*CA(I,J)+CK4*CA(I,J-1)+DIJ*CA(I,J+1)
GO TO 480
370 IF(J.EQ.MPIPE) GO TO 380
F(I)=DIJ+D(I,J+1)*CA(I,J+1)+FIJ+(DIJ-D(I,J+1))*CA(I,J)+CK1*(CCN-I*CA(I,J))
GO TO 480
380 F(I)=EMDA-2.0*CK4-CK3)*CA(I,J)+2.0*CK4*CA(I,J+1)*CK3*CCN
GO TO 480
390 F(I)=2.0*DIJ*CA(I,J+1)+FIJ
GO TO 480
400 IF(J.EQ.NPIPE) GO TO 410
F(I)=2.0*DIJ*CA(I,J-1)+FIJ
GO TO 480
410 F(I)=EMDA-2.0*CK4)*CA(I,J)+2.0*CK4*CA(I,J-1)
GO TO 480
C
420 B(I)=EMDA*FP*DIJ
C(I)=-FP*DIJ
430 IF(J.EQ.1) GO TO 370
IF(J.EQ.NLAND) GO TO 400
IF(J.EQ.NFIL.AND.I.LE.MFIL) GO TO 390
GO TO 350
C
440 FFJ=FIJ/FII*DIJ+D*(I-1,J)
A(I)=-FFJ
B(I)=EMP+FFJ*CK2/FII
FIJ=FIJ*CK2/FII*CC0
GO TO 430
450 B(I)=EMP+2*DD0*DIJ
C(I)=-2.000*DIJ
GO TO 430
C
460 MIN=MFIL1
GO TO 480
470 MIN=MFIL
480 CONTINUE
C
490 IF(IEND.EQ.0) MAX=MLAND-1
IF(MIN.GT.MAX) GO TO 540
IF(MIN.EQ.MFIL.AND.MAX.EQ.MFIL) GO TO 540
DO 500 I=MIN,MAX
IF(I.EQ.1) GO TO 500
IF(TAU.GT.TMAX1) GO TO 490
IF(I.NE.MIN) GO TO 490
F(I)=F(I)-A(I)*CA(I-1,J)
500 CONTINUE
IF(MIN.EQ.MAX) GO TO 510
CALL TRIDAG (MIN,MAX,A,B,C,F,CPRIM,BETA,GAMMA,WM)
GO TO 520
510 CPRIM(MIN)=F(MIN)/B(MIN)
520 CONTINUE
DO 530 I=MIN,MAX
530 CSTAR(I,J)=CPRIM(I)
540 CONTINUE
IF(TAU.GT.TMAX1) MFIL=MFIL
C
... COMPUTE CONCENTRATIONS AT THE END OF WHOLE TIME INCREMENT
C
570 CONTINUE
DO 790 I=1,MLAND
IF(IEND.EQ.0.AND.I.EQ.MLAND) GO TO 790
MIN=I
MAX=MLAND
FII=2*I-2
FIP=FII+2
FIH=FII-2.0
570 CONTINUE
DO 740 J=1,NLAND
IF(TAU.GT.TMAX1) GO TO 550
IF(LE.LT.NFIL.AND.J.LE.NFIL) GO TO 710
550 IF(I.GT.TMFL.AND.J.LT.NFIL) GO TO 720
IF(MFIL.EQ.NLALND.AND.J.LT.NFIL) GO TO 720
IF(NFIL.EQ.NLALND.AND.I.LT.MFIL) GO TO 720
DIJ=D(I,J)
IF(CK4.LT.CK5) CK4=DIJ
FIJ=(EMDA-2.*DIJ)*CSTAR(I,J)
IF(I.EQ.NLAND) FIJ=(EMDA-FIM/DIJ-D(I-1,J))*CSTAR(I,J)
IF(I.EQ.1) GO TO 620
IF(J.EQ.NLAND) GO TO 650
IF(MFIL.EQ.NLAND.AND.J.EQ.NFIL) GO TO 640
IF(J.EQ.NFIL.AND.I.LT.MFIL) GO TO 640
IF(I.EQ.NPIPE.AND.J.LE.NPIPE) GO TO 560
DPRJM=(D(I,J-1)-D(I,J-1))/4.
A(J)=DPRJM-DIJ
B(J)=EMDA+2.*DIJ
C(J)=-DIJ
GO TO 580
560 A(J)=-CK4
IF(J.EQ.NPIPE) GO TO 570
B(J)=EMDA+2.*CK4
C(J)=-CK4
GO TO 580
570 B(J)=EMDA+CK4+DIJ
C(J)=DIJ
GO TO 580
580 IF(I.EQ.1) GO TO 610
IF(I.EQ.NFLIL.AND.J.LE.NFIL) GO TO 690
IF(I.EQ.NLAND) GO TO 700
590 DPRIM=(D(I+1,J)-D(I,J))/4.
IF(IPROG.NE.0) GO TO 600
FIIP=(FIJ+1)/FIJ
FIIM=(FIJ-1)/FIJ
600 FIJ=(DIJ*FIIM-DPRI4)*CSTAR(I-1,J)+FIJ+(DIJ=FIIP+DPRI4)*CSTAR(I+1,J)
GO TO 740
610 FIJ=(EMDA-FP*DIJ)*CSTAR(I,J)+FP*DIJ*CSTAR(I+1,J)
GO TO 710
620 IF(ITOP.NQ.0) GO TO 730
IF(I.EQ.NPIPE) GO TO 630
B(J)=DIJ+DIJ+1*CK1+EMDA
C(J)=-DIJ-D(I,J+1)
FIJ=FIJ+CK1*C0
GO TO 670
630 B(J)=2.*CK4+CK3+EMDA
C(J)=-2.*CK4
FIJ=(EMDA-2.*DIJ)*CSTAR(I,J)+CK3*C0
GO TO 670
640 B(J)=EMDA+2.*DIJ
C(J)=-2.0*DIJ
GO TO 670
650 IF(I.EQ.MPIPE.AND.J.EQ.NPIPE) GO TO 660
A(J)=-2.0*DIJ
B(J)=EMDA+2.0*DIJ
GO TO 670
660 A(J)=-2.0*CK4
B(J)=2.0*CK4+EMDA
670 IF(I.EQ.1) GO TO 660
IF(I.EQ.KFIL.AND.J.LE.NFIL) GO TO 690
IF(I.EQ.MLAND) GO TO 700
GO TO 590
680 F(J)=(EMDA-FP*DIJ)*CSTAR(I,J)+FP*DIJ*CSTAR(I+1,J)
GO TO 740
690 F(J)=2.0*DIJ*CSTAR(I+1,J)+FIJ
GO TO 740
700 FFJ=FIN/FI*DIJ+D(I-1,J)
F(J)=FFJ*CSTAR(I-1,J)+FIJ*CK2*(CCD-CSTAR(I,J))/FIN
GO TO 740
710 IF(TAU.GT.TMAX1) GO TO 720
MIN=NFIL
GO TO 740
720 MIN=NFIL
GO TO 740
730 MIN=2
740 CONTINUE
IF(MIN.GT.MAX) GO TO 790
IF(MIN.EQ.NFIL.AND.MAX.EQ.NFIL) GO TO 700
J=MIN
IF(J.EQ.1.OR.J.EQ.NFIL) GO TO 750
F(J)=F(J)-A(J)*CSTAR(I,J-1)
750 CONTINUE
IF(MIN.EQ.MAX) GO TO 77 760
CALL TRIDAG (MIN,MAX,A,R,C,F,CPRIM,BETA,GAMMA,MK)
GO TO 770
760 CPRIM(MIN)=F(MIN)/B(MIN)
770 CONTINUE
DO 780 J=MIN,MAX
780 CA(I,J)=CPRIM(J)
790 CONTINUE
C
CHEK=0.
DO 800 I=1,MLAND1
DO 800 J=2,NLAND
CDIF=DABS(CSTAR(I,J)-CA(I,J))
IF(CDIF.GT.CHEK) CHEK=CDIF
800 CONTINUE
C
*** PRINT CONCENTRATIONS .......... 
IF(CO2.EQ.0) GO TO 810
CALL SOLUTE (CA,PH,ALK,HRD,RTS,TAU,TMAX1)
810 IF(DARS(TAU-TMAX1).LT.DTAU) ICOUNT=IFREQ
811 IF(ICOUNT.NE.IFREQ) GO TO 210
812 I_COUNT=0
813 GO TO 120

C

820 RETURN

C

830 FORMAT (15/(2F10.0))
840 FORMAT ('HISTORY OF FILL CONCENTRATIONS'/10 TIME (DAYS) VOL
1E FRACTION'/(' ',2F15.2/))
860 FORMAT (F10.0)
870 FORMAT (15)
880 FORMAT (2F10.0)
890 FORMAT (215,3F10.0)
900 FORMAT (45H POROSITY OF SOIL (DIMENSIONLESS) = ,F10.7/45H
1 TORTUOSITY (DIMENSIONLESS) = ,F10.7/45H MOLECULAR
2WEIGHT OF GAS B (GM/MOLE) = ,F10.7/45H MOLECULAR WEIGHT OF G
3AS A (GM/MOLE) = ,F10.7/45H PRESSURE (ATMOS)
4 = ,F10.7/45H TEMPERATURE (DEG KELVIN)
5 = ,F10.7/45H BULK DIFFUSION COEFFICIENT (CM SEC ATMS/SEC) = ,F10.7/45H
6 SPATIAL MESH SIZE (CM) = ,F10.7/45H DECOMPOSITION
7ION TIME (DAYS) = ,F10.7/45H INITIAL MOLE FRACTION
8 IN FILL = ,F10.7/45H TERMINATION MOLE FRACTION
9 = ,F10.7/45H SURFACE PERMEABILITY COEFFICIENT
$ = ,E10.3/45H END PERMEABILITY COEFFICIENT
$ PERMEABILITY COEFFICIENT FOR THE VENT = ,F10.7/45H PERMEABILITY
$TY MULTIPLIER FOR THE VENT = ,E10.3/45H INITIAL HARDNESS
$ = ,F10.7/45H INITIAL PH VALUE
$ = ,F10.7/45H DEGREE OF SATURATION
910 FORMAT (31H1MOLE FRACTION AT TIME (DAYS) = ,F9.1//14H STEP NUMBER =
1,15/)
920 FORMAT (31H1MOLE FRACTION AT TIME (DAYS) = ,F9.1,2X,12HDTAUJ (DAYS)
1=F6.1,2X,14HDTMAX (DAYS) = ,F6.1,7X,11HDTIJ (MIN) = ,E10.7,7X,11HDTIJ
2 (MAX) = ,E10.3//14H STEP NUMBER = ,15/)
930 FORMAT (' NUMBER PORE RADIUS VOLUMETRIC FRACTION'/17,7X,F12.2,
11X,F10.4/)
940 FORMAT (45H NUMBER OF STEPS BETWEEN PRINTOUTS = ,110//45H MAX
1IMUM NUMBER OF STEPS ALLOWED = ,110//45H INITIAL DTAU (DAYS)
2 (MAX) = ,F10.1//45H MAXIMUM TIME ALLOWED (DAYS) = ,1,2*DX*DXX/DIJ(M
4AX) = ,F10.1/)
950 FORMAT (' AXISYMMETRIC FLOW PROGRAM')
960 FORMAT (' 2-DIMENSIONAL FLOW PROGRAM')
970 FORMAT (' (CM),12I9')
980 FORMAT (' DISTANCE ',1P13E9.2)
990 FORMAT (10I,1PE9.2,4X,13E9.2)
1000 FORMAT (' * H/6=IMAX=xI3,5X,6H J=xI3,5X,17HMOMLE FRACTION = ,1P
IE15.5)
1010 FORMAT (''-1,1/6H-I\$X=,T3,5X,6H J =,I3,5X,17H\$OLF FR\$ACTION = .1P
1E15.5/49H CONCENTRATION STOPS INCREASING AT TIME (DAYS) = ,NF6F10.1
2)
1020 FORMAT (31H1ALKALINITY AT TIME (DAYS) = ,E9.1/14H STEP NUMBER =
1,15/)
1030 FORMAT (31H1PH VALUE AT TIME (DAYS) = ,E9.1/14H STEP NUMBER =
1,15/)
1040 FORMAT (31H1HARDNESS AT TIME (DAYS) = ,E9.1/14H STEP NUMBER =
1,15/)
1050 FORMAT (',I3)
1060 FORMAT (',14X,PO1)
1070 FORMAT (' CHEMICAL REACTION CONSIDERED')
1080 FORMAT (' CHEMICAL REACTION NOT CONSIDERED')
END
SUBROUTINE TRIDAG (IF, L, A, B, C, D, V, BETA, GAMMA, MM)

IMPLICIT REAL*6 (A-H, O-Z)
DIMENSION A(MM), B(MM), C(MM), D(MM), V(MM), BETA(MM), GAMMA(MM)

BETA(IF) = D(IF)
GAMMA(IF) = D(IF) / BETA(IF)
IFP1 = IF + 1
DO 10 I = IFP1, L
BETA(I) = B(I) - A(I) * C(I - 1) / BETA(I - 1)
10 GAMMA(I) = (D(I) - A(I) * GAMMA(I - 1)) / BETA(I)
V(L) = GAMMA(L)
LAST = L - IF
DO 20 K = 1, LAST
I = L - K
20 V(I) = GAMMA(I) - C(I) * V(I + 1) / BETA(I)
RETURN
END
SUBROUTINE SOLUTE (CA, HP, AKL, HDR, RTS, TAU, TMAX)

THIS SUBROUTINE COMPUTES REDISTRIBUTION OF CONCENTRATIONS
AFTER CHEMICAL REACTIONS

IMPLICIT REAL*8 (A-H, O-Z)
COMMON/ONE/MFIL, NFIL, MLAND, NLAND, MM, IPROG, MPIPE, NPIPE, KOUNT
1, IC02, MLC02, MLC02, MNC02, ITOP, IEND
COMMON/TWO/AK1, AK2, SK, HK, CO, CCO, PHT, AKNO, HRDO
DIMENSION CA(MLAND, NLAND), HP(MLAND, NLAND), AKL(MLAND, NLAND),
HDR(MLAND, NLAND), A(4,4), B(4), BO(6)
TOL=1.0D-18
N=4
DO 130 11=1, MLAND
DO 130 JJ=1, NLAND
IF(KOUNT.EQ.0) GO TO 20
IF(TAU.GT.TMAX) GO TO 10
IF(II.LE.MFIL.AND.JJ.LE.NFIL) GO TO 130
10 IF(II.LT.MFIL.AND.JJ.LT.NFIL) GO TO 130
KKK=1
PH=HP(II, JJ)
ALK=AKL(II, JJ)*2.0D-05
CFA=CA(II, JJ)
HRD=HDR(II, JJ)*1.0D-05
DC0=0.0D0
GO TO 30
20 DC0=(CO-CCO)/20.0D0
CFA=CCO
PH=PHT
ALK=ALK0*2.0D-05
HRD=HRDO*1.0D-05
KKK=21
30 DO 40 I=1, 6
40 DO1=0.0D0
TPH=10.0D0**(-PH)
DO 120 KK=1, KKK
CFA=CFA+DCO
C0=AK2*ALK/TPH
C9=WK/TPH
C10=HRD+C8
C1=TPH*ALK/AK1-HK*CFA
C2=1.0D0+HK+RTS
C3=AK1*(1.0D0-C2)/C2-TPH-ALK
C4=TPH-ALK
C5=AK2-C8
C6=AK2+C8+TPH
C7=AK1+C1/C2
50 B1=-C3*B0(1)-C4*B0(2)+B0(1)**2-B0(2)**2+C7*ALK+B0(4)+B0(1)*B0(4)
1-B0(2)*B0(4)
B2=-C5*B0(1)+C6*B0(2)+TPH*B0(3)+C8*B0(4)+B0(1)*B0(2)+B0(2)**2+B0(4)

1(2)*BO(4)+EO(1)*BO(3)+BO(2)*EO(3)+BN(3)*BO(4)
B(3)=-HRD*EO(2)-C1*BO(3)-EO(2)+EO(3)-EO(3)**2
B(4)=C9*BO(1)-C9*BO(2)-(C9+TPH)*BO(4)-BO(1)+AN(4)-AN(2)*AN(4)-PD
14)**2
IF(DABS(B(1)).GT.TOL) GO TO 60
IF(DABS(B(1)).GT.TOL) GO TO 60
IF(DABS(B(1)).GT.TOL) GO TO 60
IF(DABS(B(1)).GT.TOL) GO TO 60
GO TO 110
60 A(1,1)=C3-2.000*BO(1)-BO(4)
A(1,2)=C4+2.000*BO(2)+BO(4)
A(1,3)=0.D0
A(1,4)=-ALK-EO(1)+EO(2)
A(2,1)=C5-BO(2)-BO(1)
A(2,2)=-C6-BO(1)-2.000*BO(2)-BO(3)-BO(4)
A(2,3)=-TPH-EO(1)-EO(2)-BO(4)
A(2,4)=-C8-BO(2)-BO(3)
A(3,1)=0.D0
A(3,2)=PRN+RO(3)
A(3,3)=C1*BO(2)+2.000*PO(3)
A(3,4)=0.D0
A(4,1)=C9+BO(4)
A(4,2)=A(4,1)
A(4,3)=0.D0
A(4,4)=C9+TPH+PO(1)+PO(2)+2.000*BO(4)
DO 70 I=2,N
DO 70 J=1,N
R=A(J,1-I)/A(I-1,1-I)
B(J)=B(J)-R*B(I-1)
DO 70 K=I,N
70 A(J,K)=A(J,K)-R*A(I-1,K)
DO 80 I=2,N
K=N-I+2
R=B(K)/A(K,K)
DO 80 J=1,N
L=N-J+1
80 B(L)=B(L)-R*A(L,K)
DO 90 I=1,N
90 B(I)=B(I)/A(I,I)
DO 100 I=1,N
100 BO(I)=BO(I)+B(I)
GO TO 50
110 BO(N+1)=(BO(1)-C1)/C2
BO(N+2)=BO(N+1)*RTS
ALK=ALK+EO(1)-BO(2)
TPH=TPH+BO(1)+BO(2)+BO(4)
HRD=HRD+RO(3)
CAA=CFA-PO(6)
IF(KK.EQ.20) DCO=BO(6)*BO(6)/DCD
120 CONTINUE
IF(KOUNT.EQ.0) GO TO 140
AKL(I,J,J)=ALK/2.00-05
HP(I,J,J)=-DLOG10(TPH)
CA(I,J,J)=CAA
HDR(I,J,J)=HRD/1.00-05
130 CONTINUE
RETURN
140 PHO=-DLOG10(TPH)
ALKO=ALK/2.00-05
HRDO=HRD/1.00-05
RETURN
C
END
SUBROUTINE CEIL (TAU, CO)
IMPLICIT REAL*P (A-H,O-Z)
COMMON/THREE/CFO(20), TIM(20), NCO
C
C  THIS SUBROUTINE COMPUTES APPLIED MOLE FRACTIONS FROM GIVEN HISTORY
C
DO 10 I=1, NCO
IF (TAU.F0.0.DO) GO TO 20
IF (TAU - TIM(I)) 30, 30, 10
10 CONTINUE
20 CO = CFO(I)
GO TO 40
30 TX = (TAU - TIM(I-1))/(TIM(I) - TIM(I-1))
CO = CFO(I-1) + (CFO(I) - CFO(I-1)) * TX
40 CONTINUE
RETURN
END
3.2.3 Instructions for Data Preparation for Code I

The following sequence of punched cards will carry the problem data for input to the program.

**Card 1: Control Data (7I5)**

<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of mesh points to the end of the fill (MFIL)</td>
<td>1-5</td>
</tr>
<tr>
<td>Number of mesh points to the bottom of the fill (NFIL)</td>
<td>6-10</td>
</tr>
<tr>
<td>Number of mesh points to the end of the soil boundary (MLAND)</td>
<td>11-15</td>
</tr>
<tr>
<td>Number of mesh points to the bottom of the soil (NLAND)</td>
<td>16-20</td>
</tr>
<tr>
<td>Program Code (IPROG)</td>
<td>21-25</td>
</tr>
<tr>
<td>IPROG = 0 =&gt; Axisymmetric code</td>
<td></td>
</tr>
<tr>
<td>IPROG ≠ 0 =&gt; Cartesian coordinate code</td>
<td></td>
</tr>
<tr>
<td>Mesh point number at the location of a vent radially (MPIFE)</td>
<td>26-30</td>
</tr>
<tr>
<td>Number of mesh points to the bottom of a vent (NPIFE)</td>
<td>31-35</td>
</tr>
<tr>
<td>Code for considering chemical reaction (ICO2)</td>
<td>36-40</td>
</tr>
<tr>
<td>ICO2 = 0 =&gt; No chemical reaction considered</td>
<td></td>
</tr>
<tr>
<td>ICO2 ≠ 0 =&gt; Chemical reaction considered</td>
<td></td>
</tr>
<tr>
<td>Code for prescribed surface concentrations (ITOP)</td>
<td>41-45</td>
</tr>
<tr>
<td>ITOP = 0 =&gt; Surface concentration prescribed</td>
<td></td>
</tr>
<tr>
<td>ITOP ≠ 0 =&gt; Surface concentration not prescribed</td>
<td></td>
</tr>
<tr>
<td>Code for prescribed concentration at boundary ( r = r_s ) (IEND)</td>
<td>46-50</td>
</tr>
<tr>
<td>IEND = 0 =&gt; Concentration prescribed at ( r = r_s )</td>
<td></td>
</tr>
<tr>
<td>IEND ≠ 0 =&gt; Concentration not prescribed at ( r = r_s )</td>
<td></td>
</tr>
</tbody>
</table>

**Card 2: Title Card (18A4)**

This card gives the arbitrary descriptive identification of the job.

**Card Set A:** Material properties, mesh size and initial mole fraction of gas in the fill (8G 10.0)

This set consists of three cards containing the following information in the order described below:
<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tortuosity (TORT) (dimensionless)</td>
<td>1-10</td>
</tr>
<tr>
<td>Molecular weight of gas B (BM) (g/mole)</td>
<td>11-20</td>
</tr>
<tr>
<td>Molecular weight of gas A (AM) (g/mole)</td>
<td>21-30</td>
</tr>
<tr>
<td>Total pressure of mixture of gases (PR) (atm)</td>
<td>31-40</td>
</tr>
<tr>
<td>Temperature of mixture of gases (TEMP) (K)</td>
<td>41-50</td>
</tr>
<tr>
<td>Bulk diffusion coefficient (DAB) (cm² atm/s)</td>
<td>51-60</td>
</tr>
<tr>
<td>Spatial mesh size (DX) (cm)</td>
<td>61-70</td>
</tr>
<tr>
<td>Initial mole fraction of gas in fill (CO)</td>
<td>71-80</td>
</tr>
<tr>
<td>Period of decomposition (TMAX1) (days)</td>
<td>1-10</td>
</tr>
<tr>
<td>Termination mole fraction (CTOL) (dimensionless)</td>
<td>11-20</td>
</tr>
<tr>
<td>Convection coefficient for surface of soil (CK1) (cm·atm/s)</td>
<td>21-30</td>
</tr>
<tr>
<td>Convection coefficient for the boundary ( r = r_s ) (CK2) (cm·atm/s)</td>
<td>31-40</td>
</tr>
<tr>
<td>Convection coefficient for the vent top (CK3) (cm·atm/s)</td>
<td>41-50</td>
</tr>
<tr>
<td>Ratio of effective diffusion coefficient in vent to bulk diffusion coefficient (CK4) (dimensionless)</td>
<td>51-60</td>
</tr>
<tr>
<td>Initial hardness of soil water (HRDO) (mg Ca/l)</td>
<td>61-70</td>
</tr>
<tr>
<td>Initial pH - value of soil water (PHO)</td>
<td>71-80</td>
</tr>
<tr>
<td>Degree of saturation (S) ( \frac{\text{volume of water}}{\text{volume of voids}} \times 100 )</td>
<td>1-11</td>
</tr>
</tbody>
</table>

**Card 6:**

This card gives the total number of pore radii (RADII) considered for the soil (15).

<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total number of pore radii (NRADII)</td>
<td>1-5</td>
</tr>
</tbody>
</table>
Card Set B:

This set of cards gives the information about pore size distribution. A total number of NRADII cards, each containing the following information is required (2F 10.0).

**Information**

- Pore radius ($R_i$) (Å) 1-10
- Volumetric fraction ($FV_i$) (dimensionless) 11-20

**Printing and Program Termination Control Information**

One card containing the control information regarding printing of results and the termination of program is required (2I5, 3F 10.0).

**Information**

- Number of time steps between successive printouts of results (IFREQ) 1-5
- Maximum number of steps allowed before program termination (NSTEP) 6-10
- Time increment at the start of program (DTI) (days) 11-20
- Maximum time allowed for program termination (TMAX2) (days) 21-30
- Percentage change in mole fraction governing opening up of time increment (CDT) (dimensionless) 31-40

Card Set C: History of concentrations on the fill boundary (I5/(2F 10.0))

This set gives the concentration history on the fill boundary, during the decomposition period $TMAX1$, in the following sequence.

Card 1:

**Information**

- Number of points on the concentration history curve (NCO) 1-5

Set of NCO cards, each containing the following information

**Information**

- Time (TIM) (days) 1-10
- Mole fraction on the boundary of fill (CFO) (dimensionless) 11-20
In case more than one problem is to be solved, the data for the subsequent problems may be input in the sequence given above. The input is terminated by putting a blank card at the end of a problem data set.

3.2.4 Example Problem I - Diffusion of Methane

A typical fill covers an area of 20 acres. It can be approximated by a circle with a radius of 160 meters. The depth of the fill is 16 meters below the ground surface. For diffusion of methane through air the coefficient of bulk diffusion at 25°C and atmospheric pressure is 0.226 (cm² atm/s). The mole fraction of methane in the fill during decomposition process of five years is assumed to be at 0.70. A soil saturation of $k_{sat}$ was used. A spatial mesh size of 800 cm is used. The surface permeability coefficient is taken as $3.98 \times 10^{-5}$ gm mole/cm², which is the mass transfer coefficient for water evaporation due to a wind velocity of 5 mph measured at 3 m above ground surface.

3.2.4.1 Input--

The following data input were used for the problem.

<p>| | | | | | | |</p>
<table>
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<tr>
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<td>0.7</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.0</td>
<td>0.7</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>3</td>
<td>400000.0</td>
<td>0.40</td>
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<tr>
<td>40.</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>1825.0</td>
<td>0.05</td>
<td>3.98E-05</td>
<td>0.0</td>
<td>3.98E-05</td>
<td>1.0</td>
<td>25.0</td>
</tr>
<tr>
<td>0.25</td>
<td>25.0</td>
<td>15.05</td>
<td>1.0</td>
<td>290.0</td>
<td>0.226</td>
<td>800.0</td>
</tr>
</tbody>
</table>

3.2.4.2 Output--
3.2.4.2 Output—

Appendix A contains the computer output giving the results for this problem. The first page gives the input parameters while the next page gives the initial mole fraction of gas in the soil. The fill area has been underlined with asterisks. The distances along the radius and along the depth are in centimeters. Under each figure giving the distance is the corresponding column or row number of the mesh point. The third and fourth pages give the mole fraction at the end of the decomposition time and the fifth and sixth pages give the mole fraction at the time when mole fraction at the farthest point where it exceeds CTOL starts dropping.
3.2.5 Example Problem II - Diffusion of CO₂

The diffusion process is essentially the same as in Problem I. However, the mole fraction of CO₂ in the fill during decomposition period is assumed to stay at 0.30, and the coefficient of bulk diffusion for CO₂ through air at 25°C and atmospheric pressure is 0.158. The initial hardness of soil water was taken as 75.0 (mg Ca/l) with a pH value of 6.5 and degree of saturation of 40%. This gives a mole fraction of 3.15% of CO₂ in the soil for chemical equilibrium. The alkalinity of soil water is about 75.0 initially.

3.2.5.1 Input--

The following input data cards were used for example problem.

```
1 1.825 0.3
  0.0 0.3
2 500.0 1.0 736000.0 0.01
1 460000.0 0.40
  40.0
1 1.825 0.05 3.9910E-05 0.0 3.9610E-05 1.0 75.0 6.5
  2.33 28.8 44.60 1.0 250.0 0.158 800.0 0.30
```

```
```

DIFFUSION OF CO₂ THROUGH GRANULAR MATERIAL

```

```
3.2.5.2 Output--

As detailed in Section 3.2.4.2 Appendix B has been reproduced from a computer output. The first page gives the input parameters. The next four pages give the initial mole fraction, alkalinity, pH value and hardness in the soil. The corresponding values at the end of decomposition and at the termination of the program are given on the last ten pages.
3.3 CODE II - THREE DIMENSIONAL AXISYMMETRIC WITH PARTIALLY PENETRATING VENTS

In order to render sanitary landfill operations safer by reducing movement of landfill gases into the ground, venting pipes or continuous trenches may be used. A continuous trench problem can be directly solved by using Code I. Code II requires about three to four times the computer time and, as such, should be used only when Code I cannot be used. Code II must be used when venting pipes or wells are used.

The general format of the program is similar to Code I, the only difference being the requirement of three-dimensional arrays for storing mesh point values of C, C*, C** and D, and the complete cycle requiring a sweep in the θ direction in addition to the r- and z-direction sweeps. The set of equations (85a) through (110c) have been programmed in this Code. The equations ending with a apply for sweep in the r direction and give values C*; equations ending with b apply to sweep in the z direction and give values C**; and equations ending with c apply to sweep in the θ direction and give the values of mole fraction at the end of whole time increment.

To study the effectiveness of a vent, a provision is included to input the parameter for vent effectiveness. As in Code I, the maximum value of the time increment is kept below 1.2 (ΔX)^2/D_{max} and the time step is increased if the maximum difference between the mole fraction at the end of interval and C** is less than 10% of initial mole fraction. Six different sets of boundary conditions have been incorporated. The parameter NCASE is used to select a particular set of boundary conditions.

- **NCASE = 1 to 3** Landfill is treated as same as surrounding soil after decomposition period.
- **NCASE = 4 to 6** Landfill soil boundary is treated as an impervious boundary after the decomposition stops.
- **NCASE = 1, 4** Prescribed zero mole fraction on soil surface and boundary r = r_s.
- **NCASE = 2, 5** Prescribed zero mole fraction at boundary r = r_s with impervious soil top.
- **NCASE = 3, 6** Prescribed zero mole fraction at soil surface with impervious boundary at r = r_s.

A parameter NPIPS is used to give a total number of pipes along the circumference. A slice subtending an angle equal to π/NPIPS is divided by KPIPE mesh points in the θ direction. The axis (r = 0) being a singular point, is excluded from analysis. To accomplish this the boundary r = ΔX is approximated as an impervious boundary.
3.3.1 Flow Chart for Code II

The flow chart given below outlines the execution sequence of Code II.

MAIN PROGRAM

START

\[ \text{MFIL, NFIL, MLAND, NLAND, NCASE,}
\begin{align*}
\text{MPIPE, NPIPE, KPIPE, NPIPS, NPROG,}
\end{align*}
\text{HED} \]

SET UP DUMMY DIMENSIONS & ARRAYS

CALL SOLV
(for setting up coefficients and printing results)

STOP
SUBROUTINE SOLV

ENTER

TORT, BM, AM, FR, TEMP, DAB, DX, CO, TMAX1, CTOL, NRADII, R1, FV1, IFREQ, NSTEP, DTU, TMAX2, CDIT

BAN = 1.0 - \sqrt{AM/BM}
AK = 9.7 \times 10^{-5} \sqrt{TEMP/AM}
DKR1 = DAB/(AK*REQ)
DVi*DAB
D TORT* (1-BAN*CO+DKRI)

DTMAX = 1.2*DX+DX/DMAX
DTHET = \pi/NPI/PS/(KPIPE-1)

INITIALIZE CA1,jk, C*i,jk, C**j,k, X1, TAU = 0.0, KCONT = 0, ICONT = 0

IF KCONT > 0

FIND DMIN, DMAX, DTMAX

TDAYS, THETA, KCONT

20

IF KCONT > 0

FIND DMIN, DMAX, DTMAX

TDAYS, DTDAY, DTMAX, DMIN
D MAX, THETA, KCONT
CALCULATE \( D_{ijk} \)

CALCULATE COEFFICIENTS \( A_i, B_i, C_i \) AND VECTOR \( F_i \). MODIFY FOR PRESCRIBED CONCENTRATIONS AT THE BOUNDARY, CALL TRIDAG TO GET SOLUTION FOR CONCENTRATIONS \( C^* \)

CALCULATE COEFFICIENTS \( A_j, B_j, C_j \) AND VECTOR \( F_j \). MODIFY FOR PRESCRIBED CONCENTRATIONS AT THE BOUNDARY, CALL TRIDAG TO GET SOLUTION FOR CONCENTRATIONS \( C^{**} \)

CALCULATE COEFFICIENTS \( A_k, B_k, C_k \) AND VECTOR \( F_k \). MODIFY FOR PRESCRIBED CONCENTRATIONS AT THE BOUNDARY, CALL TRIDAG TO GET SOLUTION FOR CONCENTRATION AT THE END OF WHOLE TIME INCREMENT

\( I\text{COUNT} = I\text{FREQ} \) or \( T\text{AU} = T\text{MAX}1 \)

\( T \) or \( F \)

4
3.3.2 Listing for Code II

Code II consists of three subroutines including the MAIN program, subroutine SOLV and subroutine TRIDAG. The following pages include the program listings.
PROGRAM DIFFUSION AXISYMMETRIC WITH PENETRATING VENTS

FINITE DIFFUSION PROGRAM FOR DIFFUSION PROBLEM

PROGRAMMED BY I.S.RAI

IMPLICIT REAL*8 (A-H,O-Z)

COMMON/MFIL,NFIL,MLAND,NLAND,MM,NCASE,MPIPE,NPIPE,KPIPE,NPIPS,1,NPROG

DIMENSION HED(18)

COMMON A(8000)

HTOT=8000

CALL ERRSET(208,256,-1,1)

READ (5,40) MFIL,NFIL,MLAND,NLAND,NCASE,MPIPE,NPIPE,KPIPE,NPIPS,NPROG

IF(MFIL.EQ.0) GO TO 30

FL=MLAND-1

FF=MFIL-1

R1=FL/FF

FL=NLAND-1

FF=NFIL-1

R2=FL/FF

READ (5,50) HED

WRITE (6,70) HED,R1,R2,NCASE

WRITE (6,60) MFIL,NFIL,MLAND,NLAND,NPIPE,NPIPS

MN=MLAND*NLAND*KPIPE

MM=MAXO(MLAND,NLAND,KPIPE)

M1=1

M2=M1+MN

M3=M2+MN

M4=M3+MN

M5=M4+MN

M6=M5+MN

M7=M6+MN

M8=M7+MN

M9=M8+MN

M10=M9+MN

M11=M10+MN

M12=M11+MN

M13=M12+MLAND

IF(M13.LT.MTOM) GO TO 20

JJ=M13-HTOM-1

WRITE (6,80) JJ

GO TO 30

CALL SOLV(A(M1),A(M2),A(M3),A(M4),A(M5),A(M6),A(M7),A(M8),A(M9),A(M10),A(M11),A(M12))

GO TO 10

STOP
C
40  FORMAT (12I5)
50  FORMAT (10A4)
60  FORMAT (15/50H NUMBER OF MESH POINTS UP TO END OF FILL
1 *15/50H NUMBER OF MESH POINTS UP TO DEPTH OF FILL
2 NUMBER OF MESH POINTS UP TO END OF LAND
3 NUMBER OF MESH POINTS UP TO DEPTH OF LAND
4 NUMBER OF MESH POINTS UP TO PIPE LOCATION
5 DEPTH OF PIPE
6 NUMBER OF MESH POINTS UP TO PIPE LOCATION
7 TOTAL NUMBER OF PIPES ALONG CIRCUMFERENCE
8 REQUIRED CORE EXCEEDS MTOT BY "1,110"
END
SUBROUTINE SOLV (CA, CSTAR, DSTAR, D, A, B, C, F, CP, RIM, BETA, GAMMA, X)

IMPLICIT REAL*8 (A-H,O-Z)

COMMON/ONE/ MFIL, NFIL, MLAND, NLAND, MM, NCASE, MPIPE, NPIPE, KPIPE, NIPS
!
NPROG

DIMENSION CA(MLAND,NLAND,KPIPE), CSTAR(MLAND,NLAND,KPIPE),
!
DSTAR(MLAND,NLAND,KPIPE), D(MLAND,NLAND,KPIPE), A(MM),
!
B(MM), C(MM), F(MM), CP(MM), BETA(MM), GAMMA(MM), X(MLAND)

DIMENSION R(10), FV(10)

DATA STAR/1H* /

!!! READ MATERIAL PROPERTIES, MESH SIZE AND INITIAL CONCENTRATION

READ (5,920) TORT, BM, AM, PR, TEMP, DAB, DX, CO, TMAX1, CTOL
READ (5,930) NRADI1
READ (5,940) (R(I), FV(I), I=1,NRADII)

X(I)=0.
E=0.
DO 10 I=1,NRADII

E=E+FV(I)
WRITE (6,960) E, TORT, BM, AM, PR, TEMP, DAB, DX, TMAX1, CO, CTOL
WRITE (6,990) (I, R(I), FV(I), I=1,NRADII)

FACTOR=6400.00D0
READ (5,950) IFREQ, NSTEP, DTU, TMAX2, CDT

BAN=1.0-DSQRT(AM/BM)
AK=9.70-05*DSQRT(TEMP/AM)

DMAX=0.
DO 20 I=1,NRADII

E=FV(I)
REQ=R(I)

DKR=DAB/(AK*REQ)

DMAX=DMAX*E*DAB/(TORT*(1.0-BAN*CO*DKR))

DTMAX=1.2*DX*DX/(DMAX*FACTOR)

NTMAX=DTMAX

WRITE (6,1000) IFREQ, NSTEP, DTU, TMAX2, DTMAX
IF(NPROG.EQ.0) WRITE (6,910)

THMAX1=THMAX1*FACTOR
THMAX2=THMAX2*FACTOR

DTU=DTU*FACTOR

DTMAX=DTMAX*FACTOR

DTAU=DTU

MOUT=(MLAND-1)/12+1

NOUT=(NLAND-2)/12+1

NSTAR=(MFIL-2)*9/MOUT+FP=4.0D0

!!! SET INITIAL CONDITIONS

TAU=0.0D0
CDT=CDT*CO
KCONT=0
ICOUNT=0
PI=3.14159265358979adin
DTHET=PI/(NIPS*(KPIPE-1))
MFIL1=MFIL+1
NFIL1=NFIL+1
MLAND1=MLAND-1
KFILE=NFIL
I2=0

*** SET INITIAL CONDITIONS  ...............................**

DO 30 I=2,MLAND
笨(I)=(I-1)*DX
DO 30 J=1,NLAND
DO 30 K=1,KPIPE
CSTAR(I,J,K)=0.D0
DSTAR(I,J,K)=0.D0
CA(I,J,K)=0.D0
30

DO 40 I=2,MFIL
DO 40 J=1,NFIL
DO 40 K=1,KPIPE
CSTAR(I,J,K)=C0
DSTAR(I,J,K)=C0
CA(I,J,K)=C0
40

TDAYS=TAU/FACTOR
DTDAY=DTAU/FACTOR
IF(KCONT.EQ.0) GO TO 70
DMAX=0.
DMIN=999.
DO 60 I=2,MLAND
DO 60 J=1,NLAND
DO 60 K=1,KPIPE
IF(I.LT.MFIL.AND.J.LT.NFIL) GO TO 60
DIJ=DI(I,J,K)
IF(DMIN.GT.DIJ) DMIN=DIJ
IF(DMAX.LT.DIJ) DMAX=DIJ
60 CONTINUE

DTMAX=1.2*DX*CX/(DMAX*FACTOR)
NTMAX=DTMAX

70 DO 100 K=1,KPIPE
THETA=(K-1)*DTHET*180.DO/PI
IF(KCONT.GT.0) GO TO 80
WRITE (6,970) TDAYS,THETA,KCONT
GO TO 90
80 WRITE (6,980) TDAYS,DTDAY,DTMAX,DMIN,DMAX,THETA,KCONT
90 WRITE (6,1020) (X(I),I=2,MLAND,NOUT)
WRITE (6,1010) (I, I=2, MLAND, MOUT)
DO 100 J=1, NLAND, MOUT
WRITE (6,1030) X(J), (CA(I, J, K), I=2, MLAND, MOUT)
WRITE (6,1070) J
IF (J.LE.NFIL) WRITE (6,1080) (STAR, I=1, NSTAR)
100 CONTINUE
DTMAX=DTMAX*FACTOR
IF (KCONT.EQ.0) GO TO 260
110 IF (TAU.LE.TMAX) GO TO 250
I:MAX=1
CMAX=0.0 DO
DO 140 K=1, KPIPE
DO 140 J=1, KFIL
IF (J.EQ.1. AND. NCASE.EQ.2) GO TO 120
IF (J.EQ.1. AND. NCASE.EQ.5) GO TO 120
IF (J.GE.2) GO TO 120
GO TO 140
120 IAMX=1
DO 130 I=1, MLAND
CIJ=CA(I, J, K)
IF (CIJ.LT.CTOL .DR. IAMX.GT.I) GO TO 130
IAMX=I
JAMX=J
KAMX=K
CAMX=CIJ
130 CONTINUE
IF (IAMX.LT.IMAX) GO TO 140
IF (IAMX.EQ.IMAX .AND. CMAX.GT.CAMX) GO TO 140
CMAX=CAMX
JMAX=JAMX
KMAX=KAMX
IMAX=IAMX
140 CONTINUE
IF (ICOUNT.EQ.0) WRITE (6,1040) IMAX, JMAX, KMAX, CMAX
IF (I2.EQ.0) GO TO 190
IF (IMAX.GT.IOLD) GO TO 180
IF (IMAX.EQ.IOLD .AND. JMAX.EQ.JOLD .AND. COLD.GT.CMAX) GO TO 180
IF (IMAX.EQ.IOLD .AND. JMAX.NE.JOLD) GO TO 180
WRITE (6,1050) IMAX, JMAX, KMAX, CMAX, TDAYS
DO 150 K=1, KPIPE
THETA=(K-1)*DTHET+180.0/PI
WRITE (6, 970) TDAYS, THETA, KCONT
WRITE (6, 1020) (X(I), I=2, MLAND, MOUT)
WRITE (6, 1010) (I, I=2, MLAND, MOUT)
DO 150 J=1, NLAND, MOUT
WRITE (6, 1030) X(J), (CA(I, J, K), I=2, MLAND, MOUT)
WRITE (6, 1070) J
IF (J.LE.NFIL) WRITE (6,1080) (STAR, I=1, NSTAR)
150 CONTINUE
I1=MAX0{1, KPIPE-6}
DO 170 K = I1, KMAX, KOUT
WRITE (6, 1030) X(J), (CA(I, J, K), I = I1, I2)
WRITE (6, 1070) J
CONTINUE

170 CONTINUE
GO TO 900

180 CONTINUE

190 IF (TAU - TMAX1, GT DTAU) GO TO 240
IF (NCASE, GE 4) GO TO 220
NFIL1 = 1
IF (NCASE, EQ 2) GO TO 210
NFIL1 = 2
DO 200 K = 1, KPIPE
DO 200 I = 1, MFIL
CSTAR(I, 1, K) = 0.0
DSTAR(I, 1, K) = 0.0
200 CA(I, 1, K) = 0.0
210 MFIL = 0
NFIL = 0
MFIL1 = 1
GO TO 240

220 IF (NCASE, EQ 5) GO TO 240
DO 230 K = 1, KPIPE
CSTAR(MFIL, 1, K) = 0.0
DSTAR(MFIL, 1, K) = 0.0
230 CA(MFIL, 1, K) = 0.0
240 CONTINUE

IOLD = IMAX
KOLD = KMAX
JOLD = JMAX
COLD = CMAX
250 IF(CHEK.LT.CDT) DTAU=2.0*DTAU
IF(CHEK.GT.2.0*CDT) DTAU=0.5*DTAU
IF(TAU.GT.TMAX1) GO TO 260
TCHEK=TMAX1-TCHEK
IF(TCHEK.LT.DTAU) DTAU=TCHEK
IF(DADS(TAU-TMAX1)*LT.DTU) DTAU=DTU
260 TAU=TAU+DTAU
KCONT=KCONT+1
ICOUNT=ICOUNT+1
IF(TAU.GT.TMAX2.OR.KCONT.GT.NSTEP) GO TO 900
EMDA=2.0*DX*DX/DTAU
DO 270 K=1,KPIPE
DO 270 J=1,NLAND
DO 270 I=2,MLAND
270 0(1,J,K)=0.00
DO 280 L=1,NRAPI I
REQ=R(L)
E=FV(L)
ETPD=E*DRAB/TORT
DKR=DRAB/(AK*REQ)
DO 280 K=1,KPIPE
DO 280 J=1,NLAND
DO 280 I=2,MLAND
280 DIJ=D(I,J,K)+ETPD/(1.DO-BAN*CA(I,J,K)*DKR)
DO 490 K=1,KPIPE
DO 490 J=1,NLAND
MIN=2
DO 430 I=2,MLAND
MAX=MLAND
IF(TAU.GT.TMAX1.AND.NCASE.GE.4) GO TO 290
IF(I.LE.MFIL.AND.J.LE.NFIL) GO TO 400
290 IF(I.LT.MFIL.AND.J.LE.NFIL) GO TO 410
IF(NFIL.EQ.NLAND.AND.I.LE.MFIL) GO TO 410
IF(NPROG.EQ.O.AND.I.EQ.MPIPE.AND.J.LE.NPIPE) GO TO 390
IF(I.EQ.1.AND.I.EQ.MPIPE.AND.J.LE.NPIPE) GO TO 390
DIJ=D(I,J,K)
FIJ=DIJ-2.DO*DIJ*CA(I,J,K)
FISO=(11-1)*DTHET)**2
FIJ=FIJ-2.DO*DIJ*CA(I,J,K)/FISO
IF(I.EQ.MLAND) GO TO 370
IF(I.EQ.MFIL.AND.J.LE.NFIL) GO TO 360
IF(I.EQ.2) GO TO 360
FIJ=I-J-2
FIIP=(FIJ+1.DO)/FIJ
FIIM=(FIJ-1.DO)/FIJ
DPRIM=(D(I+1,J,K)-D(I-1,J,K))/4.DO
A(I)=DPRIM- DIJ*FIJM
B(I)=EMDA+2.DO*DIJ
C(I)=-DPRIM- DIJ*FIIM
300 IFJ(J.EQ.1) GO TO 340
IF(J.EQ.NLAND) GO TO 350
IF(J.EQ.NFIL.AND.I.LE.MFIL) GO TO 340
DPRJM=(D(I,J+1,K)-D(I,J-1,K))/4.DO
DIJJM=(DIJ- DPRJM)*CA(I,J-1,K)+ (DIJ+ DPRJM)*CA(I,J+1,K)

310 FIJ=FIJ+DIJJM
IF(K.EQ.1) GO TO 320
IF(K.EQ.KPIPE) GO TO 330
DPRKM=(D(I,J,K+1)-D(I,J,K-1))/4.DO
DIJKM=(DIJ- DPRKM)*CA(I,J,K-1)+ (DIJ+ DPRKM)*CA(I,J,K+1))/FISQ
F(I)=FIJ+DIJKM
GO TO 420
320 F(I)=FIJ+2.DO*DIJ*CA(I,J,K+1)/FISQ
GO TO 420
330 F(I)=FIJ+2.DO*DIJ*CA(I,J,K-1)/FISQ
GO TO 420
340 DIJJM=2.DO*DIJ*CA(I,J+1,K)
GO TO 310
350 DIJJM=2.DO*DIJ*CA(I,J-1,K)
GO TO 310
360 R(I)=EMDA+2.DO*DIJ.
C(I)=-2.DO*DIJ
IF (I.NE.MFIL) GO TO 300
MIN=MFIL
GO TO 300

C
370 IF(J.NE.1) GO TO 380
MAX=MLAND1
GO TO 420
380 A(I)=-2.DO*DIJ
B(I)=EMDA+2.DO*DIJ
GO TO 300

C
390 B(I)=1.DO
A(I)=0.DO
C(I)=0.DO
F(I)=0.DO
GO TO 420
400 MIN=MFIL
GO TO 420
410 MIN=MFIL
420 CONTINUE
430 CONTINUE

C
IF(MIN.GT.MAX) GO TO 490
IF(MIN.EQ.MFIL.AND.MAX.EQ.MFIL) GO TO 490
DO 450 I=MIN,MAX
IF(I.EQ.2) GO TO 450
IF(I.NE.MIN) GO TO 440
IF(TAU.GT.MAX AND NCASE.GE.4) GO TO 440
F(I)=F(I)-A(I)*CA(I-1,J,K)
440 IF(MIN.EQ.MAX OR MAX.NE.MLAND) GO TO 450
F(I)=F(I)-C(I)*CA(I+1,J,K)
450 CONTINUE
IF(MIN.EQ.MAX) GO TO 460
CALL TRIDAG (MIN,MAX,A,B,C,F,CPRI,M,BETA,GAMMA,H)
GO TO 470
460 CPRI(MIN)=F(MIN)/B(MIN)
470 CONTINUE
DO 480 I=MIN,MAX
480 CSTAR(I,J,K)=CPRI(I)
490 CONTINUE

COMPUTE CONCENTRATIONS C-DOUBLE STAR

DO 710 K=1,KPIPE
DO 710 I=2,MLAND
IF(I.LT.MLAND) GO TO 500
IF(NCASE.EQ.3 OR NCASE.EQ.6) GO TO 500
GO TO 710
500 MIN=1
MAX=MLAND
FISQ=(I-1)*THET)**2
DO 660 J=1,MLAND
IF(NPROG.EQ.0 AND I.EQ.MPIPE AND J.LE.NPIPE) GO TO 610
IF(K.EQ.1 AND I.EQ.MPIPE AND J.LE.NPIPE) GO TO 610
IF(TAU.GT.MAX AND NCASE.GE.4) GO TO 510
IF(I.LE.MFIL AND J.LE.NFIL) GO TO 620
510 IF(I.LT.MFIL AND J.LE.NFIL) GO TO 630
IF(MFIL.EQ.MLAND AND J.LT.NFIL) GO TO 630
IF(NFIL.EQ.MLAND AND I.LT.MFIL) GO TO 630
IF(J.GT.1) GO TO 520
IF(NCASE.EQ.2 OR NCASE.EQ.5) GO TO 520
GO TO 640
520 DIJ=D(I,J,K)
FIJ=EMD*C(I,J,K)-2.0D0*DIJ*CSTAR(I,J,K)
IF(J.EQ.1) GO TO 580
IF(J.EQ.NLAND) GO TO 600
IF(J.EQ.NFIL AND I.LE.HFIL) GO TO 580
DPRJM=(D(I+1,J,K)-D(I,J-1,K))/4.0D0
A(I)=DPRJM-DIJ
B(IJ)=EMD+2.0D0*DIJ
C(IJ)=-DPRJM-DIJ
530 FIJ=FIJ-2.0D0*DIJ*C(I,J,K)/FISQ
IF(I.EQ.MLAND) GO TO 570
IF(I.EQ.MFIL AND J.LE.NFIL) GO TO 590
IF(I.EQ.2) GO TO 590
DPRIM=(D(I+1,J,K)-D(I-1,J,K))/4.D0
FIJ=2*I-2
FIIP=(FIJ+1.D0)/FIJ
FIIM=(FIJ-1.D0)/FIJ
DIJIM=(DIJ*FIIM-DPRIM)*CSTAR(I-1,J,K)+(DIJ*FIIP+DPRIM)*CSTAR(I+1,J,K)

540 FIJ=FIJ+DIJIM
IF(K.EQ.1) GO TO 550
IF(K.EQ.KPIPE) GO TO 560
DPRKM=(D(I,J,K+1)-D(I,J,K-1))/4.D0
DIJKM=(DIJ-DPRKM)*CA(I,J,K-1)*(DIJ+DPRKM)*CA(I,J,K+1))/FISQ
F(J)=FIJ+DIJKM
GO TO 650

550 F(J)=FIJ+2.0D0*DIJ*CA(I,J,K+1)/FISQ
GO TO 650

560 F(J)=FIJ+2.0D0*DIJ*CA(I,J,K-1)/FISQ
GO TO 650

570 DIJIM=2.0D0*DIJ*CSTAR(I-1,J,K)
GO TO 540

580 B(J)=EMDA+2.0D0*DIJ
C(J)=-2.0D0*DIJ
GO TO 530

590 DIJIM=2.0D0*DIJ*CSTAR(I+1,J,K)
IF(TAU.LE.TMAX) GO TO 540
MIN=NFIL
GO TO 540

600 A(J)=-2.0D0*DIJ
B(J)=EMDA+2.0D0*DIJ
GO TO 530

610 MIN=NP1PF+1
GO TO 650

620 MIN=NFIL1
GO TO 650

630 MIN=NFIL
GO TO 650

640 MIN=2
650 CONTINUE

660 CONTINUE
IF(MIN.GT.MAX) GO TO 710
IF(MIN.EQ.NFIL.AND.MAX.EQ.NFIL) GO TO 710
J=MIN
IF(J.EQ.1.0R.J.EQ.NFIL) GO TO 670
FIJ=FIJ-A(J)*CSTAR(I,J-1,K)

670 CONTINUE
IF(MIN.EQ.MAX) GO TO 680
CALL TRIDAG (MIN,MAX,A,B,C,F,CPRIH,BETA,GAMMA,MM)
GO TO 690

680 CPRIH(MIN)=F(MIN)/B(MIN)
690 CONTINUE
DO 700 J=MIN,MAX
700 DSTAR(I,J,K)=CPRIM(J)
710 CONTINUE

** COMPUTE CONCENTRATIONS AT THE END OF WHOLE TIME INCREMENT **

DO 880 I=2,MLAND
 IF(I.NE.MLAND) GO TO 720
 IF(NCASE.EQ.3.OR.NCASE.EQ.6) GO TO 720
 GO TO 880

MAX=KPIPE
 FISO=((I-1)*D*THET)**2
 IF(I.EQ.1) GO TO 730
 FII=2*I-2
 FII=(FI+1,DO)/FI
 FIIH=(FI-1,DO)/FI
730 CONTINUE

DO 880 J=1,NLAND
 IF(NPROG.EQ.0.AND.I.EQ.KPIPE.AND.J.LE.NPIPE) GO TO 780
 IF(I.LE.MLAND.AND.J.EQ.1) GO TO 880
 IF(TAU.GT.TMAX1.AND.NCASE.EQ.4) GO TO 740
 IF(I.LE.MFIL.AND.J.LE.NFIL) GO TO 880
740 MIN=1
 IF(J.GT.1) GO TO 750
 IF(NCASE.EQ.2.OR.NCASE.EQ.5) GO TO 750
 GO TO 880

750 DO 860 J=2,MLAND
 DIJ=D(I,J,K)
 FII=(EMDA-2.0*DIJ)*DSTAR(I,J,K)-2.0DIJ*CSTAR(I,J,K)
 IF(K.EQ.1) GO TO 760
 IF(K.EQ.KPIPE) GO TO 830
 DPRK=(D(I,J,K+1)-DIJ,K-1))/4.0
 A(K)=(DPRK-2.0DIJ/FISO
 B(K)=EMDA+2.0DIJ/FISO
 C(K)=-(DPRK*DIJ/FISO

760 IF(J.EQ.1) GO TO 800
 IF(J.EQ.NLAND) GO TO 810
 IF(J.EQ.NFIL) GO TO 800
 DPRM=(D(I,J+1,K)-DIJ,J-1,K))/4.0
 DIJJM=(DIJ+DPRJ)*DSTAR(I,J-1,K)+(DIJ+DPRJM)*DSTAR(I,J+1,K)

770 IF(I.EQ.MLAND) GO TO 780
 IF(I.EQ.NFIL) GO TO 790
 IF(I.EQ.2) GO TO 790
 DPRIM=(D(I+1,J,K)-D(I-1,J,K))/4.0
 DIJH=(DIJ*FI+DPRIM)*CSTAR(I-1,J,K)+(DIJ*FI+DPRIM)*CSTAR(I+1,J,K)
 F(K)=FI*DIJH
 GO TO 850
780  F(K)=FIJ+2.00D0*DIJ*CSTAR(I-1,J,K)
  GO TO 850
790 F(K)=FIJ+2.00D0*DIJ*CSTAR(I+1,J,K)
  GO TO 850
800 DIJJM=2.00D0*DIJ*DSTAR(I,J+1,K)
  GO TO 770
810 DIJJM=2.00D0*DIJ*DSTAR(I,J-1,K)
  GO TO 770
820 IF(I.EQ.MPIPE.AND.J.LE.NPIPE) GO TO 840
  B(K)=EMDA+2.00D0*DIJ/FISQ
  C(K)=-2.00D0*DIJ/FISQ
  GO TO 760
830 A(K)=-2.00D0*DIJ/FISQ
  B(K)=EMDA+2.00D0*DIJ/FISQ
  GO TO 760
840 MIN=2
850 CONTINUE
860 CONTINUE
C
CALL TRIDAG (MIN,MAX,A,B,C,F,CPRIM,BETA,GAMMA,MM)
DO 870 K=MIN,MAX
870 CA(I,J,K)=CPRIM(K)
880 CONTINUE
C
CHEK=0.
DO 890 I=2,MLAND
  DO 890 J=1,NLAND
  DO 890 K=1,KPIPE
    CDIF=DABS(CSTAR(I,J,K)-CA(I,J,K))
    CSTAR(I,J,K)=CA(I,J,K)
    DSTAR(I,J,K)=CA(I,J,K)
    IF(CDIF.GT.CHEK) CHEK=CDIF
890 CONTINUE
C
*** PRINT CONCENTRATIONS ********
IF(DABS(TAU-TMAX1).LT.DTU) ICOUNT=IFREQ
IF(ICOUNT.NF.IFREQ) GO TO 110
ICOUNT=0
GO TO 50
C
900 RETURN
C
910 FORMAT ('-CONTINUOUS DITCH PROGRAM')
920 FORMAT (8F10.0)
930 FORMAT (I5)
940 FORMAT (2F10.0)
950 FORMAT (2I5,3F10.0)
960 FORMAT (45H POROSITY OF SOIL (DIMENSIONLESS),=F10.3/45H
  1 TORTUOSITY (DIMENSIONLESS),=F10.3/45H MOLECULAR
  2WEIGHT OF GAS B (GM/MOLE),=F10.3/45H MOLECULAR WEIGHT OF G
  3AS A (GM/MOLE),=F10.3/45H PRESSURE (ATMOS)
=F10.3/45H TEMPERATURE (DEG KELVIN)
=,F10.3/45H BULK DIFFUSION COEFFICIENT (CM SQ ATMOS/SEC)
=,F10.3/45H DIFFUSION TIME (DAYS)
=,F10.3/45H INITIAL MOLE FRACTION
=,F10.3/45H TOLERABLE MOLE FRACTION

970 FORMAT (31H1MOLE FRACTION AT TIME (DAYS) =,F9.1/1RH THETA (DEGREE 1S) =,F6.2/14H STEP NUMBER =,I5/)
980 FORMAT (31H1MOLE FRACTION AT TIME (DAYS) =,F9.1,2X,13HOTAU (DAYS)
1=F6.1,2X,14HOTMAX (DAYS) =,F6.1,2X,11HDIJ (MIN) =,E10.3,7X,11HDIJ
2 (MAX) =,E10.3/1FH THETA =,F8.2,14H STEP NUMBER =,I5/)
990 FORMAT (15H NUMBER OF STEPS BETWEEN PRINTOUTS =,I10/45M M
1AXIMUM NUMBER OF STEPS ALLOWED =,I10/45H INITIAL DTAU (DAYS)
2DAYS) =,F10.1/45H MAXIMUM DTAU ALLOWED (DAYS) =,F10.1/45H MAXIMUM DTAU (DAYS) =1.20X*0X*DIJ(M
4AX) =,F10.1/)
SUBROUTINE TRIDAG (IF, L, A, B, C, D, V, BETA, GAMMA, MM)
IMPLICIT REAL*8 (A-H, O-Z)
DIMENSION A(MM), B(MM), C(MM), D(MM), V(MM), BETA(MM), GAMMA(MM)
BETA(IF) = P(IF)
GAMMA(IF) = D(IF)/BETA(IF)
IFP1 = IF + 1
DO 10 I = IFP1, L
BETA(I) = P(I) - A(I) * C(I - 1)/BETA(I - 1)
10 GAMMA(I) = (D(I) - A(I) * GAMMA(I - 1))/BETA(I)
V(L) = GAMMA(L)
LAST = L - IF
DO 20 K = 1, LAST
I = L - K
20 V(I) = GAMMA(I) - C(I) * V(I + 1)/BETA(I)
RETURN
END
Instructions for Data Preparation for Code II

The following sequence of punched cards will carry the problem data for input to the program:

Card 1: Control Data (1015)

<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of mesh points to the end of the fill (MFIL)</td>
<td>1-5</td>
</tr>
<tr>
<td>Number of mesh points to the bottom of the fill (NFIL)</td>
<td>6-10</td>
</tr>
<tr>
<td>Number of mesh points to the end of the soil boundary (MLAND)</td>
<td>11-15</td>
</tr>
<tr>
<td>Number of mesh points to the bottom of the soil (NLAND)</td>
<td>16-20</td>
</tr>
<tr>
<td>Case Number (NCASE)</td>
<td>21-25</td>
</tr>
<tr>
<td>Mesh point number at the location of vent (MPIPE)</td>
<td>26-30</td>
</tr>
<tr>
<td>Number of mesh points over the depth of vent (NPIPE)</td>
<td>31-35</td>
</tr>
<tr>
<td>Number of mesh points along THETA direction (KPIPE)</td>
<td>36-40</td>
</tr>
<tr>
<td>Total number of pipes over circumference (NPIPS)</td>
<td>41-45</td>
</tr>
<tr>
<td>Program Type (NPROG)</td>
<td>46-50</td>
</tr>
<tr>
<td>NPROG = 0 = pipe vents</td>
<td></td>
</tr>
<tr>
<td>≠ 0 = continuous trench</td>
<td></td>
</tr>
</tbody>
</table>

Card 2: Title Card (18A4)

This card gives the arbitrary descriptive identification of the job.

Card Set A: Material properties, mesh size and initial mole fraction of gas in the fill (8G 10.0)

This set consists of two cards containing the following information in the order described below:

<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tortuosity (TORT) (dimensionless)</td>
<td>1-10</td>
</tr>
<tr>
<td>Molecular weight of gas B (BM) (g/mole)</td>
<td>11-20</td>
</tr>
<tr>
<td>Molecular weight of gas A (AM) (g/mole)</td>
<td>21-30</td>
</tr>
<tr>
<td>Total pressure of mixture of gases (PR) (atm)</td>
<td>31-40</td>
</tr>
<tr>
<td>Temperature of mixture of gases (TEMP) (K)</td>
<td>41-50</td>
</tr>
</tbody>
</table>
Information Columns

Bulk diffusion coefficient (DAB) (cm² atm/s) 51-60
Spatial mesh size (DX) (cm) 61-70
Initial mole fraction of gas in fill (CO) (dimensionless) 71-80
Period of decomposition (TMAX1) (days) 1-10
Termination mole fraction (CTOL) (dimensionless) 11-20

Card 5:
This card gives the total number of pore radii (NRADII) considered for the soil (I5).

Information
Total number of pore radii (NRADII) 1-5

Card Set B:
This set of cards gives the information about the pore side distribution. A total number of NRADII cards, each containing the following information is required (2F 10.0).

Information
Pore radius (R₁) (Å) 1-10
Volumetric fraction (FV₁) (dimensionless) 11-20

Last Card:
This card contains the control information regarding printing of the program (2I5, 3F 10.0).

Information
Number of time steps between successive printouts of mole fraction (IFREQ) 1-5
Maximum number of steps allowed before program termination (NSTEP) 6-10
Time increment at the start of program (DTU) (days) 11-20
Maximum time allowed for program termination (TMAX2) (days) 21-30
In case more than one problem is to be solved, the data for the subsequent problems may be input in the sequence given above. The input is terminated by putting a blank card at the end of a problem data set.

3.3.4 Example Problem III - Diffusion of Methane

As an example problem, diffusion of methane was considered from a landfill having a radius of 160 meters and a depth of fill of 16 meters. The boundaries at the top surface and at a depth of 32 meters were considered impervious while the boundary at \( r = r_s = 400 \) meters was considered as a prescribed zero mole fraction boundary (NCASE = 5). Six pipes distributed over a circle with a radius of 240 meters were considered. Thus the analysis is carried out for a slice subtending an angle of 30° at the axis. The plane at \( \theta = 0 \) is considered to pass through one of the pipes while the plane \( \theta = 30° \) passes halfway between two consecutive pipes. Three subdivisions were considered in the \( \theta \)-direction giving KPIPE = 4. Thus the printouts were considered 10° apart. \( \Delta X \) was taken as 800 cm. The mole fraction of methane in the fill during decomposition is assumed as 0.70 and at the end of the decomposition period of five years the landfill boundary is treated as impervious.

3.3.4.1 Input

The following input data card sequence was used.
3.3.4.2 Output—

Appendix C contains the computer output giving the results for this problem. The first page gives the input parameters. The next four pages give initial mole fractions at planes, θ = 0, 10, 20 and 30°. The values of mole fractions at the end of the decomposition period and at the time of termination of the program due to dropping of mole fraction of methane below CTOL at the farthest point where it exceeds CTOL are given on the next eight pages. The next four pages give a detail of mole fraction distribution at termination at the pipe. The last four pages give a detail of mole fraction distribution around the farthest point where the mole fraction of methane exceeds CTOL.
CHAPTER IV

FINITE ELEMENT FORMULATION

In this chapter the development of a finite element formulation is presented. The development has been divided into two parts: the variational formulation and the finite element discretization.

4.1 VARIATIONAL FORMULATION

Variational methods have been used extensively by Douglas and Dupont (1971), Varga, R. S. (1968), Washizu, K. (1968), Sandhu and Pister (1971), Oden and Reddy, (1974) and Salaam, U. (1974) among others. The problem presented in equations (15) and (16) does not have a variational formulation as such; however, an equivalent new set of equations, for which a variational formulation can be given, is obtained. Two sets of equations are said to be equivalent if their solutions are equivalent. A similar formulation was used by Wilson and Nickel (1966) for heat conduction problem.

The governing differential equations describing the transient diffusion problem are

\[(D(c)C_i)_t - \dot{C} = 0 \quad \text{in } \Omega \times (0,T] \quad (112)\]
\[n_i D C_i - n_i Q_i = 0 \quad \text{on } \partial \Omega \times (0,T] \quad (113)\]
\[C(\bar{x},0) = C_0(\bar{x}) \quad \text{in } \Omega \quad (114)\]

where

\[Q_i = \text{rate of flux} \]
\[\Omega = \text{a bounded domain in } \mathbb{R}^n\]

and

\[D(c) > 0\]

Define the total flux over a time \( t \) as

\[\dot{Q}_i = \int_0^t Q_i(\bar{x},\tau) d\tau. \quad (115)\]
Then
\[ \dot{q}_i = q_i \]
and the boundary conditions (B.C.) (113) may then be written as
\[ n_i(Dc_i - \dot{q}_i) = 0. \quad (116) \]

Taking the Laplace transform of equation (112) leads to
\[ (D(x)c(x,s),i) - sC(x,s) + C_0(x) = 0 \quad (117) \]

Now dividing by \( s \) and taking the inverse Laplace transform, and using the fact that multiplication in the transform domain is the same as the convolution in the time domain gives
\[ (D(x)*C(x,t),i) - C(x,t) + C_0(x) = 0. \quad (118) \]

Taking the Laplace transform of the B.C.'s (116) gives
\[ n_i(D(x)c_i(x,s) - sQ_i(x,s) - Q_i(x,0)) = 0 \quad (119) \]

Dividing throughout by \( s \) and taking the inverse Laplace transform, noting \( \hat{Q}_i(x,0) = 0 \) gives
\[ n_i[D(x)*C_i(x,t) - \hat{Q}_i(x,t)] = 0 \quad (120) \]

The system of equations (118) and (120) is equivalent to the system of equations (112) and (116) by uniqueness of the Laplace transform.

For a positive bounded operator \( A \) defined on a dense set \( M \subseteq V \), a Hilbert space of the field \( F \), the equations
\[ Au = f \quad \text{in } V \quad (121) \]
and
\[ B_nu = g_n \quad \text{on } S_n \quad (122) \]
where
\[ S = \bigcup_{n=1}^{m} S_n \quad \text{and} \quad S_i \cap S_j = \emptyset \quad (i \neq j) \]

have a unique solution. If the solution exists, the Gateaux differential of the function
\[ F(u) = \langle u, Au \rangle - 2\langle u, f \rangle + \sum_{n=1}^{m} \lambda_n \langle u, B_n u - 2g_n \rangle_{S_n} \quad (123) \]
assumes its minimum value for this solution where

$$\lambda_n = \pm 1 \quad n = 1, 2, \cdots, m$$

the sign being decided after taking the variation.

The function for the problem defined by equations (118) and (120) may, therefore, be written as

$$F(C) = \langle C, D(x) \ast C, i \rangle_{i} - \langle C, C \rangle + 2\langle C, C_0 \rangle + \lambda\langle C, n_i D \ast C, i \rangle_S - 2\lambda\langle C, n_i \hat{q}_i \rangle_S \quad (124)$$

The Gateaux differential of the function $F(C)$ is defined as

$$D_{C}F(C) = \frac{d}{dy} F(C + \gamma C) \bigg|_{\gamma = 0} . \quad (125)$$

where

$$F(C + \gamma C) = \langle C + \gamma C, (D \ast (C + \gamma C), i) \rangle_{i} - \langle C + \gamma C, C + \gamma C \rangle + 2\langle C + \gamma C, C_0 \rangle$$

$$+ \lambda\langle C + \gamma C, n_i D \ast (C + \gamma C), i \rangle_S - 2\lambda\langle C + \gamma C, n_i \hat{q}_i \rangle_S . \quad (126)$$

Therefore

$$D_{C}F(C) = \langle C, (D \ast C, i) \rangle_{i} + \langle \overline{C}, (D \ast C, i) \rangle_{i} - 2\langle C, C \rangle + 2\langle C, C_0 \rangle$$

$$+ \lambda\langle C, n_i D \ast \overline{C}, i \rangle_S + \lambda\langle \overline{C}, n_i D \ast C, i \rangle_S - 2\lambda\langle \overline{C}, n_i \hat{q}_i \rangle_S . \quad (127)$$

Let

$$H = C \ast D \ast \overline{C}, i \quad (128)$$

Then

$$\nabla H = C, i \ast D \ast \overline{C}, i + C \ast (D \ast \overline{C}, i), i \quad (129)$$

If $R$ is a bounded closed region in $E^3$ and $H$ is continuously differentiable on $R$ then by the divergence theorem

$$\iiint_R \nabla F \, dv = \iint_S F \cdot n \, dS . \quad (130)$$

Using equations (128), (129), and (130) and the commutative property of convolution gives

$$\langle C, (D \ast \overline{C}, i), i \rangle_R = -\langle D \ast C, i, \overline{C}, i \rangle_R + \langle C, n_i D \ast \overline{C}, i \rangle_S . \quad (131)$$
Using the divergence theorem again gives
\[
\langle C, i, D^*C, i \rangle = -\langle \overline{C}, (D^*C, i)_i \rangle + \langle \overline{C}, n_1 D^*C, i \rangle_S .
\]  
(132)

Now substitute equation (132) in equation (127), then
\[
D_C F(C) = \langle \overline{C}, (D^*C, i)_i \rangle - \langle \overline{C}, n_1 D^*C, i \rangle_S + \langle C, n_1 D^*C, i \rangle_S + \langle \overline{C}, (D^*C, i)_i \rangle
\]
\[-2\langle \overline{C}, C \rangle + 2\langle \overline{C}, C_0 \rangle + \lambda \langle C, n_1 D^*C, i \rangle_S + \lambda \langle \overline{C}, n_1 D^*C, i \rangle_S
\]
\[-2\lambda \langle \overline{C}, n_1 D^*_i \rangle_S .
\]  
(133)

Putting \( \lambda = -1 \) eliminates terms containing \( \overline{C}, i \) and gives
\[
D_C F(C) = 2\langle \overline{C}, (D^*C, i)_i \rangle - 2\langle \overline{C}, C \rangle + 2\langle \overline{C}, C_0 \rangle - 2\langle \overline{C}, n_1 D^*C, i \rangle_S + 2\langle C, n_1 D^*_i \rangle_S .
\]  
(134)

The Gateaux differential \( D_C F(C) \) vanishes for arbitrary \( \overline{C} \) iff
\[
(D^*C, i)_i - C + C_0 = 0 \quad \text{in} \, \Omega \quad (135)
\]
and
\[
n_1 (D^*C, i - \hat{\phi}_i) = 0 \quad \text{on} \, \partial \Omega . \quad (136)
\]

Equations (135) and (136) are the same as equations (118) and (120). Hence the function \( F(u) \) is verified to be the generating function for the initial boundary value problem.

**Note 1.** Using the simple identity
\[
1 * \dot{C} = \int_0^t \dot{C}(\overline{x}, \tau) d\tau = C(\overline{x}, t) - C_0(\overline{x})
\]
reduces equation (135) to the differential equation
\[
(D^*C, i)_i - \dot{C} = 0 \quad (137)
\]

**Note 2**
\[
\langle C, i, D^*C, i \rangle = -\langle C, (D^*C, i)_i \rangle + \langle C, n_1 D^*C, i \rangle_S
\]
by divergence theorem. Therefore the function \( F(C) \), equation (124), may be written as
\[
F(C) = -\langle C, i, D^*C, i \rangle - \langle C, C \rangle + 2\langle C, C_0 \rangle + 2\langle C, n_1 Q_i \rangle_S \quad (138)
\]
This is a more useful form.
Note 3. Surface flux

Flux across the boundary layer $\partial \Omega$ of the region $\Omega$ is given by

$$q = h \times (C_e - C) \tag{139}$$

where $h$ is the coefficient of mass transfer across the boundary layer and $C_e$ concentration of gas outside the soil.

This changes the boundary conditions (120) to

$$n_i (D(x) \times C_{i} - \frac{\partial C_i}{\partial n}) - hC_e \times h \times C = 0 \tag{140}$$

Remembering that $\lambda = -1$, and allowing for surface convection the function $F(C)$ may be rewritten as

$$F(C) = \langle C_i, D \times C_i \rangle + \langle C, C \rangle - 2\langle C, C_0 \rangle - 2\langle C, n_i \hat{C}_i \rangle_S$$

$$- 2h \times \langle C, C_e \rangle_S + h \times \langle C, C \rangle_S \tag{141}$$

4.2 FINITE ELEMENT APPROXIMATION

Within an element $m$ assume that the concentration distribution is given by

$$C_m(x, t) = \langle b_m(x) \rangle \{c(t)\} \tag{142}$$

where

$${\{c(t)\}}$$ is the column vector of nodal point concentrations and

$$\langle b_m(x) \rangle$$ is a row vector of interpolation functions.

Differentiating equation (142) with respect to the spatial coordinates yields a column vector of concentration gradients which may be written as

$$\{C^m_i(x, t)\} = \langle a_m(x) \rangle \{\hat{c}(t)\} \tag{143}$$

where $\langle a_m(x) \rangle$ is a matrix of spatial derivatives of $\langle b_m(x) \rangle$.

The generating function (141) can then be written in the form of a summation over all the elements:

$$F(C) = \sum_{m=1}^{M} \left[ \int_{\Omega^m} \left\{ C^m_i \times D^m \times C^m_i + C^m \times C^m - 2C^m \times C_0 \right\} dV_m \right.$$

$$\left. - \int_{S^m} \left\{ 2C^m \times n_i \hat{C}_i^m + 2h^m \times C^m \times C_e^m - h^m \times C^m \times C^m \right\} dS_m \right] \tag{144}$$
where \( M \) = total number of elements in the system. Substitution of (142) and (143) into the function (144) yields

\[
F(C) = \sum_{m=1}^{M} \left[ \int_{\Omega_m} \left[ (C(t))^T(a_m(\overline{x}))^T d\Omega_m \right] \left( C(t) \right) 
+ \int_{\Omega_m} \left[ \frac{\partial}{\partial t} \left( b_m(\overline{x}) \right)^T \left( b_m(\overline{x}) \right) \right] \left( C(t) \right) 
- \int_{\Omega_m} \left[ \frac{\partial}{\partial t} \left( b_m(\overline{x}) \right)^T \left( b_m(\overline{x}) \right) \right] \left( C(t) \right) 
+ \int_{\Omega_m} \left[ \frac{\partial}{\partial t} \left( b_m(\overline{x}) \right)^T \left( b_m(\overline{x}) \right) \right] \left( C(t) \right) \right] d\Omega_m
\]

In matrix form this may be written as

\[
F(C) = \{C\}^T \times [E] \times \{C\} \times [K] \times \{C\} \times 2\{C\}^T \times [E] \times \{C_0\}
- 2\{C\}^T \times \{\hat{Q}(t)\}
\]

where

\[
E = \text{accumulating capacity matrix}
\]

\[
[K] = \text{flow or diffusivity matrix}
\]

\[
\{\hat{Q}(t)\} = \text{diffusivity vector}
\]

The first variation of equation (146) gives

\[
[E]\{C\} + [K] \times \{C\} = E\{C_0\} + \{\hat{Q}\}
\]

4.3 SOLUTION PROCEDURE

The procedure for solving mildly nonlinear problems is similar to the one used for problems with constant diffusion coefficients, the diffusion coefficient being a function of concentration changes with time.
and space. Because the change over a small enough time step is very small and as such the coefficient of diffusion for the period \((t - \Delta t, t)\) may be based on the gas concentrations at time \(t - \Delta t\). Rewriting equation (147) as

\[
[E]C_t + [K] * C_t = [E]C_{t-\Delta t} + \hat{Q} \tag{148}
\]

and assuming that the concentration \(C\) varies linearly over a time interval \(\Delta t\) at any time \(\zeta\) such that \(t - \Delta t < \zeta < t\)

\[
C(\zeta) = C(t - \Delta t) + \frac{C(t) - C(t - \Delta t)}{\Delta t} (\zeta - (t - \Delta t)) \tag{149}
\]

so that

\[
[K] * C_t = [K] C(t) + \frac{C(t - \Delta t)}{2} \Delta t. \tag{150}
\]

The calculation of \(\hat{Q}(t)\) requires the time integration of flux and convective boundary terms. The changes due to chemical reaction, if any, are accommodated here. Again assuming that the values of this vector varies linearly over the time interval \(\Delta t\), we have

\[
\hat{Q}_m(t) = \int_{S_m} \left( b_m(\overline{x}) \right)^T n_1 \frac{Q_1(\overline{x}, t) + Q_1(\overline{x}, t - \Delta t)}{2} \Delta t dS_m \\
+ \int_{S_m} h_m \frac{C_e(t) + C_e(t - \Delta t)}{2} \Delta t(b_m(\overline{x}))^T dS_m \tag{151}
\]

or

\[
\hat{A}_m(t) = ([Q(t)] + [Q(t - \Delta t)]) \frac{\Delta t}{2} \tag{152}
\]

Substituting equation (150) and equation (152) in equation (148) gives

\[
\left[ [E] + \frac{\Delta t}{2} [K] \right] C_t = \left[ [E] - \frac{\Delta t}{2} [K] \right] C_{t-\Delta t} + \left( [Q]_t + [Q]_{t-\Delta t} \right) \frac{\Delta t}{2} \tag{153}
\]

Equation (153) gives the required algorithm for the solution procedure.

### 4.3.1 Calculation of Element Matrices and Flow Vector

The formulation developed in Section 4.2 requires that the concentration within an element be at least continuous. The author's experience with (1) triangular elements using linear variations of concentration within the element, (2) the Q-19 plate bending element (Rai, Sandhu, 1974) and
(3) isoparametric elements (Sandhu, Rai, Desai, 1973) has shown that the last type is easy to program and gives good results. Zienkiewicz (1971) has also shown that isoparametric elements first used by Irons (1968) give better results than triangular elements. A four point isoparametric element gives a hyperbolic variation within the element and is, therefore, quite adequate. If higher order elements are used it is possible to obtain the same order of accuracy with fewer elements but the increase in bandwidths of the coefficient matrices more than offsets the cost on computer time.

4.3.1.1 Diffusivity Matrix--

Using the four point isoparametric element (see Fig. 4) the concentration distribution within the element is assumed as:

\[ C_m(x,t) = \{\varphi\}^T \{\bar{C}(t)\} \]  \hspace{1cm} (154)

where

\[ \{\varphi\} = \frac{1}{4} \begin{bmatrix} (1 - \xi)(1 - \eta) \\ (1 + \xi)(1 - \eta) \\ (1 + \xi)(1 + \eta) \\ (1 - \xi)(1 + \eta) \end{bmatrix} \]  \hspace{1cm} (155)

![Fig. 4 - Four point isoparametric element.](image-url)
The concentration gradients at a point are defined by derivatives with respect to the Cartesian reference frame. It is, therefore, necessary to relate derivatives with respect to $\xi$, $\eta$ to those with respect to $x$, $y$. Using the chain rule for differentiations gives

\[
\begin{pmatrix}
\frac{\partial}{\partial \xi} \\
\frac{\partial}{\partial \eta}
\end{pmatrix}
= \begin{pmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta}
\end{pmatrix}
\begin{pmatrix}
\frac{\partial}{\partial x} \\
\frac{\partial}{\partial y}
\end{pmatrix}
\tag{156}
\]

Inverting, we obtain

\[
\begin{pmatrix}
\frac{\partial}{\partial x} \\
\frac{\partial}{\partial y}
\end{pmatrix}
= \frac{1}{J} \begin{pmatrix}
\frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi} \\
- \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \xi}
\end{pmatrix}
\begin{pmatrix}
\frac{\partial}{\partial \xi} \\
\frac{\partial}{\partial \eta}
\end{pmatrix}
\tag{157}
\]

where

\[
J = \left|\begin{array}{cc}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta}
\end{array}\right| = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i (\varphi_i, \xi, \varphi_j, \eta - \varphi_i, \eta \varphi_j, \xi) y_i
\]

\[
= \{x\}^T [P] \{y\}
\]

\[
P_{ij} = \varphi_i, \xi, \varphi_j, \eta - \varphi_i, \eta \varphi_j, \xi
\]

\[
\{\varphi, \xi\} = \frac{1}{4} \begin{pmatrix}
-(1 - \eta) \\
(1 - \eta) \\
(1 + \eta) \\
-(1 + \eta)
\end{pmatrix}
\]

and

\[
\{\varphi, \eta\} = \frac{1}{4} \begin{pmatrix}
-(1 - \xi) \\
(1 - \xi) \\
-(1 + \xi) \\
(1 + \xi)
\end{pmatrix}
\]

Using the notation explained above, the concentration gradients are written as
\[
\begin{align*}
\left\{ c, x \right\} &= \frac{1}{J} \left[ \begin{array}{cc}
\frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi} \\
- \frac{\partial x}{\partial \eta} - \frac{\partial x}{\partial \xi}
\end{array} \right] \left\{ c, \xi \right\} \\
\left\{ c, y \right\} &= \frac{1}{J} \left[ \begin{array}{cc}
0^T P_x \\
-0^T P_x
\end{array} \right].
\end{align*}
\]

Let

\[
\frac{[P](y)}{J} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \{ y \}
\]

and

\[
\frac{[P](x)}{J} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \{ x \}.
\]

Then for an interior element

\[
[K^m] = \int \int \begin{bmatrix} y_1 & x_1 \\ y_2 & x_2 \\ y_3 & x_3 \\ y_4 & x_4 \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \begin{bmatrix} y_1 & y_2 & y_3 & y_4 \\ x_1 & x_2 & x_3 & x_4 \end{bmatrix} \, dy \, dx
\]

(159)

If the element has one of its sides on the surface with a convective boundary, the surface term

\[
\int \partial \eta^m \langle b_m(\bar{x}) \rangle^T (b_m(\bar{x})) dS_m
\]

must be added to equation (159). The term \( \langle b_m(\bar{x}) \rangle \) must be evaluated with appropriate value of \( \xi \) or \( \eta \). For example, for the surface \( \eta = 1 \)

\[
\langle b_m(\bar{x}) \rangle^T (\varphi) = \frac{1}{2} \begin{bmatrix} 0 \\ 0 \\ 1 + \xi \\ 1 - \xi \end{bmatrix}
\]

and the convective term
\[ [K^m_n] = \int \frac{h^m}{\partial \xi^m} (b_m(x))^T(b_m(x)) \, d\xi \]

\[ = \frac{1}{8} h^m \int_0^1 \begin{bmatrix} 0 \\ 0 \\ 1 + \xi \\ 1 - \xi \end{bmatrix} < 0 \begin{bmatrix} 0 \\ 1 \end{bmatrix} (1 + \xi) (1 - \xi) \, d\xi \]

\[ = \frac{h^m}{6} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix} \]  

(160)

and

\[ [K^m] = [K^m] \text{ for the interior} + \frac{h^m}{6} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix} \]  

(161)

### 4.3.1.2 Capacity Matrix--

The calculation of the capacity matrix \([E^m]\) is carried out exactly on the same lines as that of \([K^m]\) by numerical integration. Using the Gaussian quadrature formulae (Zienkiewicz, 1972)

\[ [E^m] = \int_{\Omega^m} (b_m(x))^T(b_m(x)) \, dv_m \]

\[ = \int \int_{\Omega^m} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix} (\phi_1 \phi_2 \phi_3 \phi_4) \, dydx \]  

(162)

### 4.3.1.3 Convection Vector \([Q(t)]\)--

Assuming a linear boundary and a linear input/output between two points \(i, j\), input at an intermediate point is given by

\[ Q = Q_i \xi + Q_j (1 - \xi) \quad 0 \leq \xi \leq 1 \]

\[ \begin{cases} \hat{Q}_i \\ \hat{Q}_j \end{cases} = \xi \int_0^1 \begin{bmatrix} \xi \\ 1 - \xi \end{bmatrix} \begin{bmatrix} Q_i \\ Q_j \end{bmatrix} \begin{bmatrix} \xi \\ 1 - \xi \end{bmatrix} \, d\xi \]

\[ = \frac{\xi}{6} \begin{bmatrix} 2Q_i + Q_j \\ Q_i + 2Q_j \end{bmatrix} \]  

(163)
In the presence of surface convection say on boundary \( \eta = 1 \), add to \( Q \) the integral

\[
\Delta t \int h^m (c_e(t) + c_e(t - \Delta t)) \langle b_m(x) \rangle^T ds_m
\]

\[
= \frac{\Delta t}{4} h^m m (c_e(t) + c_e(t - \Delta t)) \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}
\]  

(164)

4.3.2 Modification for Prescribed Concentrations

In case of prescribed concentrations, the set of equations (153) must be modified as follows.

Let

\( C_b \) be the set of prescribed concentrations;
\( C_a \) the unknown concentrations;

then equation (153) may be written as

\[
\begin{bmatrix}
E_{aa} & E_{ab} \\
E_{ba} & E_{bb}
\end{bmatrix}
\begin{bmatrix}
C_a \\
C_b
\end{bmatrix}
+ \frac{\Delta T}{2}
\begin{bmatrix}
K_{aa} & K_{ab} \\
K_{ba} & K_{bb}
\end{bmatrix}
\begin{bmatrix}
C_a \\
C_b
\end{bmatrix}
= \begin{bmatrix}
\bar{Q}_a \\
\bar{Q}_b
\end{bmatrix}
\]  

(165)

where

\[
\begin{bmatrix}
\bar{Q}_a \\
\bar{Q}_b
\end{bmatrix}
= \begin{bmatrix}
E_{aa} & E_{ab} \\
E_{ba} & E_{bb}
\end{bmatrix}
\begin{bmatrix}
C_a \\
C_b
\end{bmatrix}
- \frac{\Delta T}{2}
\begin{bmatrix}
K_{aa} & K_{ab} \\
K_{ba} & K_{bb}
\end{bmatrix}
\begin{bmatrix}
C_a \\
C_b
\end{bmatrix}
\begin{bmatrix}
Q_a \\
Q_b
\end{bmatrix}
\begin{bmatrix}
Q_a \\
Q_b
\end{bmatrix}
\begin{bmatrix}
Q_a \\
Q_b
\end{bmatrix}
\frac{\Delta T}{2}
\]

(166)

The first of the equations may be written as

\[
E_{aa}[C_a]_t + \frac{\Delta T}{2} [K_{aa}] [C_a]_t = \bar{Q}_a
\]

(167)

where

\[
\bar{Q}_a = \{Q_a\} - [E_{ab} + \frac{\Delta T}{2} K_{ab}] [C_b]_t
\]

(168)

Thus \( \bar{Q}_a \) is completely defined and \( [C_a]_t \) can be evaluated.
4.3.3 Modification of Diffusivity Matrix, the Capacity Matrix and the Convection Vectors for an Axisymmetric Case

The treatment presented in Section 4.3.1 was developed for a two-dimensional problem and is applicable in case of gas flow from a long ditch type fill. For an axisymmetric approximation the following modifications, due to change of elementary volume to $r d\theta dr dz$, are necessary.

4.3.3.1 Diffusivity Matrix--

$$[K^m] = \iiint [B]^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} [B] r d\theta dr dz \quad (169)$$

where matrices used above are the same as defined in equation (159).

The derived matrices

$$[B] = \begin{bmatrix} Y_1 & X_1 \\ Y_2 & X_2 \\ Y_3 & X_3 \\ Y_4 & X_4 \end{bmatrix} \quad (170)$$

are functions of $(\xi, \eta)$. The variables of integration are changed to $(\xi, \eta)$ by means of the Jacobian determinant

$$J = J(\xi, \eta) = \frac{\partial r}{\partial \xi} \frac{\partial z}{\partial \eta} - \frac{\partial r}{\partial \eta} \frac{\partial z}{\partial \xi} \quad (171)$$

Using N point Gaussian integration scheme to evaluate $K^m$, we have

$$[K^m] = \sum_{i=1}^{N} [B(\xi_i, \eta_i)]^T [D_1] [B(\xi_i, \eta_i)] r_i J(\xi_i, \eta_i) w_i \quad (172)$$

where

$$r_i = \phi^T \Sigma$$

$$D_1 = \phi^T \Delta$$

$\Sigma$, $\Delta$ being the nodal point values of radial distance from axis of fill and effective diffusion coefficients at the nodes of element $m$, and $\phi$, the vector of interpolation functions, has been defined in equation (155).

Equation (172) gives the diffusivity matrix for an interior element. For an element with a convective boundary add the convective term

$$[K^m_n] = \int_{\partial A_m} \langle b_m \rangle^T \langle b_m \rangle r dS_m \quad (174)$$
For the surface $\eta = 1$ as before

\[
\langle b_m \rangle^T = \frac{1}{2} \begin{pmatrix}
0 \\
0 \\
1 + \xi \\
1 - \xi
\end{pmatrix}
\]

and

\[
r = \frac{1}{2} \begin{pmatrix} r_3 & r_4 \end{pmatrix} \begin{pmatrix} (1 + \xi) \\ (1 - \xi) \end{pmatrix}. \tag{176}
\]

Therefore

\[
[K^m] = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 3r_3 + r_4 & r_3 + r_4 \\
0 & 0 & r_3 + r_4 & r_3 + 3r_4
\end{bmatrix} \begin{pmatrix} h^m_k \end{pmatrix} \frac{m}{12} \tag{177}
\]

and

\[
[K] = [K^m] + [K^m]. \tag{178}
\]

The convective terms $[K^m]$ apply only to the elements with convective boundaries.

4.3.3.2 Capacity Matrix $[E^m] -$

\[
[E^m] = \int_{V^m} \langle b_m \rangle^T \langle b_m \rangle dV_m
\]

\[
= \int \int \int_{\Omega} [\phi]^T [\phi] r dr dz \tag{179}
\]

Using N point Gaussian integration scheme

\[
[E^m] = \sum_{i=1}^{N} \{\phi(\xi_i, \eta_i)^T \varphi(\xi_i, \eta_i)\} r_i \{\xi_i, \eta_i\} W_i \tag{180}
\]

4.3.3.3 Vector $\{\phi(t)\}$ --

Assuming linear input

\[
Q = \frac{1}{2} (Q_i \quad Q_j) \begin{pmatrix} 1 + \xi \\ 1 - \xi \end{pmatrix}
\]
\[
\begin{align*}
\left\{ \tilde{Q}_i \right\} &= \int_{\partial\Omega_m} \left\{ \varphi_1 \right\} Q_i e dS_m \\
\left\{ \tilde{Q}_j \right\} &= \int_{\partial\Omega_m} \left\{ \varphi_2 \right\} Q_j e dS_m \\
\ &= \frac{g}{16} \int_{-1}^{1} \left\{ 1 + \frac{1}{1 - \xi} \right\} \left\{ Q_i Q_j \right\} \left\{ r_i - r_j \right\} \left\{ 1 + \frac{1}{1 - \xi} \right\} d\xi \\
\ &= \frac{g}{12} \left\{ 3Q_1 r_i + Q_1 r_j + Q_2 r_i + Q_2 r_j \right\} \\
\end{align*}
\]

In the presence of surface convection add the term
\[
\Delta t \int_{\partial\Omega_m} \left( c_e(t) + c_e(t - \Delta t) \right) \left( \dot{b}_m(x) \right) e dS_m \\
\ &= \frac{\Delta t g \bar{x} \cdot m}{16} \left( c_e(t) + c_e(t - \Delta t) \right) \int_{-1}^{1} \left\{ 1 + \frac{1}{1 - \xi} \right\} \left\{ r_i - r_j \right\} \left\{ 1 + \frac{1}{1 - \xi} \right\} d\xi \\
\ &= \frac{\Delta t g \bar{x} \cdot m}{12} \left( c_e(t) + c_e(t - \Delta t) \right) \left\{ 2r_i + r_j \right\} \\
\ &= \frac{\Delta t g \bar{x} \cdot m}{12} \left( c_e(t) + c_e(t - \Delta t) \right) \left\{ 2r_i + r_j \right\} \\
\end{align*}
\]

\[
\begin{align*}
\left\{ \tilde{Q}_i \right\} &= \frac{g}{12} \left\{ 3Q_1 r_i + Q_1 r_j + Q_2 r_i + Q_2 r_j \right\} \\
\left\{ \tilde{Q}_j \right\} &= \frac{g}{12} \left\{ Q_1 r_i + Q_1 r_j + Q_2 r_i + 3Q_2 r_j \right\} \\
\ &= \frac{\Delta t g \bar{x} \cdot m}{12} \left( c_e(t) + c_e(t - \Delta t) \right) \left\{ 2r_i + r_j \right\} \\
\ &= \frac{\Delta t g \bar{x} \cdot m}{12} \left( c_e(t) + c_e(t - \Delta t) \right) \left\{ 2r_i + r_j \right\} \\
\end{align*}
\]

where
\[
c_e(t) = \text{concentration outside the boundary at time } t.
\]
It was pointed out in Chapter III that the effective diffusion coefficient may be based on the mole fractions at the nodal points in the beginning of a time interval. Within an element an isoparametric interpolation has been used. A Crank-Nicolson time marching scheme was used for discretization along the time axis. This scheme is stable and has no restriction on discretization. The approximation errors are of the order of $O((\Delta t)^2 + (h)^2)$. However, to reduce the approximation error, $\Delta t$ should be restricted to some reasonable value. As in the finite difference program this restriction is $\Delta t \leq 1.2 \frac{h^2}{D_{\text{max}}}$. Since the size of the elements can vary, the minimum value of $h$ has to be used.

All the finite element schemes introduce some oscillations in the solution. To reduce these oscillations the initial time step is taken to be less than $\frac{1}{8} \frac{h^2}{D_{\text{max}}}$. It has been seen that these oscillations die out in a few cycles.

All other features of the finite element code are the same as for the finite difference codes. The advantage of the finite element code is that it can accommodate varying material properties, arbitrary geometries and arbitrary surface convection areas.

5.1 LIST OF PRINCIPAL VARIABLES

NUMNP = Total number of nodal points in the system

NUMEL = Number of elements in the system

NUMAT = Number of different material types

NCBC = Number of prescribed nonzero convection boundaries

NPCA = Number of prescribed concentration nodal points for decomposition period

NPCAL = Number of prescribed concentration nodal points after decomposition period
NINT = Order of integration for Gaussian quadrature formulae

NT = Maximum number of steps allowed for analysis

IPROG = Code for defining program type

  IPROG = 0 = Axisymmetric analysis program
  IPROG ≠ 0 = Cartesian coordinates program

IFREQ = Number of time increments between successive printouts

ICO2 = Code for using CO₂ reaction routine

  ICO2 = 0 = No reaction considered
  ICO2 ≠ 0 = Chemical reaction considered

TMAX1 = Duration of decomposition (days)

TMAX2 = Maximum time allowed before program termination (days)

NRADII = Array specifying number of radii for each material

RAD = Array of pore radii (Å)

FV = Array of volumetric fractions for corresponding pore radii

TORTU = Array of tortuosities (dimensionless)

R = Array of radial or x-ordinates of nodal points (cm)

Z = Array of z-ordinates of nodal points

CA = Array of mole fractions $X_A$ at nodal points

ALK = Array of alkalinities at nodal points

ALKO = Initial alkalinity in the subsoil water

HRD = Array of hardness values at nodal points

HRDO = Initial hardness of subsoil water

PH = Array of pH values at nodal points

PHO = Initial pH value of the subsoil water

RTS = RT $\frac{SAT}{100 - SAT}$ where R = 0.08205, T = temperature (K)

SAT = Degree of saturation (%)
AK₁ = K₁, first acidity constant
AK₂ = K₂, second acidity constant
HK = Kₜ, Henry's law constant for CO₂
SK = Kₛ, solid solution equilibrium constant for CaCO₃
WK = Kₛ, equilibrium constant (ion product) for water
CCO = Initial mole fraction of CO₂ in the soil
CO = Mole fraction of component A on fill boundary at the time of analysis
CFO = Array of mole fractions on fill boundary during the period of decomposition
TIM = Array of corresponding times on boundary mole fraction history curve
TIME = Time of analysis (days)
DT = Time step increment (days)
DTI = Time step increment at start of analysis and at cut-off of decomposition
CDT = Check on opening up of time step. Time step is doubled if maximum change in mole fraction at any node is less than CDT
DTT = 2.0/(DT*86400.0)
KQUNT = A count on total number of time steps
ICOUNT = A count on number of time steps since last printout
IX = Array of element data
ICBC = Array of nodal point numbers for prescribed nonzero convections
JCBC = Array of nodal point numbers for prescribed nonzero convections
NCBT = A tag on convection boundary type
HE = Array of surface convection coefficients
IPCA = Array of nodal points where concentrations are prescribed
A = Coefficient matrix
B = Flow vector or the solution vector
MBAND = Maximum band-width of the coefficient matrix
S = Element diffusivity matrix
XE = Element capacity matrix
BM = Molecular weight of gas B (g/mole)
AM = Molecular weight of gas A (g/mole)
PR = Total pressure of gas mixture (atm)
TEMP = Temperature in the system (K)
DAB = Bulk diffusion coefficient of gas A through B (cm² atm/s)

5.2 COMPUTER CODE

The finite element computer code has the capability of solving both the axisymmetric and rectangular Cartesian coordinate cases. In general, the fill is approximated by an axisymmetric solid, but in cases where the fill has a long straight boundary and the region of interest is the area close to the fill, a strip of unit thickness running normal to the fill boundary is considered. The program has a capacity of handling diffusion through four different materials arbitrarily arranged, each material having ten different pore radii. However, additional variations can be treated by increasing the dimensions of arrays for RAD, FV, NRADII and TORT. Three different surface convection coefficients have been incorporated. Any element surface can be arbitrarily assigned one of these surface coefficients. Surfaces with nonprescribed convection are taken as impervious surfaces by default. Mole fractions in the beginning of a time step are stored in array CA. To solve for mole fractions at the end of a step, coefficient matrix A and the flow vector B are set up. Matrix A and flow vector B are then modified to incorporate prescribed concentrations. The solution vector is stored back in vector B. In case of CO₂ and partially saturated soil, solution of CO₂ in ground water and resulting chain of reactions is considered in subroutine SOLUTE to get the new equilibrium concentrations. If the difference between mole fraction at the end of time increment and that at the beginning of time step is less than CDT, a specified input mole fraction (10% of maximum fill concentration), the time step ΔT is doubled subject to a maximum of ΔT of 1.2(ΔX)²/D₉₉, where ΔX is the least dimension of any element of the mesh. Mole fractions are printed out after every IFREQ steps.
5.2.1 Flow Chart

The flow chart given below gives a detail of the sequence of execution steps of the finite element code.

MAIN PROGRAM

START

HED,NUMNP,NUMEL,NUMAT,
NCBC,NPCA,NINT,NT,NPCAL,
TMAX1,TMAX2,IPROG,IFREQ,ICO2

SET UP DUMMY DIMENSIONS & ARRAYS

CALL INPUT

1

CALL SOLVE

2

STOP
SUBROUTINE INPUT

1
ENTER

Material properties—NRADIIj, TORTUj, RAD_ij, FV_ij
Nodal point data—N, Rn, Z_n, CA_n; interpolate missing
nodal points if any
Element data—N, IXni; generate missing elements
if any
Prescribed convection boundaries—NCBT_n, ICBC_n, JCBC_n
Prescribed concentrations points IPCA_i

CALCULATE BANDWIDTH—MBAND
SET UP DIMENSIONS FOR COEFFICIENT
MATRIX A AND FLOW VECTOR B

RETURN
SUBROUTINE SOLVE

ENTER

BM, AM, PR, TEMP, DAB, DTI, HE, HRDO, PHO, SAT, CDT
(TIMi, CFOi, i = 1, NCO)

FACTOR = 86400.0
TIME = 0.0
RII = 1.0
RJJ = 1.0
RIJ = 1.0
BAN = 1 - AM/BM
AK = 9.7x10^-5 TEMP/AM
DT = DTI
KOUNT = 0
ICOUNT = 0
NPC1 = 1
NPCF = NPCA - NPCAL
CCO = 0.0

INITIALIZE CONCENTRATION VECTOR

T

ICO2 = 0

F

SAT.GT.0.1

F

STOP

CALCULATE INITIAL ALKALINITY IN SOIL WATER; pH-VALUE, HARDNESS AND ALKALINITY ON SOIL FILL INTERFACE AND INITIALIZE THESE VECTORS
M, Rm, CA_m, PH_m, HDet_m, ALK_m, m = 1, NUMNP

IF MAX|CA_t - CA_t - CA_t| < CDT
   DOUBLE DT
ELSE IF MAX|CA_t - CA_t - CA_t| > 2.5*CDT
   HALVE DT

KOUNT = KOUNT + 1
ICOUNT = ICOUNT + 1
TIME = TIME + DT
DTT = 2.0/(DT*FACTOR)

TIME < TMAX1
   CALL CFIL (TIME, CO)
TIME > TMAX1 or KOUNT > NT
   INITIALIZE CONCENTRATIONS ON FILL BOUNDARY

RETURN
130

ASSEMBLE COEFFICIENT MATRIX, FLOW VECTOR MODIFY FOR PRESCRIBED CONVECTION AND PRESCRIBED CONCENTRATION BOUNDARIES

CALL BANSOL

ICO2 ≠ 0

IF

CALL SOLUTE

TIME-TMAX1 < DT

IF

ICOUNT = IFREQ

ICOUNT ≠ IFREQ

T

F

T

F

3

8

9
SUBROUTINE CFIL

4

ENTER

INTERPOLATE CONCENTRATION
ON FILL BOUNDARY AT TIME
OF ANALYSIS FROM CONCENTRATION
HISTORY DATA

RETURN
SUBROUTINE ELEMEN

ENTER

INITIALIZE \( X_{jk}, S_{jk} = 0 ; \ j, k = 1,4 \)

\( RR_1, ZZ_1, CC_1 \ i = 1,4 \)

\( MTYPE = IX(N,5) \)

\( NRAD = NRADII(MTYPE) \)

\( TORT = TORTU(MTYPE) \)

\[
D_i = \frac{1}{NRAD} \sum_{j=1}^{NRAD} \frac{F_{V_j} D_{AB}}{TORT \left( 1 - BAN \times C_i + DAB / (AK \times R_j) \right) }, \ i = 1,4
\]

CALCULATE ELEMENT DIFFUSIVITY AND ELEMENT CAPACITY MATRICES

RETURN
SUBROUTINE BANSOL

TRIANGULIZE A AND MODIFY B
BACK SUBSTITUTE TO SOLVE
FOR CONCENTRATIONS STARTING
WITH LAST NODE. VECTOR B
NOW CARRIES THE SOLUTION

RETURN
SUBROUTINE SOLUTE

K = 21
DCO = (C0 - C00)/20
CFA = CCO
PH = PHO
ALK = ALKO*2*10^-5
HRH = HRDO*10^-5

INITIALIZE BO_i = 0, i = 1, 6
TPH = 10^-PH
SET UP NONLINEAR EQUATIONS
SOLVE FOR BO_i, i = 1, 4
BY ITERATION
SOLVE FOR BO_5, BO_6
ALK = ALK + BO(1) - BO(2)
TPH = TPH + BO(1) + BO(2) + BO(4)
HRD = HRD + BO(3)
CAA = CFA - BO(6)
UPDATE VALUES FOR NODE II
5.2.2 Listing

The finite element code consists of seven routines including the MAIN program, subroutine INPUT, subroutine SOLVE, subroutine ELEMEN, subroutine BANSOL, subroutine CFIL and subroutine SOLUTE. The following pages give the program listing.
PROGRAM DIFFUSION FINITE ELEMENT
FINITE ELEMENT PROGRAM FOR DIFFUSION OF GASES FROM SANITARY LANDFILLS
PROGRAMMED BY I.S. RAI, THE OHIO STATE UNIVERSITY
IMPLICIT REAL*P(A-H,N-Z)
COMMON/OEF/NUMNP,NUMEL,NUMAT,NCBC,NPCA,MPAND,NPCA1,IPROG
1,NINT,NMC0,KOUNT
COMMON/TWO/DTT,TIMF,TMAX1,TMAX2,NF,FREQ,IC02
COMMON/THREE/MTOT,N7,N8,NQ,NAT,DAS,TORT,XE(A,A),X1,TMRTU(A)
COMMON/FOUR/FV(A,1G),RAD(A,10),HE(3),S(4,4),NRAII(4),BAN,AK,SAT,
1 DAB,TORT,XE(4,4),XJ,TORTU(4)
COMMON/FIVE/CFO(20),TIM(20),NC0
COMMON/CO8/AK1,AK2,SK,HW,HC,CO,CC0,PHO,ALKO,HRDO
DIMENSION HED(10)

THE FOLLOWING THREE CARDS SPECIFY THE STORAGE REQUIREMENTS FOR MAIN REAL AND INTEGER ARRAYS
COMMON AA(2000),IA(800)
MTOT=2000
MTOT=800

CALL ERRSET (208,256,-1,1)
10 READ (5,30) HED,NUMNP,NUMEL,NUMAT,NCBC,NPCA,NINT,N7,N8,NQ,NAT,
1 DAS,TORT,XE(4,4),XJ,TORTU(4)
I F(NUMNP.EQ.0) STOP
WRITE (6,40) HED,NUMNP,NUMEL,NUMAT,NCBC, NPCA, NINT,N7,N8,NQ,NAT,
1 DAS,TORT,XE(4,4),XJ,TORTU(4)
I F(IPROG.EQ.0) WRITE (6,50)
I F(IPROG.NE.0) WRITE (6,60)
I F(IC02.EQ.0) WRITE (6,70)
I F(IC02.NE.0) WRITE (6,80)
HCBC=NCBC
NPCA=NPCA
I F(NCEC.EQ.0) NCBC=1
I F(NPCA.EQ.0) NPCA=1
NMC0=NUMNP
I F(IC02.EQ.0) NMC0=1
N1=1
N2=N1+NUMNP
N3=N2+NUMNP
N4=N3+NUMNP
N5=N4+NMC0
N6=N5+NMC0
N7=N6+NMC0
N8=N7+NUMNP
M1=1
M2=M1+5*NUMEL
M3=M2+NCBC
M4=M3+NCBC
M5=M4+MCBC
M6=M5+MPAND
JJ=M6-MTDT-1
IF(JJ.LE.0) GO TO 20
WRITE (6,90) JJ
CALL EXIT
20 CONTINUE
CALL INPUT (AA(N1),AA(N2),AA(N3),IA(M1),IA(M2),IA(M3),IA(M4),IA(M5))
CALL SOLVE (AA(N1),AA(N2),AA(N3),AA(N4),AA(N5),AA(N6),AA(N7),AA(NP)
 1),IA(M1),IA(M2),IA(M3),IA(M4),IA(M5))
GO TO 10
C
C
C
30 FORMAT (18A4/8F15.0,3(5)I5)
40 FORMAT (1H1,18A4/35HO NUMBER OF NODAL POINTS =, I5/35HO NUMBER OF ELEMENTS =,
15/35HO NUMBER OF MATRICES =,
15/35HO NUMBER OF CONVECTION B.C. =,
15/35HO NUMBER OF INTEGRATION POINTS =,
15/35HO MAXIMUM # OF STEPS =,
15/35HO # OF CYCLES BETWEEN PRINTOUTS =,
15/35HO DECOMPOSITION TIME (DAYS) =,
15/35HO TERMINATION =,
15/35HO EXECUTION TERMINATED, REQUIRED CORE EXCEEDS MT 10 BY ,110)
END
SUBROUTINE INPUT (R, Z, CA, IX, ICBC, JCBC, NCRT, IPCA)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON/ONE/NUMNP, NUMFL, NUMAT, NCRC, MCBC, NPCA, MPCA, MPAND, NPCA1, IPPCG
NINT, NPCG, KOUNT
COMMON/TWO/TIME, TMAX1, TMAX2, NT, IFREQ, ICPO
COMMON/THREE/NTOT, NT, N7, N8, N9, N6
COMMON/FOUR/FV(4,10), RAD(4,10), HE(3), S(4,4), NRAD1(4), PAN, AK, CAT,
DAB, TORT, XE(4,4), XJ, TORTU(4)
DIMENSION R(NUMNP), Z(NUMNP), CA(NUMNP), IX(NUMEL,5), ICBC(MCBC),
JCBC(MCBC), NCRT(MCBC), IPCA(MPCA)
WRITE (6, 250)
READ MATERIAL PROPERTIES
DO 10 I=1, NUMAT
READ (5,150) NRADII(I), TORTU(I)
NRAD=NRADII(I)
READ (5,180) (RAD(I,J), FV(I,J), J=1, NRAD)
10 WRITE (6,260) I, TORTU(I), (J, RAD(I,J), FV(I,J), J=1, NRAD)
READ OR GENERATE NODAL POINT COORDINATES
WRITE (6,190)
L=0
20 READ (5,150) N, R(N), Z(N), CA(N)
NL=L+1
IF(N.EQ.1) GO TO 30
Z=X=N-L
DR=(R(N)-R(L))/ZX
DZ=(Z(N)-Z(L))/ZX
DC=(CA(N)-CA(L))/ZX
30 L=L+1
IF(N=L) GO TO 60, 50, 40
R(L)=R(L-1)+CR
Z(L)=Z(L-1)+DZ
CA(L)=CA(L-1)+DC
GO TO 30
50 WRITE (6,200) (K, R(K), Z(K), CA(K), K=NL, N)
IF(NUMNP-N) GO TO 60, 70, 20
60 WRITE (6,210) N
CALL EXIT
70 CONTINUE
WRITE (6,220)
READ OR GENERATE ELEMENT DATA
N=0
80 READ (5,160) M, (IX(M,I), I=1, 5)
90 N=N+1
IF(M.LE.N) GO TO 100
\( IX(N,1) = IX(N-1,1) + 1 \)
\( IX(N,2) = IX(N-1,2) + 1 \)
\( IX(N,3) = IX(N-1,3) + 1 \)
\( IX(N,4) = IX(N-1,4) + 1 \)
\( IX(N,5) = IX(N-1,5) \)

100 WRITE (6,230) N, (IX(N,I), I=1,5)
IF(M.GT.N) GO TO 90
IF(N.LT.NUMEL) GO TO 80
IF(NCBC.EQ.0) GO TO 110

C
C PRESCRIBED CONVECTION BOUNDARIES DATA
C
READ (5,170) (NCBT(N),ICBC(N),JCPC(N),N=1,NCBC)
WRITE (6,240) (ICBC(N),JCPC(N),NCBT(N),N=1,NCBC)
110 IF(NPCA.EQ.0) GO TO 120

C
C PRESCRIBED CONCENTRATIONS
C
READ (5,160) (TPCA(I),I=1,NPCA)
WRITE (6,270)
WRITE (6,280) (1,TPCA(I),I=1,NPCA)
120 CONTINUE
J=0
DO 130 N=1,NUMEL
DO 130 I=1,4
DO 130 L=1,4
KK=IABS(IX(N,I)-IX(N,L))
IF(KK.GT.J) J=KK
130 CONTINUE
MPAND=J+1
WRITE (6,290) MPAND
NB=N7+NUMNP*MPAND
N9=NB+NUMP
JJ=N9-NTOT-1
IF(JJ.LE.0) GO TO 140
WRITE (6,300) JJ
CALL EXIT
140 CONTINUE
WRITE (6,310) N9,M6
RETURN
C
C
150 FORMAT (I5,3F10.0)
160 FORMAT (I6I5)
170 FORMAT (3I5)
180 FORMAT (2F10.0)
190 FORMAT (54H1NODAL POINT X ORDINATE Y ORDINATE CONCENTRATION/
  1)
200 FORMAT (I12,2F13.2)
210 FORMAT (2EH0 NODAL POINT CARD ERROR N= ,I5)
220 FORMAT (50H1 ELEMENT NO. I J K L MATERIAL /)
230 FORMAT (I13,4I6,I12)
240 FORMAT (1H1,30X,'CONVECTION BOUNDARY CONDITIONS'/1H0,'NODAL POINT
 1I NODAL POINT J BOUNDARY TYPE'/(?I12))
250 FORMAT ('- MATERIAL NUMBER TORTUOSITY SERIAL NUMBER POR
1E RADIUS VOLUMETRIC FRACTION')
260 FORMAT ('-',I17,F12.3,'/',',29X,I15,2F20.4))
270 FORMAT (1H1,30X,'PREScriBED CONCENTRATION CONDITIONS'// SERIAL
1NUMBER NODAL POINT ')
280 FORMAT (' ',2I15)
290 FORMAT (PHOMPAND =,I5)
300 FORMAT (70H PROGRAM EXECUTION TERMINATED. REQUIRED CORE EXCEEDS VT
1OT BY
 9,i10)
310 FORMAT ('-FOR THIS PROGRAM THE FIRST LOCATION NOT USED IN AA IS ' ,I
110,' AND IA IS ',I10)
END
SUBROUTINE ELEMEN (R, Z, CA, IX, N)

FORM ELEMENT DIFFUSIVITY AND CAPACITY MATRICES

IMPLICIT REAL*8(A-H, O-Z)

COMMON/ONE/NUMNP, NUMEL, NUMAT, NCRC, CERC, NPCA, MCPA, MBAND, NPCA1, PROG

COMMON/NINT, NPCO, KOUNT

COMMON/FOUR/FV(4, 10), RAD(4, 10), HE(3), S(4, 4), NRADIT(4), PAN, AK, CAT,

1 DAB, TORT, XE(4, 4), XJ, TORTU(4)

DIMENSION WGT(4, 4), XXX(4, 4), O(4), PHIS(4), PHIT(4), RR(4), ZZ(4), PY(4)

1, PX(4), P(4, 4), CC(4), t(4)

DIMENSION R(NUMNP), Z(NUMNP), CA(NUMNP), IX(NUMEL, 5)

DATA WGT/ 2.000, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00/
1 1.0000000000000, 1.0000000000000, 0.00, 0.00, 0.00, 0.00/
2 5.555555555555560, 8.0(8888888000, 5.555555555555560, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00/
3 3.478548451400, 1.524151548600, 8.524151548600, 3.478548451400/
4 3.478548451400, 3.478548451400, 3.478548451400, 3.478548451400/
5 5.773502691900, 5.773502691900, 5.773502691900, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00/
6 7.745966692400, 7.745966692400, 7.745966692400, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00/
7 8.613631155900, 3.39810435900, 3.39810435900, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00/

DO 10 J = 1, 4

DO 10 K = 1, 4

XE(J, K) = C. 0

10 S(J, K) = C. 0

DO 20 I = 1, 4

J = IX(N, I)

RR(I) = R(J)

Z2(I) = Z(J)

20 CC(I) = CA(J)

M_TYPE = IX(N, 5)

NRAD = NRADIT(M_TYPE)

TORT = TORTU(M_TYPE)

DO 30 I = 1, 4

D(I) = 0.

CCC = CC(I)

DO 30 K = 1, NRAD

E = FV(M_TYPE, K) * (100.00 - SAT) / 100.00

RR = RAD(M_TYPE, K)

ETPD = E * DAR / TORT

DKR = DAB / (AK * RR)

30 D(I) = D(I) + ETPD / (1.0000 - BAN * CCC * DKR)

DO 90 M1 = 1, NINT

SS = XXX(M1, NINT)

SM = (1.0 - SS) * 0.25

SP = (1.0 + SS) * 0.25

PHIT(1) = -SM

PHIT(2) = -SP

PHIT(3) = SP

PHIT(4) = SM

DO 90 M2 = 1, NINT

TT = XXX(M2, NINT)

TM = (1.0 - TT) * 0.25
TP=(1.0+TT)*0.25
PHIS(1)=-TM
PHIS(2)=TM
PHIS(3)=TP
PHIS(4)=-TP
Q(1)=SM*TM/0.25
Q(2)=SP*TM/0.25
Q(3)=SP*TP/0.25
Q(4)=SM*TP/0.25
DO 40 I=1,4
DO 40 J=1,4

40 P(I,J)=PHIS(I)*PHIT(J)-PHIT(I)*PHIS(J)
XJ=0.0
DO 50 I=1,4
DO 50 J=1,4

50 XJ=XJ+RR(I)*P(I,J)*ZZ(J)
DD=0.0
RI=0.0
DO 70 I=1,4
PX(I)=0.0
PY(I)=0.0
DO 60 J=1,4
PX(I)=PX(I)+P(I,J)*RR(I)

60 PY(I)=PY(I)+P(I,J)*ZZ(I)
DD=DD+D(I)*Q(I)
RI=RI+RR(I)*Q(I)
PX(I)=-PX(I)/XJ

70 PY(I)=PY(I)/XJ
IF(IPROG.NE.0) RI=1.0
GT=WGT(M1,NINT)*WGT(K2,NINT)*XJ*RI
DO 80 I=1,4
DO 80 J=1,4
XE(I,J)=XE(I,J)+Q(I)*Q(J)*GT

80 S(I,J)=S(I,J)+(PY(I)*PY(J)+PX(I)*PX(J))*DD*GT
CONTINUE
RETURN
END
SUBROUTINE SOLVE (R, Z, CA, ALK, PH, HRD, X, ICBC, JCB, NCBT, IPCA)

IMPLICIT RFAL*RF(A-H,0-9)

COMMON/ONE/NUMNP, NUMEL, NUMAT, NCEC, MCBC, NPCA, MPCA, MBAND, NPCA1, IPRNG
1*INT, N*COMRT, KOUNT,

COMMON/THD/TIME, TMAX1, TMAX2, NT, IFREQ, ICO2

COMMON/FVE/TV(14,10), RAD(4,10), HE(5), S(4,4), HRADII(4), PAN, AK, SAT,

1 DB, TORT, XE(4,4), XJ, TORTU(4)

COMMON/FIV/CF0(20), TVM(20), NCO

COMMON/CO2/AC1, AK2, SK, WK, HK, CO, CC0, PHO, AK0, HRD0

DIMENSION R(NUMNP), Z(NUMNP), CA(NUMNP), IX(NUMEL), ICBC(0.5), NCBT(MNCB)

1 JCB(MCB), NCBT(MCBB), IPCA(MPCA), A(NUMNP, MBAND), R(NUMNP)

2*ALK(NMNC), PH(NMNC), HRD(NMNC)

READ (5,290) RH, AM, PR, TEMP, DAB, CDT, GTI, HE, HRD0, PHO, SAT
WRITE (6,300) AM, PR, TEMP, DAB, CDT, GTI, HE, HRD0, PHO, SAT

READ (5,310) NCO, (TIM(I), CFO(I), I = 1, NCO)
WRITE (6,320) (TIM(I), CFO(I), I = 1, NCO)

FACTOR = 86.400/0.0

TIME = 0.0

DTMAX = 22.0

PI = 3.14159265358979

ELL = 1600.0

P1 = PI/ELL

RII = 1.0

RJ = 1.0

BAN = 1.0 - C3RT(AM/BM)

AK = 9.70 - 05*DSR(TMP/AM)

DT = DTI

KOUNT = 0

ICOUNT = 0

NPC1 = 1

NPCF = NPCA - NPCA1

CO = 0.0

IF (CO2.EQ.0) GO TO 60

IF (SAT.GT.0.1) GO TO 10

WRITE (6,280)

CALL EXIT

TPH = 10.0D0**(-PHO)

RTS = 0.0E205*TEMP*SAT/(100.0D0 - SAT)

AK1 = 4.44E0 - 07

AK2 = 4.6E0 - 11

HK = 3.3E0 - 02

SK = 4.5E0 - 09

WK = 1.0D0 - 14

H1 = TPH

D1 = HRD0*1.00 - 5

B1 = (H1 + 2.0*D1 - WK/H1)/(1.0 + 2.0*AK2/H1)

ALK0 = B1/2.0 - 0.05

CO = H1*B1/(AK1*HK)

CO = CFO(I)
DO 20 M=1,NUMNP
CA(M)=CC0
ALK(M)=ALKO
PH(M)=PHO

20 HRD(M)=HRDO

CALL SOLUTE (CA, PH, ALK, HRD, RTS, TIME, TMAX1)
DO 30 M=1,NPCF
CA(M)=CO
ALK(M)=ALKO
PH(M)=PHO

30 HRD(M)=HRDO

IF(ICO2.EQ.0) GO TO 60
WRITE (6,I30) TIME, DT, KOUNT
DO 50 M=1,NUMNP

50 WRITE (6,I30) M, R(M), Z(M), CA(M), ALK(M), PH(M), HRD(M)
GO TO 80

60 WRITE (6,I30) TIME, DT, KOUNT
DO 70 M=1,NUMNP
70 WRITE (6,I30) M, R(M), Z(M), CA(M)

80 IF(KOUNT.EQ.0) GO TO 100
QQ=0.0
DO 90 I=1,NUMNP

90 CONTINUE
IF(QQ.LT.CD1) DT=2.0*DT
IF(DT.GT.DTMAX) DT=DTMAX
IF(QQ.GT.(2.5*CDT)) DT=0.5*QQ*CDT
IF(TIME.GT.TMAX1) GO TO 100
TCHEK=TMAX1-TIME
IF(TCHEK.LT.DT) DT=TCHEK
IF(DABS(TCHEK).LT.DT1) DT=DT1

100 DO 110 I=1,NUMNP
110 CA(I)=B(I)

120 KCOUNT=KCOUNT+1
ICOUNT=ICOUNT+1
TIME=TIME+DT
DTT=2.0/(DT*FACTOR)
IF(TIME.GT.TMAX1) GO TO 140

CALL CFIL (TIME,CO)
DO 130 M=1,NPCF
130 I=IPCA(M)

140 DO 150 M=1,NUMNP
B(M)=0.0
DO 150 N=1,MRAND
150 A(M,N)=0.0
IF(TIME.GT.TMAX2.OR.KCOUNT.GT.NT) RETURN
IER=0
DO 170 N=1,NUMEL
CALL ELEMEN (R,Z,CA,IX,N)
IF(XJ.GT.0.) GO TO 160
IER=1
WRITE (6,?20) N,XJ
160 CONTINUE
DO 170 J=1,4
II=IX(N,I)
DO 170 J=1,4
SIJ=S(I,J)
XEIJ=XE(I,J)*DTT
JJ=IX(N,J)
B(IJ)=B(IJ)+(XEIJ-SIJ)*CA(JJ)
JJ=JJ-1+1
IF(JJ.LE.0) GO TO 170
A(IJ,JJ)=A(IJ,JJ)+XEIJ+SIJ
170 CONTINUE
IF(IER.EQ.1) CALL EXIT
IF(INCBC.EQ.0) GO TO 210
C
C ALLOW FOR BOUNDARY CONVECTIONS
C
DO 200 N=1,NCBC
II=ICBC(N)
JJ=JCBC(N)
LL=NCBT(N)
DL=DSQRT((R(II)-R(JJ))^2+(Z(II)-Z(JJ))^2)
IF(IPROG.NF.0) GO TO 180
RII=(3.0*R(II)+R(JJ))/4.0
RJJ=(3.0*R(JJ)+R(II))/4.0
RIJ=(R(II)+R(JJ))/2.0
180 HFI=HE(II)
A(IJ,1)=A(IJ,1)+HE1*DL/3.*RII
A(JJ,1)=A(JJ,1)+HE1*DL/3.*RJJ
KK=JJ-II+1
IF(KK.GT.0) GO TO 190
KK=II-JJ+1
A(JJ,KK)=A(JJ,KK)+HE1*DL/6.*RIJ
GO TO 200
190 A(IJ,KK)=A(IJ,KK)+HE1*DL/6.*RIJ
200 CONTINUE
210 IF(NPCA.EQ.0) GO TO 270
C
C MODIFY FOR PRESCRIBED CONCENTRATIONS
C
IF(TIME.GT.TMAX) NPC1=NPCF+1
DO 260 I=NPC1,NPCA
II=IPCA(I)
IF(II.EQ.1) GO TO 230
DO 260 II=1,II
NPCA=II
260 CONTINUE
JJ=II-MBAND+1  
IF(JJ.LE.0) JJ=1  
LL=II-1  
DO 220 NN=JJ,LL  
KK=II-NN+1  
B(NN)=B(NN)-A(NN,KK)*CA(II)  
220 A(NN,KK)=0.0  
230 A(II,1)=1.0  
B(II)=CA(II)  
IF(II.EQ.NUMNP) GO TO 250  
LL=MBAND-1  
KK=NUMNP-II  
IF(KK.LT.MBAND) LL=KK  
DO 240 NN=1,LL  
B(II+NN)=B(II+NN)-A(II,NN+1)*CA(II)  
240 CONTINUE  
250 CONTINUE  
260 CONTINUE  
C  
C  
270 CALL BANSOL(A,E,NUMNP,MEAND)  
IF(ICOZ2.NE.0) CALL SOLUTE(E,PH,ALK,PRD,RTS,TIMF,TMAX1)  
IF(DABS(TIME-TMAX1).LT.0.1) GO TO 100  
C  
PRINTER CONCENTRATIONS AND ALLOW FOR CHANGE IN T  
C  
ICOUNT=0  
GO TO 40  
C  
C  
280 FORMAT ('ANALYSIS TERMINATED. DEGREE OF SATURATION LESS THAN 1 0.1%')  
290 FORMAT ('G10.0')  
300 FORMAT ('G10.3/45 MOLECULAR WEIGHT OF GAS B (GM/MOLE) '  
1H MOLECULAR WEIGHT OF GAS A (GM/MOLE) =F10.3/45 PRESSURE  
21(AMOS) =F10.3/45H TEMPERATURE (DEG KEL  
3VIN) =F10.3/45BULK DIFFUSION COEFFICIENT (CM S  
4Q ATMOS/SEC)=F10.3/45H MOLE FRACTION FOR DT CHECK  
5 =F10.3/45H INITIAL DT =F10.3/45H  
6H SURFACE PERMEABILITY COEFFICIENT =E13.5/45H END PERME  
7ABILITY COEFFICIENT =E13.5/45H PERMEABILITY COEFFIC  
8= =E13.5/45H INITIAL HARDNESS  
9 =F10.3/45H INITIAL PH VALUE =F10.3/45H DEGREE OF SATURATION  
10 =F10.3/45H  
310 FORMAT ('G10.3/45')  
320 FORMAT ('G10.0')  
330 FORMAT ('G10.3/45 HISTORt OF FILL CONCENTRATIONS'/0 TIME (DAYS) MOLE  
1E FRACTION'/1'G10.3/45')  
340 FORMAT ('G10.3/45')  
350 FORMAT ('G10.3/45')  
360 FORMAT ('G10.3/45')  
END
SUBROUTINE CFIL (TAU, CO)
IMPLICIT REAL*P (A-H,O-Z)
COMMON/FIVE/CFO(20), TIM(20), NCO

THIS SUBROUTINE COMPUTES APPLIED MOLE FRACTIONS FROM GIVEN HISTORY

DO 10 I=1, NCO
IF(TAU*FO.0.0 DO) GO TO 20
IF(TAU-TIM(I)) 30,30,10
10 CONTINUE
20 CO=CFO(I)
GO TO 40
30 TX=(TAU-TIM(I-1))/(TIM(I)-TIM(I-1))
CO=CFO(I-1)+(CFO(I)-CFO(I-1))*TX
40 CONTINUE
RETURN
END
SUBROUTINE SOLUTE (CA,HP,AKL,HDR,RTS,TAU,TMAX1)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONF/NUMP,NUMAT,NCBC,MCBC,NPCA,MPCA,MNAME,NPCAI,IPRNG
1,NINT,NUMC0,KOUNT
COMMON/C02/AK1,AK2,SK,WK,HK,CO,CCP,PHD,ALK0,HRO0
DIMENSION CA(NUMP),HP(NUMP),AKL(NUMP),HDR(NUMP),A(4,4),B(4,4)

1 BO16
TOL=1.0D-18
N=4
DO 120 II=1,NUMP
IF(KOUNT.EQ.0) GO TO 10
KKK=1
PH=HP(II)
ALK=AKL(II)*2.0D-05
CFA=CA(II)
HRD=HDR(II)*1.0D-05
DC0=0.00
GO TO 20
10 DCO=(DC0-CC0)/2.0D-05
CFA=CC0
PH=PH0
ALK=ALK0*2.0D-05
HRD=HRD0*1.0D-05
KKK=2
20 DO 30 I=1,6
30 B0(I)=0.00
TPH=10.0D0**(-PH)
DO 110 KK=1,KKK
CFA=CFA+DC0
C8=AK2*ALK/TPH
C9=WK/TPH
C10=HRD/TPH
C1=TPH*ALK/AK1-HK*CFA
C2=1.0D0+HK*RTS
C3=AK1*(1.0D0-C2)/C2-TPH-ALK
C4=TPH-ALK
C5=AK2-C8
C6=AK2+C8+TPH
C7=AK1*C1/C2
40 B(1)=-C3*B0(1)-C4*B0(2)+BO(1)**2-BO(2)**2+C7+ALK**50(4)+90(1)**90(4)
1-BO(2)**10(4)
B(2)=-C5*B0(1)+C6*B0(2)+TPH*PO(3)+C8*PO(4)+PO(1)**2+PO(2)**2+PO(3)**2
B(3)=HRD*BO(2)-C10*BO(3)-PO(2)**2+PO(3)**2
B(4)=-C9*BO(1)-C9**2+PO(2)**2+PO(3)**2
41**2
IF(DABS(B(1)).GT.TOL) GO TO 50
IF(DABS(B(2)).GT.TOL) GO TO 50
IF(DABS(B(3)).GT.TOL) GO TO 50
IF(DABS(B(4)).GT.TOL) GO TO 50
GO TO 100

50 A(1,1)=C3-2.0D0*BO(1)-BO(4)
A(1,2)=C4+2.0D0*BO(2)+BO(4)
A(1,3)=0.0D0
A(1,4)=ALK-BO(1)+BO(2)
A(2,1)=C5-BO(2)-BO(3)
A(2,2)=-C6-BO(1)-2.0D0*BO(2)-5.0D0*BO(3)-BO(4)
A(2,3)=TPH-BO(1)-5.0D0*BO(2)-BO(4)
A(2,4)=-C6-BO(2)-BO(3)
A(3,1)=0.0D0
A(3,2)=HRD+BO(3)
A(3,3)=C10+BO(2)+2.0D0*BO(3)
A(3,4)=0.0D0
A(4,1)=C5+BO(4)
A(4,2)=A(4,1)
A(4,3)=0.0D0
A(4,4)=C9+TPH+BO(1)+BO(2)+2.0D0*BO(4)

DO 60 J=2,N
DO 60 K=J,N
Q=A(J,J-1)/A(J-1,J-1)
B(J)=B(J)-R*B(J-1)
DO 60 K=J,N

60 DO 70 J=2,N
K=N-J+2
R=B(K)/A(K,K)
DO 70 J=J,N
L=N-J+1

70 DO 80 I=1,N
B(I)=B(I)-R*A(L,I)
DO 80 I=1,N

80 B(I)=B(I)/A(I,I)
DO 90 I=1,N

90 BO(I)=BO(I)+B(I)
GO TO 50

100 BD(N+1)=(BO(1)-C1)/C2
BD(N+2)=BD(N+1)*RTS
ALK=ALK+BD(1)-BD(2)
TPH=TPH+BD(1)+BD(2)+BD(4)
HRD=HRD+BD(3)
CAA=CFA-BO(6)
IF(KK.EQ.20) DCO=BO(6)*BO(6)/DC0

110 CONTINUE
IF(KCOUNT.EQ.0) GO TO 130
ALK(I)=ALK/2.0D-05
HP(I)=-DLOG10(TPH)
CA(I)=CAA
HDR(I)=HRD/1.0D-05

120 CONTINUE
RETURN

130 PHO=-DLOG10(TPH)
ALKD=ALK/2.0D-05
HRDD=HRD/1.0D-05
RETURN

END
SUBROUTINE BANSOL (A, B, NN, MM)

C
C  BANDED SYMMETRIC EQUATION SOLVER
C
IMPLICIT REAL*8 (A-H, O-Z)
DIMENSION A(NN, MM), B(NN)
DO 30 N=1, NN
IF(A(N+1) .EQ. 0.) GO TO 30
B(N)=B(N)/A(N+1)
DO 20 L=2, MM
IF(A(N+L) .EQ. 0.) GO TO 20
C=A(N+L)/A(N+1)
I=N+L-1
J=0
DO 10 K=L, MM
J=J+1
A(I, J)=A(I, J)-C*A(N, K)
B(I)=B(I)-A(N, L)*B(N)
A(N, L)=C
20 CONTINUE
30 CONTINUE
DO 50 W=1, NN
N=NN+1-W
DO 40 K=2, MM
L=N+K-1
IF(L .GT. NN) GO TO 50
B(N)=B(N)-A(N, K)*B(L)
40 CONTINUE
50 CONTINUE
RETURN
C
END
### Instructions for Data Preparation

The following sequence of punched cards will carry the problem data for input to the program.

**Card 1: Title Card (18A4)**

This card gives a descriptive information for identification of the job.

**Card 2: Control Data (8I5, 2F10.0, 3I5)**

This card carries the following information:

<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of nodal points (NUMNP)</td>
<td>1-5</td>
</tr>
<tr>
<td>Number of elements (NUMEL)</td>
<td>6-10</td>
</tr>
<tr>
<td>Number of materials (NUMAT)</td>
<td>11-15</td>
</tr>
<tr>
<td>Number of convection boundary conditions (NCBC)</td>
<td>16-20</td>
</tr>
<tr>
<td>Number of prescribed concentration nodes (NPCA)</td>
<td>21-25</td>
</tr>
<tr>
<td>Number of integration points for the element (NINT)</td>
<td>26-30</td>
</tr>
<tr>
<td>Maximum number of execution steps allowed before program termination (NT)</td>
<td>31-35</td>
</tr>
<tr>
<td>Number of prescribed concentration nodes after decomposition time (NPCAL)</td>
<td>36-40</td>
</tr>
<tr>
<td>Decomposition time (TMAX1) (days)</td>
<td>41-50</td>
</tr>
<tr>
<td>Time for termination of analysis (TMAX2)</td>
<td>51-60</td>
</tr>
<tr>
<td>Program code (IPROG)</td>
<td>61-65</td>
</tr>
<tr>
<td>IPROG = 0 = Axisymmetric code</td>
<td></td>
</tr>
<tr>
<td>IPROG ≠ 0 = Cartesian coordinates code</td>
<td></td>
</tr>
<tr>
<td>Number of time steps between successive printouts (IFREQ)</td>
<td>66-70</td>
</tr>
<tr>
<td>Chemical reaction code (ICO2)</td>
<td>71-75</td>
</tr>
<tr>
<td>ICO2 = 0 = CO₂ reaction not considered</td>
<td></td>
</tr>
<tr>
<td>ICO2 ≠ 0 = CO₂ reaction considered</td>
<td></td>
</tr>
</tbody>
</table>
Card Set A:

This set of cards consists of subsets of cards giving material properties. Total number of subsets is equal to the total number of material types considered. A provision has been built in the program to cater for four different types of materials, each having 10 different pore radii. Each subset carries the following information:

1st card: \((15, F10.0)\)

<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total number of pore radii (NRADII)</td>
<td>1-5</td>
</tr>
<tr>
<td>Tortuosity (TORTU)</td>
<td>6-15</td>
</tr>
</tbody>
</table>

Card Subset consisting of NRADII cards, each containing the following information \((2F10.0)\)

<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pore radius (RAD) (Å)</td>
<td>1-10</td>
</tr>
<tr>
<td>Volumetric fraction (FV) (dimensionless)</td>
<td>11-20</td>
</tr>
</tbody>
</table>

Card Set B: Nodal point data \((15, 3F10.0)\)

This set consists of cards containing the nodal point data as given below:

<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nodal point number (N)</td>
<td>1-5</td>
</tr>
<tr>
<td>R-ordinate R(N)</td>
<td>6-15</td>
</tr>
<tr>
<td>Z-ordinate Z(N)</td>
<td>16-25</td>
</tr>
<tr>
<td>Initial concentration CA(N)</td>
<td>26-35</td>
</tr>
</tbody>
</table>

Any missing nodal point data is generated by linear interpolation.

Card Set C: Element data \((6I5)\)

A set of cards containing the following information is required:

<table>
<thead>
<tr>
<th>Information</th>
<th>Columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Element number</td>
<td>1-5</td>
</tr>
<tr>
<td>Nodal point I</td>
<td>6-10</td>
</tr>
</tbody>
</table>
Information Columns

Nodal point J 11-15
Nodal point K 16-20
Nodal point L 21-25
Material type 26-30

Note: Nodal points I, J, K, L are to be input as if the boundary of the element is traversed anticlockwise. Missing elements are generated by incrementing the element and nodal point number of the previous element by 1 each, whereas the material type is kept the same.

Card Set D: Convection boundary cards (315)

A set of cards containing NCBC cards with the following information is required.

Information Columns

Convection boundary type (NCBT) 1-5
Nodal point I (ICBC) 6-10
Nodal point J (JCBC) 11-15

Card Set E: Prescribed concentration points (1615)

A set of cards giving nodal point numbers for NPCA nodal points is required. Nodal points at which the concentration remains prescribed (NPCA) after the decomposition time also should be input towards the end of the list.

Card Set F:

This set consists of two cards containing the following information in the sequence described below.

Information Columns

Molecular weight of gas B (BM) (g/mole) 1-11
Molecular weight of gas A (AM) (g/mole) 11-20
Total pressure of mixture of gases (PR) (atm) 21-30
Temperature of mixture of gases (TEMP) (K) 31-40
Bulk diffusion coefficient (DAB) (cm² atm/s) 41-50
### Information Columns

| Time increment at the start of program (DTI) (days) | 51-60 |
| Convection coefficient for surface type 1 (HE(1)) (cm atm/s) | 61-70 |
| Convection coefficient for surface type 2 (HE(2)) (cm atm/s) | 71-80 |
| Convection coefficient for surface type 3 (HE(3)) (cm atm/s) | 1-10 |
| Initial hardness of subsoil water (HRDO) | 11-20 |
| Initial pH-value of subsoil water | 21-30 |
| Degree of saturation (S) | 31-40 |

**Card Set G: History of concentrations on the soil boundary ([5/12F10.0])**

This set gives the concentration history on the fill boundary, during the decomposition period TMAX1, in the following sequence

1st card:

| Information | Columns |
| Number of points on the concentration history curve (NCO) | 1-5 |

Set of NCO cards each containing the following information.

| Information | Columns |
| Time (TIM) (days) | 1-10 |
| Mole fraction on the boundary of fill (CFO) (dimensionless) | 11-20 |

### 5.2.4 Example Problem IV - Diffusion of Methane

As an example problem, diffusion of methane from a landfill of the shape of the city of Hopkins, Minnesota fill was selected. The boundary at 100 meters is taken as a prescribed zero concentration boundary, surface convection was allowed on top. The convection coefficient was used for a 5 mph wind velocity. The boundary at a depth of 8.1 meters is taken to be impervious due to the presence of the groundwater table at that depth. The surrounding soil is assumed to consist of two layers, silt and clay, with a trench filled with gravel acting as a vent. Figure 5 shows the physical problem and the finite element mesh used for getting the solution.
Fig. 5a - Example problem IV using finite element analysis.
Fig. 5b - Finite element mesh for example problem IV.
5.2.4.1 **Input**-

The following sequence of input was used.

```
DIFFUSION OF METHANE THROUGH LAYERED SOIL WITH VFNT
90 68  3 12  14 2 500 6 1825.0 3665.00 1 10
   1  1.50
120000.0 0.400
  10 3.0
   63.5 0.0220
  138.5 0.0380
  300.0 0.0440
  655.0 0.0480
  1450.0 0.0456
  3150.0 0.0464
  6850.0 0.0480
  15200. 0.0480
  35000.0 0.0380
  72500.0 0.0220
   1  1.05
200000.0 0.400
  1  0.0  0.0
  3  0.0  270.0
  6 550.0  0.0
  7 1100.0  0.0
  9 1100.0  270.0
 10 1650.0  0.0
 12 1650.0  270.0
 13 2200.0  0.0
 15 2200.0  270.0
 18 2700.0  810.0
 19 2800.0  0.0
 21 2800.0  270.0
 24 2800.0  808.0
 25 3400.0  0.0
 27 3400.0  270.0
 30 2900.0  806.0
 31 3500.0  0.0
 33 3500.0  270.0
 36 3500.0  800.0
 37 3600.0  0.0
 39 3600.0  270.0
 42 4100.0  795.0
 43 3900.0  0.0
 45 3900.0  270.0
 48 4200.0  793.0
 49 4300.0  0.0
 51 4300.0  270.0
 54 4300.0  790.0
 55 4800.0  0.0
 57 4800.0  270.0
 60 4800.0  785.0
 61 5400.0  0.0
```
<table>
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<th>67</th>
<th>69</th>
<th>72</th>
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<td>11</td>
<td>5</td>
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</tr>
</tbody>
</table>

The table continues with similar entries.
5.2.4.2 Output—

The following two pages present the computer output of mole fractions at the end of the decomposition period of five years. Figures 6a through 6d give the mole fraction contours at times equal to 335, 1825, 2140 and 3500 days. A contour interval of 0.05 has been used.
Fig. 6a - Mole fraction contours for example problem IV for $t = 335$ days.
Fig. 6b - Mole fraction contours for example problem IV for $t = 1825$ days.
Fig. 6c – Mole fraction contours for example problem IV for t = 2140 days.
Fig. 6d - Mole fraction contours for example problem IV for $t = 3500$ days.
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>43</td>
<td>3900.0</td>
<td>0.0</td>
<td>0.327573</td>
</tr>
<tr>
<td>44</td>
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<td>4200.0</td>
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CHAPTER VI

COMPARISON BETWEEN FINITE DIFFERENCE AND
FINITE ELEMENT METHODS

The finite element method (FEM) and the finite difference method (FDM) are extensively used for solution of initial boundary value problems. The FEM starts with a variational statement of the problem and introduces piecewise definitions of the functions defined by a set of meshpoint values. The FDM starts with a differential statement of the problem and proceeds to replace the derivatives with their discrete analogs.

Both methods result in a set of algebraic equations relating a discrete set of variables in place of relations in continuous variables. These algebraic equations are remarkably similar and provide the basis for identifying the methods as essentially similar. While the two approaches actually rely on very different descriptions for their discussions, they have closely related applications. Both approaches are adopting features of the other that prove to be attractive. The FDM has found the variations approach (Bushnell, 1973) of the FEM useful in producing symmetric difference equations, the FEM rather than using a time dimension on an element invariably uses a step forward finite-difference technique in the time domain. In short, both methods arrive at a discrete analog to the problem, the FEM by minimizing an extremum principle over a family of functions, having compact support, and defined piecewise, the FDM by using discrete approximations to integrals and derivatives occurring in balance equations. Zienkiewicz and Cheung (1965) observed similarities in algebraic equations resulting from FEM and FDM. Gondreau (1970) has an extensive treatment on "Evaluation of Discrete Methods for Linear Dynamic Response of Elastic and Viscoelastic Solids." Pian (1971) has discussed a variety of element patterns along with several finite-difference approaches and compares the resulting discrete analogs. There are so many approaches in each of the two procedures that it is very difficult to pinpoint the method and approach that will be best suited for the problem under study.

6.1 COST EFFECTIVENESS

R. L. Schiffman, (1972) has discussed at length cost-effective computations for soil engineering problems in his paper, "The Efficient Use of Computer Resources." He has presented a comparison between explicit, implicit and Crank-Nicolson FDM's and the FEM's using linear,
quadratic and cubic elements. He compares the CPU time, storage require-ment and accuracy for the above mentioned six cases and concludes that for the consolidation problem, which is quite similar to a diffusion problem, the finite element method always requires more storage capacity and more solution time as compared to FDM. However, once the procedure is set up it requires no additional effort to solve problems with different geometries or boundary conditions.

6.2 ACCURACY AND STABILITY

It is difficult to determine exactly how much error is involved in the two methods and which of the two is more stable. The procedure for error analysis depends on the method of error estimation and the error bounds are, in turn, based on the procedure adopted in each of the two methods. In the recent years, mathematicians and analysts have shown a considerable interest in the error and stability analysis of the FEMs, almost on the same lines as is done in the case of FDMs. Some of the recent papers are: (1) Donea, J., (1974), "On the Accuracy of Finite Element Solutions to Transient Heat Conduction Equations;" (2) Price and Varga (1968), "Numerical Methods of High Order Accuracy for Diffusion-Convection Equations;" (3) Babuska, I., (1973), "Finite Element Method with Penalty;" (4) Douglas and Dupont (1973), "A Finite Element Colocation Method for Quasilinear Parabolic Equations;" and Oden, J. T., (1974), in his supplementary notes on Mathematical Theory of Finite Element Methods, has a chapter on Time Dependent Problems. Oden claims that "this chapter is a very new and incomplete addition." However, he has given several distinct methods for study of the problem of accuracy, convergence and stability. He has characterized these techniques into four categories:

1. Semigroup Theoretic Estimates
2. Energy Methods
3. $L_2$ Methods
4. Other Methods

For example, in the semigroup theoretic estimates Oden uses norms, $\| \cdot \|_m$, to calculate the error bounds. Let

$$e = \text{approximation error},$$
$$\sigma = \text{semidiscrete approximation error},$$
$$\tau = \text{temporal approximation error}.$$

The approximation error may be evaluated following the work of Oden.

Consider the set of time-dependent problems characterized by equations of the form
\[ \frac{\partial u(x,t)}{\partial t} + A(x)u(x,t) = f(x,t) \]

\[ x \in \Omega; \quad t \in (0,T] \]

\[ D^m(x,t) = 0 \]

\[ x \in \partial \Omega; \quad |g| \leq m - 1 \]

\[ u(x,0) = u_0(x) \quad x \in \Omega. \]  

(184)

and \( A \) is the \( m \)th order differential operator. Equation (184) can be replaced by the equivalent variational problem

\[ \left( \frac{\partial u(t)}{\partial t},v \right)_0 + a(u(t),v) = (f(t),v)_0 \]

\[ (u(\cdot,0),v)_0 = (u_0,v)_0 \quad v \in H^m_0(\Omega) \]

\[ t \in (0,T) \]  

(185)

where \( H^m_0(\Omega) \) is the Sobolev space of \( H^m(\Omega) \) functions with compact support in \( \Omega \).

Now consider a Galerkin approximation of equation (185) which involves the search of a function \( U(x,t) \in S_h(\Omega) \times C^1(0,T) \) such that

\[ \left( \frac{\partial U(t)}{\partial t},v \right)_0 + a(U(t),v) = (f(t),v)_0 \quad t \in (0,T] \]

\[ (U(\cdot,0),v)_0 = (u_0,v)_0 \quad v \in S_h(\Omega) \]  

(186)

If \( u(x,n\Delta t) \) is the solution to equation (185) at time \( t = n\Delta t \) and \( U(x,n\Delta t) \) is the solution to equation (186) at time \( t = n\Delta t \), then the semidiscrete approximation error (Oden, 1974)

\[ \| \sigma(x,n\Delta t) \|_m = \| u(x,n\Delta t) - U(x,n\Delta t) \| \]

\[ \leq c_1 h^{k+1-m} |u(x,n\Delta t)|_{k+1} \]

(187)

For the problem described by equation (15), \( m = 1 \), and using quadratic element, \( k = 2 \). This gives

\[ |\sigma(x,n\Delta t)| \leq c_1 h^2 |u(x,n\Delta t)| \]

(188)

To evaluate the temporal approximation error we proceed as follows. The Crank-Nicolson difference approximation to equation (186) is
\[ (\delta_t u^n, v)_o + \frac{1}{2} a(u^{n+1}, v) + \frac{1}{2} a(u^n, v) = (f(t), v)_o \quad t \in (0, T] \]

\[ (u^0, v)_o = (u^o, v) \quad v \in \mathcal{S}_h(\Omega) \quad (189) \]

where \( \delta_t \) denotes the forward difference operator, i.e.,

\[ \delta_t u^n = \frac{u^{n+1} - u^n}{\Delta t} \quad (190) \]

\[
\| \mathcal{T}(x; n\Delta t) \|_m = \| u(x; n\Delta t) - u^n(x) \|_m \\
= \left\| E_h(x; n\Delta t, 0) - E_h^{\Delta t, \frac{1}{2}}(x; n\Delta t, 0) u^o(x) \right\|_m \\
= \left\| \sum_{\nu=1}^{n} E_h^{\Delta t, \frac{1}{2}}(x; n\Delta t, \nu\Delta t) \left[ E_h^{\Delta t, \frac{1}{2}}(x; \nu\Delta t, (\nu - 1)\Delta t) - E_h(x; \nu\Delta t, (\nu - 1)\Delta t, 0) u^o(x) \right] \right\|_m \\
\leq \sum_{\nu=1}^{n} \| E_h^{\Delta t, \frac{1}{2}}(x; n\Delta t, \nu\Delta t) \| \| E_h^{\Delta t, \frac{1}{2}}(x; \nu\Delta t, (\nu - 1)\Delta t) \| \\
- E_h(x; \nu\Delta t, (\nu - 1)\Delta t) \| \| E_h(x; (\nu - 1)\Delta t, 0) u^o(x) \|_m \quad (191) \]

If the finite difference-Galerkin problem is assumed to be stable and well posed, the fundamental solution operator and the amplification matrix are bounded, i.e.,

\[
\| E_h(x; (\nu - 1)\Delta t, 0) u^o(x) \|_m \leq C_2 \| u(x) \|_m \quad \nu = 0, 1, \ldots, N \\
U \in \mathcal{S}_h(\Omega) \quad (192) \\
\| E_h^{\Delta t, \frac{1}{2}}(x; n\Delta t, \nu\Delta t) v(x) \|_m \leq C_4 \| v(x) \|_m \\
= \sup_{v \in \mathcal{S}_h(\Omega)} \left\| E_h^{\Delta t, \frac{1}{2}}(x; n\Delta t, \nu\Delta t) v(x) \right\|_m / \| v(x) \|_m \\
\leq C_3 \quad 0 \leq \nu \leq n \leq N \quad (193) \]

and using Pade's approximations

\[
\| E_h(x; \nu\Delta t; (\nu - 1)\Delta t) - E_h^{\Delta t, \frac{1}{2}}(x; \nu\Delta t, (\nu - 1)\Delta t) \| \leq C_4 \Delta t^3 \quad (194) \]

Substituting equations (192), (193), and (194) in equation (191) gives
\[ \| \tau(x, n \Delta t) \|_m \leq \sum_{n=1}^{\infty} \nu C_3 C_4 \Delta t^3 C_2 \| u(x) \|_m \leq \nu C_3 \Delta t^2 \| u(x) \|_m \] (195)

Then the approximation error

\[ \| e \| \leq \| u \| + \| \tau \| \leq C_1 h^2 \| u(x, n \Delta t) \| + C_5 \Delta t^2 \| u_0(x) \| \] (196)

In the finite difference field Douglas, Varga, Ames, Bellman, Lees, and Peaceman, among others, have discussed at length the error estimates. For Crank-Nicolson discretization the error

\[ \| e \| \leq K_1 (\Delta t)^2 + K_2 (\Delta x)^2 \] (197)

where \( K_1 \) and \( K_2 \) are bounded.

Thus, it is seen that the approximation error in both the finite difference and the finite element methods is of the order of \( O((\Delta x)^2 + (\Delta t)^2) \).

6.3 EXAMPLE PROBLEM V - A COMPARATIVE CASE IN ONE DIMENSION

An example problem was solved for a one-dimensional problem with prescribed concentrations at two ends assuming diffusion coefficient to be constant. A series solution to this problem is given by Crank (1975), p. 50. Table 3 and Figure 7 give a comparison of the accuracy of the two methods. The computation time for the finite element is twice as much as taken for the finite difference method.

The finite element method, while relatively slow, is very useful in solving a multitude of problems with different geometries and changing material properties, whereas the finite difference method is simple, fast and more accurate for simple regular geometries.
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Comparison of accuracy of finite element and finite difference methods.

$C_T$ = series solution value of concentration

$C_N$ = numerical solution value of concentration

Fig. 7 - Comparison of accuracy of finite element and finite difference methods.
CHAPTER VII

APPLICATIONS TO FIELD PROBLEMS

In this Chapter the solutions of two representative field situations are presented. The first problem, the Azusa landfill, compares the present model with field data and with a simpler theoretical treatment. In the second problem, the city of Hopkins landfill, several alternative designs for alleviating a methane hazard to apartment buildings are presented. Additional studies using the model may be found in Moore (1975).

7.1 AZUSA LANDFILL

The Azusa, California landfill is a three-fourth acre (approximately 3100 sq. m) test site chosen in a gravel pit (Bishop et al., 1966). The landfill was filled with domestic rubbish and filling was completed by the end of March, 1962. A plan view of the site is given in Figure 8. The groundwater table is approximately 200 ft (61 m) below the fill bottom.

Fifteen gas sampling wells were drilled in the soil surrounding the fill including one well through the fill center. Seventy gas sampling probes were placed in the wells before backfilling. Figure 9 gives the average CO$_2$ concentration in the bottom layer of the fill.

For the purpose of calculation of the quantity of CO$_2$ entering the ground the following input was used.

- Fill radius = 62.1 meters
- Depth of fill = 6.9 meters
- Radius of boundary of soil = 310.5 meters (assumed)
- Depth of impervious bottom layer = 69 meters (after Bishop)
- Soil porosity = 0.20 (after Bishop)
- Tortuosity = 1.10 (assumed)
- Surface transfer coefficient = 3.981 cm atm/s (assumed)
- Temperature = 298 K (assumed)
- Pressure = 1 atm
- Molecular diffusion coefficient = 0.158 cm$^2$ atm/s

No chemical reaction or solution of gas in subsoil water was considered. The concentration values at the fill boundary used were as given on the concentration history curve given in Figure 9.
Fig. 8 - Topographical and location map of test refuse fill at Azusa, California, (after Bishop, 1966).
Fig. 9 - Gas concentrations at bottom layer vs. time at Azusa test refuse fill (after Bishop, 1966).
Table 4 shows (1) field observations, (2) the values predicted by Bishop et al. using simple error function solution and a constant effective diffusion coefficient, and (3) the results obtained by the finite difference model. The observed values presented in the table are average values for wells within 4.9 meters of the side of the fill, whereas for the finite difference model the results presented are for points 4.6 meters from the radial boundary of the fill. The results for the points at 13.8 meters depth show good agreement with the field values. The results for other depths are considerably better than those predicted by the simple error function solution.

7.2 CITY OF HOPKINS LANDFILL

The city of Hopkins, Minnesota, sanitary landfill (Wefald, E., 1975) constitutes a potential hazard to adjacent apartment buildings when organic refuse decomposes generating methane gas. The sanitary landfill consists of 37.2 acres and is located in the NW 1/4 of the SW 1/4, section 25, Township 117 North, Range 22 West in the city of Hopkins, Hennepin County, Minnesota (Figure 10). The study by Wefald was limited to an area adjacent to the Westbrook Patio Homes. Figure 11 shows the landfill venting cross-section as proposed by Wefald.

A finite element analysis was carried out to study the effect of venting. A preliminary analysis showed that the vent provided in the fill itself does not affect the diffusional flow. Diffusional flow is caused by concentration gradients. For a given concentration at the fill boundary the concentration gradients in the surrounding soil are
Fig. 10a - Location map, City of Hopkins landfill (after Wefald, 1975)
Fig. 10b - Detail map for City of Hopkins landfill (after Wefald, 1975)
Fig. 11a - Cross-section showing proposed venting (after Wefald, 1975)
Fig. 11b - Cross-section used for finite element analysis.
not affected; however, any pressure buildup in the fill will definitely be eased. It was, therefore, decided to study the effect of providing a vent outside the fill. In this analysis the soil surrounding the landfill was assumed to be silt with a pore radius of $1.2 \times 10^3 \ \text{Å}$, porosity 0.4, and tortuosity 1.50. The vent is assumed to be filled with gravel having a pore radius of $2 \times 10^8 \ \text{Å}$, porosity 0.4, tortuosity 1.05, and of cross section shown in Figure 11b. The temperature is assumed to be 298 K and pressure 1 atmosphere. The corresponding value for the coefficient of diffusion for methane into air was 0.226. For a decomposition period of five years, the boundary of the fill is assumed to have a mole fraction of methane equal to 0.70. The boundary at 100 m is assumed to have a prescribed zero concentration of methane. The top surface of the soil is assumed to be impervious and the boundary at a depth of 8.1 m is assumed to be impervious because of the presence of groundwater. After the decomposition period, the fill boundary is also assumed to be impervious. The analysis was carried out for three different cases:

1. Diffusion into surrounding soil without vent and without surface convection.

2. Diffusion into surrounding soil with vent but no surface convection at top of vent.

3. Diffusion into surrounding soil with vent and with surface convection over the vent.

This study indicates the following:

1. Venting provided in the fill itself does not help in reducing the diffusion into the adjacent soil. It will however help to reduce pressure flows if any.

2. Vents having the top sodded do not help. Sodding will hamper surface convection and the concentrations of methane under the buildings will even be higher as seen from Figures 12 and 13.

3. Vents with open tops allowing for surface convection reduce the concentrations of methane in the soil (Figure 14).
Fig. 12a - Mole fraction contours for methane for City of Hopkins landfill without trench at $t = 220$ days.
Fig. 13h - Mole fraction contours for methane for City of Hopkins landfill without trench at $t = 1825$ days.
Fig. 12c - Mole fraction contours for methane for City of Hopkins landfill without trench at \( t = 2140 \) days.
Fig. 12d - Mole fraction contours for methane for City of Hopkins landfill without trench at $t = 3500$ days.
Fig. 13a - Mole fraction contours for methane for City of Hopkins landfill with trench but without convection on top surface of trench at $t = 270$ days.
Fig. 13b - Mole fraction contours for methane for City of Hopkins landfill with trench but without convection on top surface of trench at $t = 1825$ days.
Fig. 13c - Mole fraction contours for methane for City of Hopkins landfill with trench but without convection on top surface of trench at $t = 2140$ days.
Fig. 13d - Mole fraction contours for methane for City of Hopkins landfill with trench but without convection on top surface of trench at 3460 days.
Fig. 14a: Mole fraction contours for methane for City of Hopkins landfill with trench and with convection allowed on trench surface at $t = 350$ days.
Fig. 14b - Mole fraction contours for methane for City of Hopkins landfill with trench and with convection allowed on trench surface at \( t = 1825 \) days.
Fig. 14c - Mole fraction contours for methane for City of Hopkins landfill with trench and with convection allowed on trench surface at $t = 2140$ days.
Fig. 14d - Mole fraction contours for methane for City of Hopkins landfill with trench and with convection allowed on trench surface at $t = 3460$ days.
CHAPTER VIII

SUMMARY AND CONCLUSIONS

The purpose of this study was to develop an analytical technique for the prediction of flow of gases through soil adjoining sanitary landfills. The summary and conclusions of this study are:

1. Based on the available literature, differential equations were formulated describing multicomponent diffusional flow with chemical reaction through a porous medium assumed to consist of capillaries of circular cross-section. Emphasis was placed on methane and on carbon dioxide together with its chemical reactions with groundwater which result in changes in hardness, pH value and alkalinity of groundwater.

2. A simplified geometric representation for sanitary landfills was used. The fill was treated as axisymmetric with a provision for analyzing long trench type cases. The boundary conditions incorporated were:

   a. An impervious boundary at a depth $d_s$ due to the presence of a subsoil water table or to bedrock.

   b. A specified concentration or a specified flux boundary at a radial distance $r_s$. In fact if $r_s$ is taken greater than five times the radius of the fill the concentrations at that distance are so low that it is immaterial which of the two boundary types are selected.

   c. The axis of the fill, being an axis of symmetry, was taken as an impervious boundary.

   d. The ground surface may have either a prescribed concentration or a prescribed convection. Convection was related to wind velocity.

   e. The interface between the soil and the fill was treated as a prescribed concentration boundary for the period of decomposition, $t_0$, assumed to be 5 years. After this period it was treated as an impervious boundary.

3. A finite difference formulation was developed to treat situations where the boundaries are relatively simple. The finite difference codes use the alternating direction implicit methods which proved quite accurate and stable. Code I, an axisymmetric program, allows for surface convectons for which the wind coefficients given in Table 2 were used. Code II, a three dimensional program allows for locating vents at a radial distance $r_v$ from the axis of fill. Any number of vents
equally spaced along the circumference may be used. The effectiveness of the vents was arbitrarily specified and needs to be investigated further. Example problems were solved for the following cases:

a. Diffusion of methane using Code I.

b. Diffusion of carbon dioxide along with its chemical reactions with groundwater using Code I.

c. Diffusion of methane through a vented soil using Code II.

4. A variational formulation was developed to be used in a finite element solution. Code III implements a finite element formulation using isoparametric quadrilateral elements in space and Crank-Nicolson finite difference approximation in time.

5. A comparison of cost effectiveness, stability and accuracy of the finite difference and finite element methods was made. Example problem V illustrates the application to a one dimensional problem using a constant diffusion coefficient. The solutions are compared with a series solution given by Crank, J. (1975). Both of the numerical methods proved stable; however, as seen from Figure 7, for the simple problem considered the results are more accurate in case of finite difference solution than the finite element solution. To obtain physically meaningful results in the beginning of analysis the time increment $\Delta T$ is taken such that $\lambda = \frac{D \Delta T}{(\Delta X)^2}$ is restricted to less than $1/4$ in both techniques. The finite difference code is fast but for every new geometry a new code must be developed. On the other hand the finite element code requires more computer time but the versatility with which it can be applied to different geometries, in homogeneous strata and varying boundary conditions without requiring any change in the code more than offsets this objection.

6. The computer codes developed were applied to the following field problems:

a. The Azusa fill was chosen as an example for a verification problem where field data currently exists. The finite difference code was used to predict the migration of gases generated by decomposition of refuse. A variable concentration on the soil-fill boundary was used. The results obtained compared well with those obtained experimentally during 3 years of experimentation.

b. The city of Hopkins, Minnesota is faced with the problem of venting a fill to avoid possible development of concentrations of methane under the adjoining apartment buildings. The finite element code was used to study the effect of venting. It was concluded that venting reduces the gas concentrations in the adjoining soil. The vents should be placed outside the fill to obtain maximum effectiveness. In addition, keeping the top of the trenches free of grass significantly improves convection transfer of gas from the soil to the atmosphere.
APPENDIX A

SAMPLE OUTPUT PROBLEM I

DIFFUSION OF METHANE THROUGH GRANULAR MATERIAL
DIFFUSION OF METHANE THROUGH GRANULAR MATERIAL

NUMBER OF MESH POINTS UP TO END OF FILL = 21
NUMBER OF MESH POINTS UP TO DEPTH OF FILL = 3
NUMBER OF MESH POINTS UP TO END OF LAND = 51
NUMBER OF MESH POINTS UP TO DEPTH OF LAND = 5
NUMBER OF MESH POINTS UP TO VENT = 20
NUMBER OF MESH POINTS UP TO DEPTH OF VENT = 1

POROSITY OF SOIL (DIMENSIONLESS) = 0.400
TORTUOSITY (DIMENSIONLESS) = 2.250
MOLECULAR WEIGHT OF GAS B (GM/MOLE) = 28.800
MOLECULAR WEIGHT OF GAS A (GM/MOLE) = 16.050
PRESSURE (ATMOS) = 1.000
TEMPERATURE (DEG KELVIN) = 298.000
DULK DIFFUSION COEFFICIENT (CM SQ ATOMS/SEC) = 0.226
SPATIAL MESH SIZE (CM) = 800.000
DECOMPOSITION TIME (DAYS) = 1825.000
INITIAL MOLE FRACTION IN FILL = 0.700
TERMINATION MOLE FRACTION = 0.050
SURFACE PERMEABILITY COEFFICIENT = 0.398D-04
END PERMEABILITY COEFFICIENT = 0.0
PERMEABILITY COEFFICIENT FOR THE VENT = 0.398D-04
PERMEABILITY MULTIPLIER FOR THE VENT = 0.1000+01
INITIAL HARDNESS = 75.000
INITIAL PH VALUE = 6.500
DEGREE OF SATURATION = 40.000

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HISTORY OF FILL CONCENTRATIONS
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1825.00  0.70

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APPENDIX B

SAMPLE OUTPUT PROBLEM II

DIFFUSION OF CARBON DIOXIDE THROUGH GRANULAR MATERIAL
DIFFUSION OF CO-2 THROUGH GRANULAR MATERIAL

NUMBER OF MESH POINTS UP TO END OF FILL = 21
NUMBER OF MESH POINTS UP TO DEPTH OF FILL = 3
NUMBER OF MESH POINTS UP TO END OF LAND = 51
NUMBER OF MESH POINTS UP TO DEPTH OF LAND = 5
NUMBER OF MESH POINTS UP TO VENT = 20
NUMBER OF MESH POINTS UP TO DEPTH OF VENT = 1

POROSITY OF SOIL (DIMENSIONLESS) = 0.400
TORTUOSITY (DIMENSIONLESS) = 2.250
MOLECULAR WEIGHT OF GAS B (GM/MOLE) = 28.800
MOLECULAR WEIGHT OF GAS A (GM/MOLE) = 44.000
PRESSURE (ATMOS) = 1.000
TEMPERATURE (DEG KELVIN) = 298.000
BULK DIFFUSION COEFFICIENT (CM SQ ATMOS/SEC) = 0.158
SPATIAL MESH SIZE (CM) = 800.000
DECOMPOSITION TIME (DAYS) = 1825.000
INITIAL MOLE FRACTION IN FILL = 0.300
TERMINATION MOLE FRACTION = 0.050
SURFACE PERMEABILITY COEFFICIENT = 0.398D-04
END PERMEABILITY COEFFICIENT = 0.0
PERMEABILITY COEFFICIENT FOR THE VENT = 0.398D-04
PERMEABILITY MULTIPLIER FOR THE VENT = 0.1000+01
INITIAL HARDNESS = 75.000
INITIAL PH VALUE = 6.500
DEGREE OF SATURATION = 40.000

NUMBER PORE RADIUS VOLUMETRIC FRACTION
1  400000.00  0.4000

HISTORY OF FILL CONCENTRATIONS
TIME (DAYS) MOLE FRACTION
0.0  0.30
1825.00  0.30

NUMBER OF STEPS BETWEEN PRINTOUTS = 500
MAXIMUM NUMBER OF STEPS ALLOWED = 2000
INITIAL DTAU (DAYS) = 1.0
MAXIMUM TIME ALLOWED (DAYS) = 730000.0
MAXIMUM DTAU (DAYS) = 1.2*DX*DX/DIJ(MAX) = 565.0

AXISYMMETRIC FLOW PROGRAM
CHEMICAL REACTION CONSIDERED
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214
## HOLE FRACTION

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IMAX = 27     J = 3     MOLE FRACTION = 5.66276D-02
APPENDIX C

SAMPLE OUTPUT PROBLEM III

DIFFUSION OF METHANE THROUGH A VENTED SOIL
GAS DIFFUSION THROUGH GRANULAR MATERIAL

NUMBER OF MESH POINTS UP TO END OF FILL  21
NUMBER OF MESH POINTS UP TO DEPTH OF FILL  3
NUMBER OF MESH POINTS UP TO END OF LAND  51
NUMBER OF MESH POINTS UP TO DEPTH OF LAND  5
NUMBER OF MESH POINTS UP TO PIPE LOCATION  31
NUMBER OF MESH POINTS UP TO DEPTH OF PIPE  4
NUMBER OF MESH POINTS ALONG THETA DIRECTION  4
TOTAL NUMBER OF PIPES ALONG CIRCUMFERENCE  6

POROSITY OF SOIL (DIMENSIONLESS)  =  0.400
TORTUOSITY (DIMENSIONLESS)  =  2.250
MOLECULAR WEIGHT OF GAS B (GM/MOLE)  =  28.800
MOLECULAR WEIGHT OF GAS A (GM/MOLE)  =  16.050
PRESSURE (ATMOS)  =  1.000
TEMPERATURE (REG KELVIN)  =  298.000
BULK DIFFUSION COEFFICIENT (CM SQ ATMOS/SFC)  =  0.226
SPATIAL MESH SIZE (CM)  =  800.000
DECOMPOSITION TIME (DAYS)  =  1825.000
INITIAL MOLE FRACTION IN FILL  =  0.700
TOLERABLE MOLE FRACTION  =  0.050

NUMBER   PORE RADIUS   VOLUMETRIC FRACTION
         400000.00   0.4000

NUMBER OF STEPS BETWEEN PRINTOUTS  =  20
MAXIMUM NUMBER OF STEPS ALLOWED  =  1000
INITIAL DTAU (DAYS)  =  1.0
MAXIMUM TIME ALLOWED (DAYS)  =  730000.0
MAXIMUM DTAU (DAYS) = 1.2*(DX*DX/DIJ(MAX))  =  182.0
MOLE FRACTION AT TIME (DAYS) = 0.0

THETA (DEGREES) = 0.0

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225
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THETA = 10.00  STEP NUMBER = 52

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THETA = 30.00 STEP NUMBER = 52

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MOLE FRACTION AT TIME (DAYS) = 20848.0  DTAU (DAYS) = 512.0  DTMAX (DAYS) = 198.0  

THETA = 0.0  STEP NUMBER = 192  

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| 7.00D-01 | 7.00D-01 | 7.00D-01 | 7.00D-01 | 1.50D-01 | 8.93D-02 | 1.16D-02 | 2.73D-02 | 1.99D-02 | 9.72D-03 |

******************************************************************************

8.00D+02  

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1.60D+03  

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2.40D+03  


******************************************************************************

3.20D+03  

| 3.98D-01 | 3.89D-01 | 3.29D-01 | 2.51D-01 | 1.60D-01 | 8.98D-02 | 1.57D-02 | 2.74D-02 | 1.99D-02 | 9.82D-03 |
**Mole Fraction at Time (Days) = 20848.0  DTAU (Days) = 512.0  DMAX (Days) = 198.0**

**Theta = 10.00  Step Number = 192**

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MOLE FRACTION AT TIME (DAYS) = 20848.0  DTAU (DAYS) = 512.0  DTMAX (DAYS) = 198.0  
THETA = 20.00  STEP NUMBER = 192

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MOLE FRACTION AT TIME (DAYS) = 20848.0  DTAU (DAYS) = 512.0  DTMAX (DAYS) = 198.0
THETA = 30.00  STEP NUMBER = 192

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IMAX= 38  J = 3  K = 4  MOLE FRACTION = 5.21087D-02

IMAX= 38  J = 3  K = 4  MOLE FRACTION = 5.21087D-02
CONCENTRATION STOPS INCREASING AT TIME (DAYS) = 20848.0
**MOLE FRACTION AT TIME (DAYS) = 20848.0**

**THETA (DEGREES) = 0.0**

**STEP NUMBER = 192**

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**THETA (DEGREES) = 10.00**

**STEP NUMBER = 192**

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**THETA (DEGREES) = 20.00**

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THETA (DEGREES) = 30.00
STEP NUMBER = 192

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**Step Number = 192**

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THETA (DEGREES) = 10.00

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REFERENCES


Oden, J. T., (1974), Supplementary Notes on Mathematical Theory of Finite Element Methods," The Ohio State University, Columbus.


