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Development of Computer Simulations for Landfill Methane Recovery

J. W. Massman, C. A. Moore, and R. M. Sykes

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DEVELOPMENT OF COMPUTER SIMULATIONS
FOR LANDFILL METHANE RECOVERY

prepared by

Joel W. Massman, Charles A. Moore,
and Robert M. Sykes

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for

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DEVELOPMENT OF COMPUTER SIMULATIONS FOR LANDFILL METHANE RECOVERY

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ABSTRACT

Two- and three-dimensional finite-difference computer programs simulating methane recovery systems in landfills have been developed. These computer programs model multi-component combined pressure and diffusional flow in porous media. Each program and the processes it models are described in this report. Examples of the capabilities of each program are also presented. The two-dimensional program was used to simulate methane recovery systems in a cylindrically shaped landfill. The effects of various pump locations, geometries, and extraction rates were determined. The three-dimensional program was used to model the Puente Hills landfill, a field test site in southern California. The biochemical and microbiological details of methane generation in landfills are also given. Effects of environmental factors, such as moisture, oxygen, temperature, and nutrients on methane generation are discussed and an analytical representation of the gas generation rate is developed.

1 INTRODUCTION

Methane gas generated within landfills constitutes a hazard when it migrates through the adjacent soil. Design criteria have been presented (Moore, 1979) for control facilities to alleviate this problem. However, facilities constructed solely to control methane migration represent a significant expenditure of funds that provides no financial return. Only recently, with the growing need for new energy sources, has a potential for profit been discerned in controlling landfill methane migration in conjunction with a methane recovery program. As this opportunity has become more widely recognized, interest has grown in the energy recovery aspects of landfill operation.

The recovery of landfill methane for energy use adds complexity to the analytical approaches that must be developed to optimize methane production. Landfills have historically been constructed in an uncontrolled manner, resulting in a high degree of uncertainty with respect to the types and distribution of materials, geometry of the fill boundaries, and control of moisture routing through the fill. In contrast, in many manufacturing processes, a high degree of control is maintained over operations. The heterogeneities inherent in landfills must be explicitly incorporated into the analytical techniques for optimizing methane production.

Another important contrast between landfills and conventional manufacturing processes is that landfills are one-batch systems. In a conventional manufacturing process, it is relatively easy to make major process modifications from run to run. However, for any given landfill, there is only one opportunity to perform methane extraction; thus, the process must be carried out in the optimum manner initially. Moreover, because of variations among sites, lessons learned at one site may have limited applicability to another.

It is thus important that a strong analytical basis be provided for designing operating procedures to recover methane from landfills. The techniques designed will then insure that methane recovery will be maximized. Moreover, the analytical basis can be used to predict conditions that signal irregularities in recovery operations so that remedial measures can be taken before irreparable damage has been done to the landfill.

2 GAS FLOW IN A POROUS MEDIUM

2.1 MECHANICS OF FLOW IN A SINGLE CAPILLARY TUBE

Because of the small total pressure gradients and large partial pressure gradients generally found in landfills, the flow processes involved in gas migration from these fills are complex. Both diffusional and pressure flow contribute equally to the transport process and must therefore both be investigated (Alzaydi, Moore, and Rai, 1978). Further complicating the flow process, the pores found in soils are of such a size that, in flows at atmospheric pressure, the gas molecules collide with soil as well as with each other.

2.1.1 Diffusional Flow

Concentration gradients are the driving forces behind diffusional flow. Gases flow isobarically from points of higher to lower concentration. Several physical mechanisms may interact to impede this flow. Figure 2.1 illustrates the various flow mechanisms of the diffusion process as it occurs in a single capillary tube of radius r under a constant total pressure.

Figure 2.1a shows the process known as Knudsen diffusion. The gas molecules collide only with the walls of the capillary tube and behave independently of each other. The retardation effect depends upon the molecular weight and temperature of the gas and the radius of the capillary tube and is not influenced by the presence of other species of gas.

The molecular diffusion process is illustrated in Fig. 2.1b. The gas molecules collide only with other gas molecules; however, these collisions may occur between either like or unlike molecules. The retardation effect depends on the molecular weights and temperature of the gases in the capillary tube and is unaffected by the physical nature of the pore walls.

The more general process of transition region diffusion is illustrated in Fig. 2.1c. Molecules collide with each other and with the capillary wall. The flow depends on the radius of the pore, the molecular weights and temperature of the gases, and the physical nature of the pore walls.

In summary, the various types of diffusional flow can be categorized according to the type of collisions that the gas molecules experience. Knudsen diffusion is characterized by molecule-to-wall collisions, while molecular diffusion involves collisions between like or unlike molecules. Transition region diffusion is a combination of Knudsen and molecular diffusion and therefore involves both types of collisions.

2.1.2 Pressure Flow

If a total pressure gradient exists in a capillary tube, gases will flow from points of higher pressure to points of lower pressure. Viscous flow (Poiseuille flow) and slip flow along the capillary walls are the two mechanisms involved in the pressure flow process.

(a) Knudsen Diffusion

(b) Molecular Diffusion

(c) Transition Region Diffusion

Fig. 2.1 Diffusional Flow Mechanisms

Poiseuille flow is analogous to the flow of compressible fluids in tubes. The driving force behind Poiseuille flow is the total pressure gradient, while the resistance is caused by the viscosity of the gas and the drag created by the small pores of the medium.

If the radius of the capillary tube is very small, the gas molecules will frequently collide with the walls of the tube and will behave as though in the Knudsen region. The slip flow mechanism, whereby the molecules slide along the capillary walls, is of increased importance under these conditions.

2.1.3 Combined Flow

If both partial pressure and total pressure gradients are present in a capillary tube, the transport process will involve a combination of diffusional and pressure flows. Figure 2.2 illustrates possible flow mechanisms when such conditions exist.

In Fig. 2.2a, the partial pressures of gases A and B, as well as the total pressure of the gas mixture, decrease from left to right. The direction of flow for both components under these conditions is also from left to right.

Figure 2.2b illustrates the more general case of partial pressure and total pressure gradients existing in opposite directions. Both the total pressure and the partial pressure of gas A decrease from left to right. However, the partial pressure of gas B decreases from right to left. Gas A will clearly migrate to the right under both partial and total pressure gradients. The flow direction of gas B is not so easily determined. The diffusional process will transport gas B from right to left while pressure flow tends to move the gas from left to right. The net direction of flow for gas B cannot be determined a priori but is dependent upon the predominating flow mechanism.

2.2 EQUATIONS OF FLOW IN A SINGLE CAPILLARY TUBE

The mechanics of flow of a gas in a single capillary tube were described in Sec. 2.1. Included were diffusional flow, pressure flow, and combined flow. This section introduces the mathematical expressions that govern each of these flow processes.

2.2.1 Concept of Mean Free Path of a Molecule

To determine which type of flow predominates under a given set of conditions, a quantitative measure is needed for the average distance a molecule travels before it collides with another molecule. This average distance is called the mean free path of the molecule, and is given by Bird, Stewart, and Lightfoot (1960) and Geankoplis (1972) as:

$$\lambda = \frac{3.2\mu}{P} \sqrt{\frac{RT}{2\pi gM}} \quad (1)$$

where:

λ = mean free path (cm),

μ = viscosity (poise),

P = pressure (g/cm²),

T = temperature (K),

g = gravitational constant (980 cm/s),

M = molecular weight (g/gmole), and

R = gas constant (84,780 g-cm/K-gmole).

Fig. 2.2 Flow under Partial Pressure and Total Pressure Gradients

2.2.2 Equations of Diffusional Flow

Under a given set of conditions, the type of diffusional flow that will predominate (Knudsen, molecular, or transition region flow) depends on the relationship between the mean free path of a molecule (λ) and the diameter of the capillary tube. If λ is on the order of 10 times the capillary diameter, molecule-to-wall collisions will predominate. Molecule-to-molecule collisions will prevail if the ratio of $\lambda/2r$ is on the order of 0.01. Both types of collisions will be present if the $\lambda/2r$ ratio is between 0.01 and 10.

The governing equation describing Knudsen diffusion is given by Alzaydi (1975) as:

$$N_i^K = 9.7 \cdot 10^{-5} \left(\bar{r} \sqrt{\frac{T}{M_i}} \right) \left(\frac{\partial C_i}{\partial Z} \right) \quad (2)$$

where:

N_i^K = Knudsen flow rate for component i (gmole/cm²-s),

$\bar{r}$ = average pore radius (A),

T = temperature (K),

M_i = molecular weight of component i (g/gmole),

C_i = concentration of component i (gmole/cm³), and

Z = distance (cm).

This equation assumes $\lambda \gg 2r$, cosine wall reflection (i.e., the molecules leave the wall in a direction independent of their incident direction but with an equal probability for all directions), slowly varying pressure gradients along the capillary tube, and no radial pressure gradient (Knudsen, 1909).

If the mean free path of a molecule is very small relative to the diameter of the capillary tube ($\lambda/2r \ll 0.01$), the primary impedance to flow will be produced by molecule-to-molecule collisions. The equation describing this molecular diffusion is given by Alzaydi (1975) as:

$$\frac{-\partial C_i}{\partial Z} = \sum_{\substack{j=1 \\ i \neq j}}^n \frac{N_i^M X_j - X_i N_j^M}{D_{ij}} \quad (3)$$

where:

N_i^M = total molecular diffusion of i relative to fixed coordinates (gmole/cm²-s),

C_i = concentration of component i (gmole/cm³),

Z = distance (cm),

X_i = mole fraction of component i ($C_i / \sum C_i$), and

D_{ij} = molecular diffusion coefficient of component i diffusing in component j (cm/s) (Geankoplis, 1972).

As can be seen from Eq. 3, molecular diffusion depends on the physical properties of each of the gas species present in the capillary tube and is independent of the physical or geometrical properties of the pore.

Alzaydi (1975) used a momentum balance proposed by Rothfield (1963) and Scott and Dullien (1962) to derive an equation describing transition region diffusion for those cases when $\lambda/2r$ is between 0.01 and 10. Alzaydi showed that the total concentration gradient causing flow in the transition region is the sum of the concentration gradient causing Knudsen flow plus the concentration gradient causing molecular flow:

$$\frac{-\partial C_i}{\partial Z} = \frac{N_i^D}{DK_i} + \sum_{\substack{j=1 \\ i \neq j}}^n \frac{N_i^D X_j - X_i N_j^D}{D_{ij}} \quad (4)$$

where:

N_i^D = total diffusional flow rate (gmole/cm²-s), and

$$DK_i = (9.7 \cdot 10^{-5}) \bar{r} \sqrt{\frac{T}{M_i}}$$

2.2.3 Equations of Pressure Flow

Two mechanisms contribute to the forced flow transport process when total pressure gradients exist in a capillary tube. Poiseuille flow and slip flow along the capillary wall combine to give the total pressure flow.

Alzaydi (1975) gives the Poiseuille flow equation as:

$$F_p = \frac{-\bar{r}^2 P}{8\mu_{\text{mix}} RT} \left(\frac{\partial P}{\partial Z} \right) \quad (5)$$

where:

F_p = Poiseuille flow rate (gmole/cm²-s),

r = average radius of pores,

P = total pressure (dyne/cm²),

μ_{mix} = viscosity of mixture (poise),

R = gas constant (dyne cm/gmole-K), and

T = temperature (K).

The viscosity of the mixture is given by a semiempirical formula developed by Wilke (1950):

$$\mu_{\text{mix}} = \sum_{i=1}^n \frac{X_i \mu_i}{\sum_{j=1}^n X_j \phi_{ij}} \quad (6)$$

where:

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-\frac{1}{2}} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{\frac{1}{2}} \left(\frac{M_j}{M_i} \right)^{\frac{1}{4}} \right]^2$$

μ_i = viscosity of component i (poise), and

X_i = mole fraction of component i.

Equation 5 represents an extension of the equations that describe the flow of fluids in tubes. It assumes that the gas behaves as a compressible continuum in relatively large capillaries. It also assumes that the total pressure gradients are small so that the flow is laminar. This assumption is valid if the Reynolds number is less than 2100 (Geankoplis, 1972).

Should the pressure or capillary diameter be reduced so that the mean free path becomes an appreciable fraction of the capillary diameter, Eq. 5 will underestimate the experimental flow rate. The excess flow is due to slippage along the capillary walls. An additional term to include this slip flow was given by Scott and Dullien (1962) as:

$$F_s = \frac{-4\bar{r}}{3 \sum_{i=1}^n M_i \bar{V}_i X_i} \left(\frac{\partial P}{\partial Z} \right) \quad (7)$$

where:

F_s = slip flow rate (gmole/cm²-s),

r = average pore radius (cm),

M_i = molecular weight of gas i (g/gmole),

V_i = mean thermal velocity of component i (cm/s),

X_i = mole fraction of component i , and

P = total pressure (dyne/cm²).

The mean thermal velocity, as defined by the kinetic theory of gases, is given by Scott and Dullien (1962) as:

$$\bar{V}_i = \left(\frac{8RT}{\pi M_i} \right)^{1/2} \quad (8)$$

The total forced flow rate (F_T) due to a total pressure gradient is simply the sum of the flow rate due to Poiseuille flow plus the flow rate due to slip flow:

$$F_T = - \left(\frac{\bar{r}^2 P}{8\mu_{\text{mix}}} + \frac{4\bar{r}RT}{3 \sum_{i=1}^n M_i \bar{V}_i X_i} \right) \left(\frac{1}{RT} \right) \left(\frac{\partial P}{\partial Z} \right) \quad (9)$$

2.2.4 Equations of Combined Flow

In a generalized flow, the transport process is a combination of diffusional and pressure flows. Evans, Watson, and Mason (1962) have shown that the equation for combined flow can be expressed as a summation of the flow rate due to pressure flow plus the flow rate due to diffusional flow, provided that the pressure dependency of the D_{ij} term in Eq. 3 is accounted for:

$$D_{ij} = \frac{\text{constant}}{P}$$

$$= \frac{\bar{D}_{ij}}{P} \quad (10)$$

Substitution of Eq. 10 into Eq. 4 and solving for N_i^D gives:

$$N_i^D = - \left[\frac{1}{DK_i} + \sum_{\substack{j=1 \\ i \neq j}}^n \frac{x_j - x_i \left(\frac{N_j^D}{N_i^D} \right)}{D_{ij}/P} \right]^{-1} \left(\frac{1}{RT} \right) \left(\frac{\partial P_i}{\partial Z} \right) \quad (11)$$

For component i, the combined flow is:

$$N_i^T = N_i^D + X_i F_T$$

$$= N_i^D + N_i^P \quad (12)$$

Substituting Eqs. 9 and 11 into Eq. 12 gives:

$$N_i^T = - \left[\frac{1}{DK_i} + \sum_{\substack{j=1 \\ i \neq j}}^n \frac{x_j - x_i \left(\frac{N_j^D}{N_i^D} \right)}{D_{ij}/P} \right]^{-1} \left(\frac{1}{RT} \right) \left(\frac{\partial P_i}{\partial Z} \right)$$

$$- x_i \left(\frac{\bar{r}^2 P}{8\mu_{\text{mix}}} + \frac{4\bar{r}RT}{3 \sum_{i=1}^n M_i \bar{V}_i X_i} \right) \left(\frac{1}{RT} \right) \left(\frac{\partial P}{\partial Z} \right) \quad (13)$$

Equation 13 represents all of the mechanisms involved in gas transport in a single capillary, including Knudsen diffusion, molecular diffusion, transition region diffusion, viscous flow, and slip flow.

2.3 MECHANICS OF FLOW IN A POROUS MEDIUM

The concepts introduced in Sec. 2.1 to describe the flow of gas in a single capillary are extended in this section to describe flow in a porous medium. A physical model representative of the porous medium is assumed. The gas transport process discussed in Secs. 2.1 and 2.2 is then applied to this model.

2.3.1 Flow in a Porous Medium

The flow of gas through a porous medium such as soil differs in several respects from flow in a single capillary. Figure 2.3 illustrates a general example of gas flow in a porous medium.

Fig. 2.3 Flow of Gas Particles through a Porous Medium

As the gas molecule approaches point a, its flow domain is reduced because the size of the pore space decreases, thereby effectively reducing the cross sectional area available for flow. The porosity of the soil (ϵ) is used as a quantitative measure for the area available for flow per unit area of soil and is defined as the volume of voids divided by the total volume:

$$\epsilon = \frac{V_v}{V_T} \quad (14)$$

where:

ϵ = porosity,
 V_v = volume of voids in the soil, and
 V_T = total volume of soil.

At point b, the direction of flow for the gas molecule is changed because of the arrangement of soil particles. A tortuosity factor is introduced to account for the circuitous path that the gas molecule must travel. Tortuosity is a function of the average size of the soil particles. The tortuosity factor (τ) is defined as the effective length the gas molecule must travel, divided by the length of the soil sample:

$$\tau = \frac{L_e}{L} \quad (15)$$

where:

τ = tortuosity,

L_e = effective path length of a gas element flowing through a pore space, and

L = length of a porous sample in the direction of flow.

Between points a and b, the transport process involves any or all of the flow mechanisms shown in Fig. 2.2. However, because of the scales of length involved, slip flow is of negligible importance in gas migration in soils. The pore sizes of soils and the distances the gas travels from landfills are very large compared to the small spatial scales necessary before slip flow will contribute significantly to the transport process.

2.3.2 Modeling the Porous Medium

Before applying the mechanics and equations for flow in a single capillary to that in a porous medium, it is necessary to introduce a physical model that will idealize the interactions between the transport processes and the porous medium. Several models have been proposed, the majority of which are variations of the series and/or parallel pore model (Alzaydi, 1975).

The model used in this study (shown in Fig. 2.4) assumes that:

- The porous medium consists of a bundle of capillary tubes of various radii,
- The radius of each capillary is constant along its length, and
- The mechanics and equations of flow in a single capillary can be applied to each of these capillaries.

The total flow consists of a summation over the entire pore size distribution. The flow per unit area of soil is then determined by multiplying the total flow by the porosity and dividing it by the tortuosity. The porosity of a porous medium consisting of capillaries of various radii is given by:

$$\epsilon = \sum_{r=r_{\min}}^{r_{\max}} f_v(r) \quad (16)$$

section a-a

Fig. 2.4 Model Used to Represent the Porous Medium

where:

ϵ = porosity, and

$fv(r)$ = void fraction of radius r .

2.4. EQUATIONS OF FLOW IN A POROUS MEDIUM

In Secs. 2.2.2 and 2.2.3, the general equations for diffusional and pressure flow in a single capillary were introduced. By combining these equations with the porous medium model discussed in Sec. 2.3, the equations for diffusional and forced flow in a porous medium can be developed. This can be accomplished by summing the flows in each of the pores over the entire pore size distribution.

Equation 11 gives the diffusional flux for component i in a single capillary as:

$$N_i^D = - \left[\frac{1}{DK_i} + \sum_{\substack{j=1 \\ i \neq j}}^n \frac{X_j - X_i (N_j^D / N_i^D)}{\bar{D}_{ij}/P} \right]^{-1} \left(\frac{\partial C_i}{\partial Z} \right) \quad (17)$$

where:

$$DK_i = 9.7 \cdot 10^{-5} \left(r \sqrt{\frac{T}{M_i}} \right) \\ = K_i r$$

The flow in a porous medium is given by summing the flows in each of the pores, multiplying this summation by the porosity, and dividing it by the tortuosity. Combining Eqs. 16, 17, and 18 and introducing the tortuosity factor gives:

$$N_i^D = \frac{1}{\tau} \left[\sum_{r_{\min}}^{r_{\max}} \frac{-fv(r)}{\frac{1}{K_i r} + \sum_{\substack{j=1 \\ i \neq j}}^n \frac{X_j - X_i (N_j^D / N_i^D)}{\bar{D}_{ij}/P}} \right] \frac{\partial C_i}{\partial Z} \quad (18)$$

Equation 18 represents the diffusional flow of a multicomponent gas in a porous medium.

As discussed in Sec. 2.3.1, the equation for forced flow in a single capillary can be simplified by neglecting the slip flow term when applied to a porous medium. Combining Eqs. 5 and 16 and again introducing tortuosity gives:

$$F_p = \frac{1}{\tau} \sum_{r_{\min}}^{r_{\max}} \left[\frac{-r^2 P f v(r)}{8 \mu_{\text{mix}} R T} \left(\frac{\partial P}{\partial Z} \right) \right] \quad (19)$$

The equation for both diffusional and forced flow is obtained by combining Eqs. 12, 18, and 19 as follows:

$$N_i^T = \frac{1}{\tau} \sum_{r_{\min}}^{r_{\max}} \left[\frac{-f v(r)}{\frac{1}{K_i r} + \sum_{\substack{j=1 \\ i \neq j}}^n \frac{X_j - X_i (N_j / N_i^D)}{\bar{D}_{ij} / P}} \left(\frac{1}{R T} \right) \left(\frac{\partial P_i}{\partial Z} \right) - \frac{r^2 P}{8 \mu_{\text{mix}}} \left(\frac{X_i}{R T} \right) \left(\frac{\partial P}{\partial Z} \right) \right] \quad (20)$$

Equation 20 represents all the relevant mechanisms involved in gas transport in a porous medium, including Knudsen, molecular, and transition region diffusion as well as viscous flow.

3 FINITE DIFFERENCE FORMULATION

The equations introduced in Chapter 2 to describe pressure and diffusional flow of a multicomponent gas through a porous medium are classified as parabolic partial differential equations. These equations can be solved analytically if the diffusion coefficient and the boundary conditions remain constant. However, if the diffusion coefficient is a function of gas concentration or if the boundary conditions change with time, analytical solutions are virtually impossible. Such is the case for the equations presented in Chapter 2.

Numerical methods involving finite differences are often used to solve nonlinear partial differential equations similar to those describing gas flow in a porous medium. In this chapter are formulated the finite difference algorithms necessary to solve the equations in Chapter 2.

3.1 EQUATIONS OF FLOW IN MATRIX FORM

The general equations describing multicomponent gas flow in a porous medium are given by Eqs. 18, 19, and 20. These expressions can be rewritten in a more tractable form for solution by a finite difference method.

Equation 18 can be rewritten as:

$$N_i^D = \sum_{r_{\min}}^{r_{\max}} \frac{fv(r)}{\tau} \left[\frac{\left(\sum_{j=1}^n \frac{X_i N_j P}{D_{ij}} \right) - \frac{\partial C_i}{\partial Z}}{\frac{1}{K_i r} + \sum_{j=1}^n \frac{X_j P}{D_{ij}}} \right], \quad i \neq j \quad (21)$$

By definition,

$$X_i = \frac{P_i}{P} \quad (22)$$

and

$$\frac{\partial C_i}{\partial Z} = \left(\frac{1}{RT} \right) \left(\frac{\partial P_i}{\partial Z} \right) \quad (23)$$

Substituting Eqs. 22 and 23 into Eq. 21 gives:

$$N_i^D = \sum_{r_{\min}}^{r_{\max}} \frac{fv(r)}{\tau} \left[\frac{\left(\sum_{j=1}^n \frac{N_j P_i}{\bar{D}_{ij}} \right) - \left(\frac{1}{RT} \right) \left(\frac{\partial P_i}{\partial Z} \right)}{\frac{1}{K_i r} + \sum_{j=1, j \neq i}^n \frac{P_j}{\bar{D}_{ij}}} \right] \quad (24)$$

Equation 24 in matrix form is written as:

$$[A] \{ \tilde{N}^D \} = - \frac{1}{RT} \{ \nabla \tilde{P} \} \quad (25)$$

where:

$$\tilde{N}^D = N_1^D, N_2^D, \dots, N_n^D, \text{ and}$$

$$\tilde{P} = P_1, P_2, \dots, P_n.$$

The elements of matrix [A] are:

$$a_{ii} = \sum_{r_{\min}}^{r_{\max}} \left(\frac{fv(r)}{\tau} \cdot \frac{1}{K_i r} \right) + \sum_{j=1, j \neq i}^n \frac{P_j}{\bar{D}_{ij}}$$

and

$$a_{ij} = -P_i / \bar{D}_{ij}$$

Solving Eq. 25 for the diffusive flux vector gives:

$$\{ \tilde{N}^D \} = \frac{1}{RT} [A^{-1}] \{ \nabla \tilde{P} \} \quad (27)$$

In a similar manner, the term representing pressure flow in Eq. 20 can also be written in matrix form. The pressure flow term is given as:

$$N_i^P = \frac{-C_o}{\mu_{\text{mix}}} \frac{P X_i}{RT} \frac{\partial P}{\partial Z} \quad (28)$$

where:

$$C_o = \sum_{r_{\min}}^{r_{\max}} \frac{r^2 f_v(r)}{8}$$

Combining Eq. 28 with Eq. 22 gives, in matrix form:

$$\{\tilde{N}^P\} = \frac{-C_o}{RT\mu_{\text{mix}}} \nabla P \{\tilde{P}\} \quad (29)$$

Total flow rate can now be expressed in matrix form by combining diffusive and pressure fluxes as follows:

$$\{\tilde{N}^T\} = \frac{-1}{RT} [A^{-1}] \{\nabla \tilde{P}\} - \frac{C_o \nabla P}{RT\mu_{\text{mix}}} \{\tilde{P}\} \quad (30)$$

Substituting $[A^{-1}] = [D]$ gives:

$$\{\tilde{N}^T\} = \frac{-1}{RT} \left(D \{\nabla \tilde{P}\} - \frac{C_o \nabla P}{RT\mu_{\text{mix}}} \{\tilde{P}\} \right) \quad (31)$$

The continuity equation for component i is:

$$\frac{1}{RT} \frac{\partial P_i}{\partial t} = -\nabla N_i \quad (32)$$

Combining Eq. 32 with the spatial derivative of Eq. 31 gives:

$$\frac{\partial P_i}{\partial t} = \nabla \cdot \sum_{j=1}^n D_{ij} \nabla P_j + \nabla \cdot \left(\frac{C_o P_i \nabla P}{\mu_{\text{mix}}} \right) + S_i \quad (33)$$

where S_i is the change in pressure of component i per unit volume due to a sink/source term.

Equation 33 gives the general system of equations for flow in a porous medium. The elements of D_{ij} are determined by inverting matrix $[A]$. Both D_{ij} and $C_o P_i / \mu_{\text{mix}}$ are functions of P .

3.2 LANDFILL GEOMETRY AND BOUNDARY CONDITIONS

Before a finite difference solution for the equations of flow in a porous medium can be developed, a geometrical representation of the landfill must be assumed. This representation must be flexible enough to approximate the wide variety of actual landfill geometries, yet simple enough to permit solution by a numerical method. The geometry and boundary conditions for modeling the landfill are developed in this section.

3.2.1 Geometric Simulation of Landfills

This study treats the geometry of the landfill as a cylindrical volume that is circular in plan with a radius r_f and a depth d_f , as shown in Fig. 3.1. The soil surrounding the fill extends radially to a distance r_s and vertically to a depth d_s . Gas wells extending to a depth d_v may be placed at any radial distance r_v . These wells are assumed to be equally spaced around the circle of radius r_v . The spacing of these wells can attain any value, and any number of well circles can be used; however, the spacing in all circles must be constant.

3.2.2 Landfill Boundary Conditions

The landfill boundary conditions can be divided into three general types: boundaries with prescribed concentrations, boundaries with prescribed convective flows, and boundaries with sinks or sources such as wells or vents.

At boundaries with prescribed concentrations, the mole fraction of the gas component under consideration at a given time and coordinate is known. (For example, the concentration of methane at a radial boundary far from the fill may be assumed to be zero.)

Boundaries with prescribed convective flows generally either are impervious (e.g., at the interface between the water table and the dry soil below a fill) or have convective flows that are linearly related to the difference in gas concentrations across the boundary (e.g., at the ground surface). The coefficients that relate the amount of convective flow to the concentration gradient are unique for each gas component considered. MacKay and Matsugu (1973) developed the following semiempirical formula to determine these convection coefficients:

$$CK_i = 0.0292V^{0.78}L^{-0.11}Sc_i^{-0.67} \quad (34)$$

where:

CK_i = convection coefficient for component i ,

V = wind velocity at 10 m above ground surface (m/hr),

L = fill size (m), and

Sc_i = Schmidt number for component i .

Sink/source boundaries are used to accommodate either the generation or loss of material at a given point (e.g., a well location). These sink or source terms give the change in concentration of a given gas component per unit volume of soil. They can be functions of time, space, or gas concentration.

Figure 3.1 illustrates the various boundary conditions imposed on the landfill geometry. The base of the soil is assumed impervious, while the edge of the soil at a radial distance r_s can have either prescribed concentrations

Fig. 3.1 Landfill Geometry and Boundary Condition Types

or prescribed convective flows. The soil surface is assumed to be a prescribed convective flow boundary, and the axis of the fill is impervious by symmetry. The well locations are sink/source boundaries.

3.2.3 Mathematical Representation of Boundary Conditions

In this section, the boundary conditions described above are represented mathematically. The condition numbers refer to the boundaries shown in Fig. 3.1.

Condition 1: Axisymmetry

$$\partial X_i / \partial r = 0 \quad \text{for } r = 0 \text{ and } 0 \leq z \leq d_s \quad (35)$$

In this case the Laplacian operator with respect to r becomes:

$$\nabla^2 = 2(\partial^2 / \partial r^2) \quad (36)$$

Condition 2: Impervious Base of Soil

$$\partial X_i / \partial z = 0 \quad \text{for } z = d_s \quad (37)$$

Condition 3: Prescribed Concentration at Radial Soil Boundary

$$X_i = \text{constant} \quad \text{for } r = r_s \text{ and } z \leq d_s \quad (38)$$

Condition 4: Convective Flow at Ground Surface

$$2CK_i(\partial X_i / \partial z) = S_i \quad \text{for } z = 0 \quad (39)$$

Condition 5: No Circumferential Flow at Radial Line through Vent/Pump

$$\partial X_i / \partial \theta = 0 \quad \text{for } \theta = 0 \text{ and } r \neq r_v \quad (40)$$

Condition 6: No Circumferential Flow at Radial Line Midway between Vent/Pump Pairs

$$\partial X_i / \partial \theta = 0 \quad \text{for } \theta = \theta_v / 2 \quad (41)$$

Condition 7: Imperviousness at Surface of Pump Location

$$\partial X_i / \partial z = 0 \quad \text{for } r = r_p \text{ and } z = 0 \quad (42)$$

Condition 8: Sink/Source Terms at Well Location

$$QX_i = S_i \quad \text{for } r = r_v \text{ and } 0 < z \leq d_v \quad (43)$$

3.3 FINITE DIFFERENCE ALGORITHMS

Various finite difference methods are available to solve partial differential equations. The optimum method depends, among other things, on the degree of nonlinearity inherent in the equations. Equation 33 is solved in this study by using a modified version of the alternating direction implicit (ADI) method applied by Rai (1975) to the solution of the gas flow problem with uniform total pressure.

Because the transport coefficients in Eq. 33 have a large variation with respect to concentration, a predictor-corrector technique (Douglas and Jones, 1963) is used. Concentrations are predicted for the mid-time interval through several explicit steps. Transport coefficients and total pressure gradients are based on these concentrations, and a corrector step is applied to give concentrations at the end of the time interval. This procedure differs from Rai's solution of the flow problem with uniform total pressure in which transport coefficients were based on concentrations at the beginning of the time step.

To reduce the solution time, the ADI method is used for the corrector step; however, the ADI methods developed by Brian (1961), Douglas and Gunn (1964), and Brakat and Clark (1966) are not directly applicable because of the presence of additional terms due to total pressure gradients and pumping.

The predictor and corrector steps used to solve Eq. 33 are detailed in Secs. 3.3.1 and 3.3.2. The more general three-dimensional case is also described, along with the modifications necessary to represent the two-dimensional case.

3.3.1 Predictor Step

$$\frac{P_i^{n+(1/2k)} - P_i^n}{\Delta T/2k} = \nabla \cdot \sum_{j=1}^n D_{ij}^n \nabla P_i^n + \nabla \cdot \left(\frac{C_{oi} P_i^n}{\mu_{mix}^n} \nabla P^n \right) + S_i^n \quad (44)$$

where:

P_i^n = partial pressure of component i at time n ,

k = number of predictor steps required to reach the mid-interval of corrector steps,

D_j^n = effective diffusion coefficient based on partial pressure at time n ,

μ_{mix}^n = viscosity of mixture at time n , and

s_i^n = sink/source term at time n .

Knowing P_i^n , the partial pressure of each component at time n , the elements of matrix A (Eq. 25) are evaluated for each pore radius and are summed over all pore radii. Inversion of matrix A gives elements of D_{ij}^n ,

and $P_i^{n+(1/2k)}$ is then calculated. This process is repeated k times to reach time $n + (1/2)$, yielding $P_i^{n+(1/2)}$.

ΔT is selected in such a way that:

$$\lambda = D_{\max} \Delta T (\Delta X^{-2} + \Delta Y^{-2} + \Delta Z^{-2}) / k \leq 0.5 \quad (45)$$

3.3.2 Corrector Step

$$\begin{aligned} \frac{P_i^{n+1} - P_i^n}{\Delta T} = & \nabla \cdot \sum_{j=1}^n \left[D_{ij}^{n+(1/2)} \cdot \nabla \left(\frac{P_j^{n+1} + P_j^n}{2} \right) \right] \\ & + \nabla \cdot \left[\frac{C_o P_i^{n+(1/2)}}{\mu_{\text{mix}}^{n+(1/2)}} \nabla P^{n+(1/2)} \right] + S_i^{n+(1/2)} \end{aligned} \quad (46)$$

The terms $P_i^{n+(1/2)}$, $P^{n+(1/2)}$, $S_i^{n+(1/2)}$, $D_{ij}^{n+(1/2)}$, and $\mu_{\text{mix}}^{n+(1/2)}$ are based on the predictor step calculations. Equation 46 can be solved for $P_i^{n+(1/2)}$ using the implicit technique. However, for large bandwidths, particularly in three-dimensional problems, implicit solutions require large computational times. The ADI method, which is also known as operator-splitting, is used to reduce computational times and resultant computer costs.

In cylindrical coordinates:

$$\begin{aligned} \nabla(D\nabla\phi) &= \left[\frac{1}{r} \frac{\partial}{\partial r} \left(D r \frac{\partial}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left(\frac{D}{r} \frac{\partial}{\partial \theta} \right) + \frac{\partial}{\partial z} \left(\frac{D}{\partial z} \right) \right] \phi \\ &= \frac{2}{\Delta T} (\lambda_\theta + \lambda_r + \lambda_z) \phi \end{aligned} \quad (47)$$

where:

$$\lambda_r = \frac{\Delta T}{2} \frac{1}{r} \frac{\partial}{\partial r} \left(D r \frac{\partial}{\partial r} \right),$$

$$\lambda_\theta = \frac{\Delta T}{2} \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{D}{r} \frac{\partial}{\partial \theta} \right), \text{ and}$$

$$\lambda_z = \frac{\Delta T}{2} \frac{\partial}{\partial z} \left(D \frac{\partial}{\partial z} \right).$$

Let:

$$\frac{C_o P_i^{n+(1/2)}}{\mu_{mix}^{n+(1/2)}} = \bar{D}_i,$$

$$\eta_r = \frac{\Delta T}{2} \frac{1}{r} \frac{\partial}{\partial r} \left(\bar{D}_i r \frac{\partial}{\partial r} \right),$$

$$\eta_\theta = \frac{\Delta T}{2} \frac{1}{r} \frac{\partial}{\partial \theta} \left(\frac{\bar{D}_i}{r} \frac{\partial}{\partial \theta} \right), \text{ and} \quad (48)$$

$$\eta_z = \frac{\Delta T}{2} \frac{\partial}{\partial z} \left(\bar{D}_i \frac{\partial}{\partial z} \right).$$

Substituting Eqs. 47 and 48 into Eq. 46 gives:

$$\begin{aligned} P_i^{n+1} - P_i^n &= (\lambda_r + \lambda_\theta + \lambda_z)(P_i^{n+1} + P_i^n) \\ &\quad + 2(\eta_r + \eta_\theta + \eta_z)P_i^{n+(1/2)} + \Delta TS_i^{n+(1/2)} \end{aligned} \quad (49)$$

or

$$(1 - \lambda_r - \lambda_z - \lambda_\theta)P_i^{n+1} = (1 + \lambda_r + \lambda_z + \lambda_\theta)P_i^n + f_i \quad (50)$$

where:

$$\begin{aligned} f_i &= 2 \sum_j^m (\bar{\lambda}_r + \bar{\lambda}_z + \bar{\lambda}_\theta)P_j^n + (\eta_r + \eta_z + \eta_\theta)P_i^{n+(1/2)} \\ &\quad + \Delta TS_i^{n+(1/2)}, \quad j \neq i \end{aligned} \quad (51)$$

where: m = number of gas components.

Now add $(\lambda_r \lambda_z + \lambda_z \lambda_\theta + \lambda_\theta \lambda_r - \lambda_r \lambda_z \lambda_\theta)P_i^{n+1}$ to the left side and $(\lambda_r \lambda_z + \lambda_z \lambda_\theta + \lambda_\theta \lambda_r - \lambda_r \lambda_z \lambda_\theta)P_i^n$ to the right side of Eq. 50. Direct substitution yields:

$$(1 - \lambda_r)P_i^* = (1 + \lambda + 2\lambda_r + 2\lambda_z)P_i^n + f_i$$

$$(1 - \lambda_z)P_i^{**} = P_i^* - \lambda_z P_i^n \quad (52)$$

$$(1 - \lambda_\theta)P_i^{n+1} = P_i^{**} - \lambda_\theta P_i^n$$

Equation 52 gives a tridiagonal system of equations using the Crank-Nicholson method (Carnahan, Luther, and Wilkes, 1969). The finite difference analogues for operators r , z , and θ are given by:

$$\begin{aligned}\lambda_r f &= \frac{\Delta T}{2} \frac{1}{r} \frac{\partial}{\partial r} \left(D r \frac{\partial f}{\partial r} \right) \\ &= \frac{\Delta T}{2} \delta_r D \delta_r f + \frac{D}{r} \delta_r f + D \delta_r^2 f\end{aligned}\quad (53)$$

$$\delta_x f = (f_{\ell+1} - f_{\ell-1}) / (2\Delta X) \quad (54)$$

$$\delta_x^2 f = (f_{\ell-1} - 2f_{\ell} + f_{\ell+1}) / (\Delta X)^2 \quad (55)$$

where:

$$\ell = i, j, \text{ or } k,$$

$$X = r, \theta, \text{ or } z, \text{ and}$$

$$X = r, r\Delta\theta, \text{ or } \Delta z.$$

Therefore:

$$\lambda_r f = \frac{\Delta T}{2\Delta r^2} \left\{ \left[\frac{D'_i}{4} + \frac{(2i-1)D}{2i-2} \right] f_{i+1} - 2Df_i + \left[\frac{(2i-3)D}{2i-2} - \frac{D'}{4} \right] f_{i-1} \right\} \quad (56)$$

$$\lambda_z f = \frac{\Delta T}{2\Delta z^2} \left[\left(\frac{D'_j}{4} + D \right) f_{j+1} - 2Df_j + \left(D - \frac{D'_j}{4} \right) f_{j-1} \right] \quad (57)$$

$$\lambda_\theta f = \frac{\Delta T}{2[(i-1)\Delta r\Delta\theta]^2} \left[\left(\frac{D'_k}{4} + D \right) f_{k+1} - 2Df_k + \left(D - \frac{D'_k}{4} \right) f_{k-1} \right] \quad (58)$$

Similar expressions are written for η_r , η_z , and η_θ by replacing D with $\bar{D}_i$. In the two-dimensional codes, due to axisymmetry, $\lambda_\theta P_i^n$ vanishes, and Eq. 51 reduces to:

$$(1 - \lambda_r) P_i^* = (1 + \lambda_r + 2\lambda_z) P_i^n + f_i$$

and

$$(1 - \lambda_z) P_i^{n+1} = P_i^* - \lambda_z P_i^n \quad (59)$$

Only small changes in the algorithm are required, i.e., all terms containing derivatives with respect to θ are dropped. The solution requires only two sweeps, one in the r -direction and the other in the z -direction.

3.3.3 Finite Difference Algorithms for Boundaries

This section gives the finite difference algorithms for the boundary conditions described in Sec. 3.2.3.

Condition 1

To avoid a singularity, the boundary must be placed one grid point beyond $r = 0$ and the boundary $r = \Delta r$ treated as an impervious boundary. Therefore Eq. 53 reduces to:

$$\lambda_{rf} = \frac{D\Delta T}{2} \delta_{rf}^2 \quad (60)$$

and Eq. 56 becomes:

$$\lambda_{rf} = \frac{D\Delta T}{\Delta r^2} (f_{i+1} - f_i) \quad (61)$$

Condition 2

In Eq. 57,

$$\lambda_{zf} = \frac{D\Delta T}{\Delta z^2} (f_{j-1} - f_j) \quad (62)$$

Condition 3

$v = \text{constant}$

Condition 4

In Eq. 51,

$$S_i^{n+(1/2)} = 2CK_1 \frac{(v_{i1} - v_{i0})}{Z} \quad (63)$$

where:

v_{i1} = partial pressure of component i outside the fill above the ground surface, and

v_{i0} = partial pressure of component i just below the ground surface.

Condition 5

In Eq. 58,

$$\lambda_{\theta f} = \frac{D\Delta T}{[(i-1)\Delta r\Delta\theta]^2} (f_{k+1} - f_k) \quad (64)$$

Condition 6

In Eq. 58,

$$\lambda_{\theta f} = \frac{D\Delta T}{[(i-1)\Delta r\Delta\theta]^2} (f_{k-1} - f_k) \quad (65)$$

Condition 7

In Eq. 47,

$$\lambda_{zf} = \frac{D\Delta T}{\Delta z^2} (f_{j+1} - f_j) \quad (66)$$

Condition 8

In Eq. 51,

$$S_i^{n+(1/2)} = QP_i^{n+(1/2)} \quad (67)$$

where Q = flow rate.

4 FINITE DIFFERENCE COMPUTER CODES

The finite difference computer codes used to solve the gas transport equations (see Eq. 33) are presented in this chapter. The codes use the finite difference algorithms introduced in Secs. 3.3.3 and 3.3.4 to determine gas concentration as a function of time and distance from the landfill. The computer programs described are as follows:

- Code IV: A two-dimensional, finite difference code that can be applied in Cartesian coordinates for relatively long, straight-sided fills with trench-type recovery systems, or that can be applied in cylindrical coordinates to fills that are circular in plan view with annular trench-type recovery systems.
- Code V: A three-dimensional, finite difference code that can be applied in cylindrical coordinates to fills that are circular in plan view and that have circular pipe recovery systems.

4.1 CODE IV

As previously noted, the transport coefficients of Eq. 33 are highly dependent upon gas concentration. In particular, the pressure flow of a given component is directly proportional to the concentration of that component at the point under consideration. Because of this nonlinearity, Code IV uses explicit predictor steps to evaluate the transport coefficients at the middle of the time interval. These coefficients are then used in an alternating-direction implicit corrector step to determine the gas concentrations at the end of the time interval. The time increment for the predictor step is based on the following limitations established by Carnahan, Luther, and Wilkes (1969):

$$\lambda = D_{\max} T (\Delta X^{-2} + \Delta Y^{-2} + \Delta Z^{-2}) / K \leq 0.5 \quad (68)$$

where:

- D = transport coefficient,
- T = predictor step time increment,
- X = horizontal grid size, and
- Z = vertical grid size.

The time increment for the corrector step is restricted to four times that used by each predictor step.

Code IV can accommodate trench-type recovery systems or hybrid systems consisting of trenches with adjacent low permeability barriers. The program can handle ten different pore radii; however, more pore radii can be treated by simply changing several program statements. It should be noted that the effective transport coefficients are obtained by summing the elements of a

matrix over pore radii, the elements being obtained by inverting a square matrix of a size equal to the number of gas components considered. As such, the cost of running the program increases rapidly with an increasing number of pore radii.

The program user can specify the time steps taken between printouts. At each printout, the partial pressures and the total pressure are given. At the soil surface, partial pressures are modified to make the total pressure atmospheric; however, at the location of the pump this pressure is allowed to float, assuming that the trench top can be sealed so that pumping effectiveness can be realized. Pump characteristic curves can be used to determine the relationship between pressure at the pump and pumping rates. These characteristic curves allow the specific attributes of the pump being used to be introduced into the program.

Program execution is terminated after a specific time has been reached or after a specified number of steps have been computed, whichever occurs first.

A listing of Code IV is given in Appendix A.

4.1.1 Principal Variables

The principal variables used in Code IV are listed below.

MF = Number of mesh points up to end of fill ($r = r_f$)
 NF = Number of mesh points over the depth of fill
 ML = Number of mesh points up to the radial boundary ($r = r_s$)
 NL = Number of mesh points over the depth of soil
 MP = Mesh point number at the location of vent/trench
 NP = Number of mesh points over the depth of vent/trench
 KP = Number of mesh points in θ -direction
 NPIPS = Total number of pipes along the circumference
 NCMP = Number of gas components
 NHIST = Number of points on the generation history curve
 IIN = Code for reading in initial concentrations
 IIN = 0 = Initialize uniform concentrations in fill and soil separately
 IIN = 1 = Initial concentrations are read in for each mesh point for all components
 IOUT = Code for punching out final concentrations
 IOUT = 0 = Do not punch out
 IOUT = 1 = Punch out
 IPUMP = Code for pumping in/out
 IPUMP = 1 = Air is pumped in
 IPUMP = 2 = Mixture is pumped out
 IBARR = Code for barrier
 IBARR = 0 = No barrier
 IBARR $\neq$ 0 = Barrier is present
 ITR = Code for iterating to determine pressures in wells
 ITR = 0 = No iterations for well pressures
 ITR = 1 = Pressures are iterated over the depth of the pipe

MTOT = Variable array size. Set MTOT equal to the dimension of array A in common block. If the number of mesh points is increased, the program capacity should be changed 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)

TEMP = Temperature in the system (K)

DX = Spatial mesh size (cm)

DTI = Initial increment of time (days)

TMAX1 = Maximum time allowed before program termination (days)

IFREQ = Number of time increments between successive printouts

NSTEP = Maximum number of steps allowed before program termination

NPRDC = Number of predictor steps between successive corrector steps

CK1 = Convection coefficients for soil surface

CK2 = Convection coefficients for trench top

NRADII = Number of pore radii considered for soil

R = Pore radii of soil

FV = Volumetric fraction

TTIM = Time on generation history curve

ROO = Generation rates for various components at times TTIM

PO = Initial concentration in the fill; used if IIN = 0

PRS = Initial concentrations in the soil; used if IIN = 0

AM = Molecular weights of various components (g/mole)

AMU = Viscosity of various components (poise)

DAB = Bulk diffusion coefficients

NPUMP = Number of points on the pump characteristic curve

QPUMP = Pump discharge

PPUMP = Pump pressure corresponding to QPUM

AK = Knudsen diffusion coefficient

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 (days)

Q = Discharge at pump (ft^3/min)

DD = A matrix of effective diffusion coefficients for a component i diffusing through a component j ($i, j = 1, \text{NCMP}$)

DP = A matrix of transport coefficients for pressure flow

A = Array of coefficients on lower diagonal of coefficient matrix

B = Array of coefficients on the diagonal coefficient matrix

C = Array of coefficients on upper codiagonal of coefficient matrix

F = Vector containing values on the right side of Eq. 52

CPRIM = Temporary array used to store partial pressures computed in subroutine TRIDAG

BETA = Temporary array used in subroutine TRIDAG

GAMMA = Temporary array used in subroutine TRIDAG

X = Distance along radius or along depth of soil

PN = Partial pressure at the beginning of a time interval

PS = Partial pressure at the end of predictor step

PP = Temporary array used to store partial pressures during corrector step

4.1.2 Flow Chart

Code IV consists of ten subroutines, including the MAIN program and subroutines SOLV, CFIL, PREDIC, PRBDIC, CORECT, CORBCT, PUMP, INVERT, and TRIDAG. The flow charts for each of these subroutines are given in Figs. 4.1-4.7.

4.1.3 Instructions for Data Preparation

The sequence of punched cards shown in Table 4.1 contains the problem data for input to the program.

4.2 CODE V

Code V can accommodate landfills that are circular in plan view and use well-type recovery systems. It is assumed that the wells are located in a circular pattern with equal distances between the wells. The user can specify the number of pipe sets and the depth, location, and discharge for each set. Any number of pipe sets can be specified; however, the number of pipes in each circle (NPIPS) must be the same for all sets.

An explicit numerical scheme is used in Code V to solve the three-dimensional finite difference algorithms given in Chapter 2. Code V requires approximately four times as much computer time as Code IV and therefore should be used only when a three-dimensional analysis is required. The addition of the θ -direction is accomplished by dividing a slice subtending an angle equal to θ/NPIPS into KL mesh points. The axis ($r = 0$) is a singular point and is excluded from analysis.

A modified version of Code V, Code VB, can be used to model landfills with irregular geometries. Initial pressures and generation rates are specified at each nodal point.

The general input and output format for Code V is similar to that given in Sec. 4.1 for Code IV.

A listing of Code V is given in Appendix B.

4.2.1 Principal Variables

The principal variables listed in Sec. 4.1.1 for Code IV are also used in Code V. Several additional variables must be introduced to accommodate the extra dimension in Code V. These variables are:

- KL = Number of mesh points along the θ -direction,
- NPIPS = Number of pipes over the circumference,
- NPOR = Point of symmetry for maximum resolution output, and
- NPC = Number of pipe sets.

Fig. 4.1 Code IV, Subroutine SOLV

Fig. 4.1 (Cont'd)

Fig. 4.2 Code IV, Subroutine CFIL

Note: PRBDIC is used if a barrier exists; if not, PREDIC is used.

Fig. 4.3 Code IV, Subroutine PREDIC/PRBIC

Note: CORBCT is used if a barrier exists; if not, CORECT is used.

Fig. 4.4 Code IV, Subroutine CORRECT/CORBCT

Fig. 4.5 Code IV, Subroutine PUMP

Fig. 4.6 Code IV, Subroutine INVERT

Fig. 4.7 Code IV, Subroutine TRIDAG

Table 4.1 Instructions for Data Preparation, Code IV

Card, Field Description	Columns
Card 1: Control data (13I5)	
Number of mesh points up to the end of fill (MF)	1-5
Number of mesh points up to the depth of fill (NF)	6-10
Number of mesh points up to the end of soil boundary (ML)	11-15
Number of mesh points up to the depth of soil boundary (NL)	16-20
Number of mesh points up to the vent (MP)	21-25
Number of mesh points over the depth of vent (NP)	26-30
Number of gas components considered (NCMP)	31-35
Number of points on the fill history curve (NHIST)	36-40
Code for inputting the initial concentrations (IIN)	41-45
Code for punching out the partial pressures at the end of time of analysis (IOUT)	46-50
Code for pumping in or out (IPUMP)	51-55
Code for barrier (IBARR)	56-60
Code for well pressure iterations (ITR)	61-65
Card 2: Title card (10A8)	
Arbitrary descriptive identification of the job	1-80
Card 3: Partial pressures outside the fill (8F10.0)	
Initial discharge at well, ft^3/min (Q)	1-10
Partial pressure for component 1 outside fill (POUT_1)	11-20
Partial pressure for component 2 outside fill (POUT_2)	21-30
etc.	
Card 4: (8F10.0)	
Tortuosity of soil, dimensionless (TORT)	1-10
Temperature of gases, K (TEMP)	11-20
Spatial mesh size, cm (DX)	21-30
Period of analysis, days (TMAX)	31-40
Time step, days (DTI)	41-50
Card 5: (3I5)	
Number of steps between printouts (IFREQ)	1-5
Maximum number of steps of analysis (NSTEP)	6-10
Number of predictor steps (NPRDC)	11-15
Card Set 6 (total of NCMP cards): Surface transfer coefficients for each component (2F10.0)^a	
Mass transfer coefficients for top of fill (CK1)	1-10
Mass transfer coefficients for top of vent (CK2)	11-20
Card 7: (I5)	
Total number of pore radii (NRADII)	1-5

Table 4.1 (Cont'd)

Card, Field Description	Columns
Card Set A: Pore size distribution (2F10.0)	
Pore radius, Å (R_i)	1-10
Volumetric fraction, dimensionless (FV_i)	11-20
Card Set B (total of NHIST cards): Fill history (8F10.0)	
Time (days)	1-10
Rate of generation for component 1	11-20
Rate of generation for component 2	21-30
Rate of generation for component 3	31-40
etc.	
Card Set C (total of NCMP cards): (8F10.0)^a	
Initial partial pressure in the fill (PO_i)	1-10
Initial partial pressure in the soil (PRS_i)	11-20
Molecular weight (AM_i)	21-30
Viscosity (AMU_i)	31-40
Card Set D (total of NCMP cards): (8F10.0)	
<u>Card 1</u>	
Bulk diffusion coefficient of component 1 through 1	1-10
Bulk diffusion coefficient of component 1 through 2	11-20
Bulk diffusion coefficient of component 1 through 3	21-30
etc.	
<u>Card 2</u>	
Bulk diffusion coefficient of component 2 through 1	1-10
Bulk diffusion coefficient of component 2 through 2	11-20
etc.	
⋮	
<u>Card NCMP</u>	
Card Set E: Pump characteristic curve	
<u>Card 1: (I5)</u>	
Number of points on pump characteristic curve (NPUMP)	1-5
<u>Cards 2 through (NPUMP+1): (2F10.0)</u>	
Discharge of pump ($QPUMP_i$)	1-10
Pressure at pump ($PPUMP_i$)	11-20

^aOne card for each component.

4.2.2 Flow Chart

Code V consists of six subroutines, including the MAIN program and subroutines SOLV, CFIL, INVERT, PREDIC, and PUMP. The flow charts for each of these subroutines are similar to those given in Sec. 4.1.2, the primary difference being a sweep in the θ -direction in addition to the r- and z-directions. This changes subroutine PREDIC, but the general format as indicated by the flow charts does not differ from that given for Code IV.

4.2.3 Instructions for Data Preparation

The sequence of punched cards shown in Table 4.2 contains the problem data for input to the program.

Table 4.2 Instructions for Data Preparation, Code V

Card, Field Description	Columns
Card 1: (11I5)	
Number of mesh points up to end of fill (MF)	1-5
Number of mesh points up to depth of fill (NF)	6-10
Number of mesh points up to end of soil boundary (ML)	11-15
Number of mesh points up to depth of soil boundary (NL)	16-20
Number of mesh points along θ -direction (KL)	21-25
Total number of pipes over circumference (NPIPS)	26-30
Number of gas components considered (NCMP)	31-35
Number of points on the fill history curve (NHIST)	36-40
Code for inputting initial concentrations (IIN)	41-45
Code for punching out partial pressures at the end of the time of analysis (IOUT)	46-50
Point of symmetry for maximum resolution output (MPOR)	51-55
Card 2: (I5)	
Number of pipe sets (NPC)	1-5
Card Set A (total of NPC cards): (2I5,F5.0)	
Number of mesh points over depth of pipe (NP)	1-5
Number of mesh points to location of pipe (MP)	6-10
Discharge at pipe (Q)	11-15
Card 4: Title card (10A8)	
Arbitrary descriptive identification of job	1-80
Card 5: (8F10.0)	
Partial pressure for component 1 outside fill (POUT ₁)	1-10
Partial pressure for component 2 outside fill (POUT ₂)	11-20
etc.	

Table 4.2 (Cont'd)

Card, Field Description	Columns
Card 6: (8F10.0)	
Tortuosity of soil, dimensionless (TORT)	1-10
Temperature of gases, K (TEMP)	11-20
Spatial mesh size, cm (DX)	21-30
Period of analysis, days (TMAX1)	31-40
Period of analysis, days (TMAX2)	41-50
Initial time step (DTI)	51-60
Card 7: (3I5)	
Number of steps between printouts (IFREQ)	1-5
Maximum number of steps of analysis (NSTEP)	6-10
Number of predictor steps (NPRDC)	11-15
Card 8: (I5)	
Total number of pore radii (NRADII)	1-5
Card Set B (total of NRADII cards): Pore size distribution (2F10.0)	
Pore radius, Å (R_i)	1-10
Volumetric fraction, dimensionless (FV_i)	11-20
Card Set C (total of NHIST cards): Fill history (8F10.0)	
Time (days)	1-10
Rate of generation for component 1	11-20
Rate of generation for component 2	21-30
Rate of generation for component 3	31-40
etc.	
Card Set D (total of NCMP cards): (8F10.0)^a	
Initial partial pressure in the fill (PO_i)	1-10
Initial partial pressure in the soil (PRS_i)	11-20
Molecular weight (AM_i)	21-30
Viscosity (AMU_i)	31-40
Surface convection coefficient for top of vent (CK1)	41-50
Surface convection coefficient for top of soil (CK2)	51-60
Card Set E (total of NCMP cards): (8F10.0)	
Card 1: (8F10.0)	
Bulk diffusion coefficient of component 1 through 1	1-10
Bulk diffusion coefficient of component 1 through 2	11-20
Bulk diffusion coefficient of component 1 through 3	21-30
etc.	

Table 4.2 (Cont'd)

Card, Field Description	Columns
Card Set E (Cont'd)	
<u>Card 2: (8F10.0)</u>	
Bulk diffusion coefficient of component 2 through 1	1-10
Bulk diffusion coefficient of component 2 through 2	11-20
Bulk diffusion coefficient of component 2 through 3	21-30
etc.	
:	
:	
<u>Card NCMP</u>	
Card Set F: Pump characteristic curve	
<u>Card 1: (I5)</u>	
Number of points on curve (NPUMP)	1-5
<u>Cards 2 through (NPUMP+1): (2F10.0)</u>	
Discharge of pump (QPUMP _i)	1-10
Pressure at pump (PPUMP _i)	11-20

^aOne card for each component.

5 COMPUTER SIMULATIONS

In this chapter, the finite difference computer codes introduced in Chapter 4 are applied to several landfills to simulate methane recovery systems. Code IV, the two-dimensional pressure flow program, is used to model a cylindrically shaped landfill. Code V, modified to accommodate irregular fill geometries, is used to model the Puente Hills landfill, a field test site that is being studied in conjunction with another project under sponsorship of the U.S. Department of Energy (DOE).

5.1 COMPUTER SIMULATION OF METHANE RECOVERY FOR A HYPOTHETICAL LANDFILL

Several methane recovery systems in a hypothetical landfill have been analyzed to illustrate the modeling capabilities of Code IV. The landfill is assumed to be circular in plan view with a radius of 160 m and a depth of 16 m. The soil surrounding the landfill is fine-grained and a gas-impervious layer is encountered at a depth of 37 m. Initially, the landfill has a concentration of 70% methane and 30% carbon dioxide. The atmosphere above the landfill and the soil surrounding the landfill initially contain air. As time progresses, the methane and carbon dioxide migrate outward, and air invades the landfill.

The soil is assumed to have a porosity of 0.4, a tortuosity of 1.55, and a pore size of 1450 Å. A surface convection coefficient corresponding to a wind velocity of 5 mph is used.

Extraction wells are placed at different locations and depths and are subjected to different extraction rates, as shown in Table 5.1. These wells are illustrated in Figs. 5.1-5.4. All other data are consistent in each of the four computer runs made. The complete input deck used is given in Table 5.2.

Figure 5.1 presents the results for Well 1. Figure 5.1a shows the relative total pressure, which refers to the ratio of the total pressure with the extraction well operating to that at the same point and time but without the well operating (expressed as a percentage). In Fig. 5.1a, the relatively low pumping rate of 1 ft³/min results in a small zone of influence around the extraction well. Figure 5.1b, which shows the relative percentage of methane, indicates that there is a significant reduction in that gas.* Thus, the well is more

Table 5.1 Wells Examined in Code IV Landfill Simulation

Well	Distance from Center of Landfill (m)	Well Depth (m)	Extraction Rate (ft ³ /min)
1	120	12	1
2	120	12	10
3	120	8	2
4	152	16	10

*The term "relative percentage" is defined as the ratio of the concentration with the extraction well operating to that at the same point and time but without the well operating.

(a) Relative Total Pressure (%)

(b) Relative Percentage of Methane

(c) Relative Percentage of Oxygen

Fig. 5.1 Code IV Landfill Simulation, Well 1 (vertical section)

(a) Relative Total Pressure (%)

(b) Relative Percentage of Methane

(c) Relative Percentage of Oxygen

Fig. 5.2 Code IV Landfill Simulation, Well 2 (vertical section)

(a) Relative Total Pressure (%)

(b) Relative Percentage of Methane

(c) Relative Percentage of Oxygen

Fig. 5.3 Code IV Landfill Simulation, Well 3 (vertical section)

(a) Relative Total Pressure (%)

(b) Relative Percentage of Methane

(c) Relative Percentage of Oxygen

Fig. 5.4 Code IV Landfill Simulation, Well 4 (vertical section)

Table 5.2 Code IV Data Deck

Card	Column	Value	Card	Column	Value
1	4-5	40	10	5-10	1450.0
	10	4		18-20	0.4
	14-15	60	11	8-10	0.0
	20	8		13-20	1.46E-09
	24-25	30		23-30	0.00E-00
	30	3		33-40	0.63E-09
	35	3	12	4-10	73000.0
	40	2		13-20	1.46E-09
	45	0		23-30	0.00E-00
	50	0		33-40	0.63E-09
	55	2	13	8-10	0.7
	60	0		18-20	0.0
	65	1		26-30	16.05
2	1-8	Code IV		35-40	0.0108
3	8-10	1.0	14	8-10	0.0
	18-20	0.0		18-20	1.0
	28-30	1.0		26-30	28.02
	38-40	0.0		35-40	0.0177
4	7-10	1.55	15	8-10	0.3
	16-20	298.0		18-20	0.0
	26-30	400.0		26-30	44.00
	35-40	3650.0		35-40	0.0145
	48-50	1.0	16	5-10	0.2225
5	4-5	50		14-20	0.21875
	8-10	200		25-30	0.1668
	15	2	17	4-10	0.21875
6	2-10	0.0000206		15-20	0.2225
	12-20	0.0000206		25-30	0.1580
7	2-10	0.0000215	18	5-10	0.1668
	12-20	0.0000215		15-20	0.1580
8	2-10	0.0000173		25-30	0.1103
	12-20	0.0000173	19	5	1
9	5	1	20	8-10	1.0

efficient at extracting methane than it is in reducing the total pressure; this is a desirable situation in practice. Figure 5.1c shows the relative percentage of oxygen. The extraction well draws in a limited amount of oxygen from the surface of the landfill. This process is undesirable because oxygen can quench the anaerobic methane generation processes and thus arrest the production of gas in the landfill.

Figure 5.2 shows the same geometric configuration as Fig. 5.1 but with the pumping rate increased to $10 \text{ ft}^3/\text{min}$. Figure 5.2a shows the relative total pressure; a large zone of influence extending into the soil beneath the landfill is apparent. Figure 5.2b shows that methane concentrations are reduced over an equally large area. Figure 5.2c shows that a considerable amount of oxygen is drawn into the landfill surface by this relatively high pumping rate.

Figure 5.3 illustrates an extraction well at the same location as those in Figs. 5.1 and 5.2, but only half as deep. The pumping rate is $2 \text{ ft}^3/\text{min}$. This arrangement was chosen as a compromise between the previous two cases with the hope that methane production would be increased. Figure 5.3a shows that the zone of influence with respect to total pressure lies primarily within the landfill. Figure 5.3b indicates that methane is being extracted over a large portion of the landfill. Figure 5.3c shows that a moderate amount of oxygen is being drawn into the landfill surface.

Figure 5.4 shows a configuration that was designed both to recover methane and to control its migration into the soil beyond the landfill. In Fig. 5.4a, a total pressure zone of influence extends to a large area around the well. Figure 5.4b shows an equally large area of reduced methane concentrations; it is evident that a significant reduction in methane migration has been achieved.

5.2 COMPUTER SIMULATION OF METHANE RECOVERY FOR THE PUENTE HILLS LANDFILL

Although studies similar to the one discussed in Sec. 5.1 are valuable in determining the effects of various pump locations, geometries, and extraction rates, actual landfills are seldom as geometrically simple or homogeneous as the hypothetical one used to illustrate Code IV. In this section, Code V, modified to accommodate multiple pipe sets and irregular fill geometries, is used to model a landfill with a relatively complex geometry.

Although detailed descriptions of the geometry, soil conditions, gas generation rates, and initial gas concentrations and pressures for the Puente Hills landfill are not presently available, sufficient information to illustrate some of the capabilities of the modified version of Code V has been obtained or assumed. A more refined analysis will be possible as more information becomes available.

The Puente Hills landfill (Fig. 5.5) was formed by filling a 2000-ft long canyon that juts into the side of a hill in Whittier, California. The floor of the canyon slopes in a north-south direction from an elevation of 525 ft at its closed end to 275 ft at the open end. A horizontal cut was made into the canyon walls at elevation 525 ft, and approximately 125 ft of fill

Fig. 5.5 Plan View of Puente Hills Landfill (showing locations of extraction wells and cross sections [K = 1-4] used for computer simulation)

were placed onto this cut. The western edge of the fill meets the side of the hill approximately 400 ft from the wall of the canyon, while the eastern edge extends from the canyon for an undesignated but relatively large distance. At the open end of the canyon, the fill has a 2:1 slope.

Three wells (Fig. 5.6), each 105 ft deep, have been placed in the fill, and a network of 34 probes surrounds the line of wells. These probes were placed in borings that are also 105 ft in depth.

For the Code V simulation, the landfill was divided into four cross sections (Fig. 5.7), each of which was subdivided by a series of nodes spaced at 8-m intervals.* Gas generation rates, initial concentrations, and total pressures were then assigned to each nodal point. The boundary conditions used were a prescribed convection at the fill top and prescribed concentrations at the edge of the fill.

The soil was assumed to have a porosity of 0.4, a tortuosity of 1.55, and a pore size of 40,000 Å. A surface convection coefficient corresponding to a wind velocity of 5 mph was used. The same generation rates as those used for the hypothetical landfill presented in Sec. 5.1 gave pressures of between

*The vertical scale has been doubled in this and subsequent figures; the landfill is actually much shallower in relationship to its length than depicted.

Fig. 5.6 Extraction Wells in Puente Hills Landfill

1.00 atm and 1.02 atm, which corresponds to a maximum gauge pressure in the fill of 8.1 in. of water.

The complete input deck used in the Puente Hills simulation is given in Table 5.3.

Figure 5.8 illustrates the 5%- and 50%-methane contours after 100 days with no pumping at the wells, assuming that the initial methane concentration in the landfill was 70%. Figure 5.9 gives pressure contours at Well 2 for extraction rates of 20 ft³/min, 100 ft³/min, and 200 ft³/min after 10 days of pumping. Comparing the one-inch vacuum contours shows that increasing the extraction rate by a factor of ten has a relatively small effect upon the size of the sphere of influence. The spheres of influence in Figs. 5.9c and 5.9e are virtually identical. However, increasing the pumping rate affects the size of the pressure gradients within the sphere of influence. Comparison of the 10-in. contour in Fig. 5.9c with the 20-in. contour in Fig. 5.9e

(a) Cross Section 1

(b) Cross Section 2

(c) Cross Section 3

(d) Cross Section 4

Fig. 5.7 Cross Sections through Landfill

Table 5.3 Code V Data Deck

Card	Column	Value	Card	Column	Value
1	4-5	48	10	5	1
	10	8			
	14-15	50	11	4-10	40000.0
	20	9		18-20	0.4
	25	4			
	30	6	12	8-10	0.0
	35	2		13-20	1.46E-09
	40	2		23-30	0.00E-09
	45	1			
	50	0	13	4-10	73000.0
	54-55	29		13-20	1.46E-09
				23-30	0.00E-09
2	5	3			
			14	8-10	0.7
3	5	4		18-20	0.0
	9-10	21		26-30	16.05
	18-20	0.0		35-40	0.0108
				42-50	0.0000215
4	5	4		53-60	1.46E-09
	9-10	29			
	18-20	0.0	15	8-10	0.3
				18-20	1.0
5	5	4		20-30	28.02
	9-10	37		35-40	0.0177
	18-20	0.0		42-50	0.0000206
				53-60	0.00E-00
6	1-8	CODE V			
			16	5-10	0.2225
7	8-10	0.0		14-20	0.21875
	18-20	1.0			
			17	5-10	0.21875
8	7-10	1.55		14-20	0.2225
	16-20	298.0			
	27-30	800	18	5	1
	35-40	3650			
	45-50	3650	19	18-20	0.0
	58-60	0.5			
9	3-5	100			
	7-10	200			
	15	2

(a) Cross Section 1

(b) Cross Section 2

(c) Cross Section 3

(d) Cross Section 4

Fig. 5.8 Percentage Methane Contours through Cross Sections
(for assumed gas generation rates and without
pumping at wells)

(a) Extraction Rate of 20 ft³/min, Cross Section 1

(b) Extraction Rate of 20 ft³/min, Cross Section 2

(c) Extraction Rate of 100 ft³/min, Cross Section 1

(d) Extraction Rate of 100 ft³/min, Cross Section 2

Fig. 5.9 Vacuum Contours at Well 2 (in. of water, for various extraction rates and cross sections)

(e) Extraction Rate of 200 ft³/min, Cross Section 1

(f) Extraction Rate of 200 ft³/min, Cross Section 2

(g) Extraction Rate of 200 ft³/min, Cross Section 3

Fig. 5.9 (Cont'd)

suggests that higher pumping rates will remove the methane in the area of the well more quickly, but will not substantially increase the net yield.

The relative percentages of methane and oxygen in the fill after 10 days of pumping at rates of 20 ft³/min, 100 ft³/min, and 200 ft³/min are given in Fig. 5.10.* Comparison of Figs. 5.10c and 5.10e shows that increasing the pumping rate from 20 ft³/min to 100 ft³/min will substantially increase the amount of methane removed after 10 days. However, doubling the rate of extraction from 100 ft³/min to 200 ft³/min seems to have only a slight effect

*As in the Code IV simulation study, the term "relative percentage" is defined as the ratio of the concentration with the extraction well operating to that at the same point and time but without the well operating.

(a) Relative Percentage of Methane at Extraction Rate of 20 ft³/min

(b) Relative Percentage of Oxygen at Extraction Rate of 20 ft³/min

(c) Relative Percentage of Methane at Extraction Rate of 100 ft³/min

(d) Relative Percentage of Oxygen at Extraction Rate of 100 ft³/min

Fig. 5.10 Relative Percentages of Methane and Oxygen at Well 2, Cross Section 1, for Various Extraction Rates

(e) Relative Percentage of Methane at Extraction Rate of 200 ft³/min

(f) Relative Percentage of Oxygen at Extraction Rate of 200 ft³/min

Fig. 5.10 (Cont'd)

upon the size or shape of the relative percentage contours. This is shown by comparing Figs. 5.10c and 5.10d with Figs. 5.10e and 5.10g, respectively.

The "figure 8" contours seen in Figs. 5.10c and 5.10e initially suggest that methane movement in the vicinity of the wells occurs in "bubbles." This is not the case, however. These shapes are a manifestation of the method of data presentation and can be explained in the following manner.

A relatively sharp gradient in methane concentration exists at the edge of the fill; outside, the methane concentration is quite low. Pumping rates less than 100 ft³/min have no appreciable effect in this area after the relatively short pumping time of 10 days. Even for quite large pumping rates (100 ft³/min and 200 ft³/min), the wells draw in only very small amounts of methane from this area. Even so, because of the low initial concentrations, this small removal of methane represents a rather large change in the relative percentage of methane. This creates an additional lobe in the well's area of influence, as presented in terms of relative percentages.

As previously mentioned, a more detailed and refined analysis will be possible when more site-specific information becomes available. While this analysis, based upon assumed landfill properties, may be of limited quantitative value, it exhibits some of the qualitative aspects of various extraction rates.

6 METHANE GENERATION IN LANDFILLS

6.1 KINETIC CONTROLS FOR LANDFILL METHANE GENERATION

6.1.1 Microbiology

The formation of methane gas from organic matter is due to the coupled activities of a variety of bacteria. These bacteria are usually divided into two functional groups: an acidogenic group that produces hydrogen, carbon dioxide, ammonia, hydrogen sulfide, and various volatile fatty acids (VFA) from the organic matter; and a methanogenic group that produces methane from the products of the acidogenic group.

The acidogenic group consists primarily of Gram-negative, nonsporulating, obligately anaerobic bacilli, generally of the family Bacteroidaceae (Kirsh and Sykes, 1971). However, obligately anaerobic members of the family Bacillaceae, especially the Clostridium spp., are also common.

The methanogenic bacteria are Gram-negative or -positive rods, cocci, sarcina, or spinula, non-sporulating, and obligately anaerobic (Zeikus, 1977). Despite the wide variety in species characteristics, all the species are collected into a single family, the Methanobacteriaceae (Buchanan and Gibbons, 1974). This is justified by the biochemical unity of the group (Ferry and Wolfe, 1977). The species generally recognized include (Buchanan and Gibbons, 1974; Zeikus, 1977) the following:

- Methanobacterium formicum,
- Methanobacterium mobile,
- Methanobacterium ruminantium,
- Methanobacterium thermoautotrophicum,
- Methanosarcina barkeri, and
- Methanococcus vanniellii.

Other species have also been reported in the literature. However, they are not generally recognized because the type cultures have been lost, the available cultures have not been purified, or the species has not yet been approved by the Judicial Commission of the International Committee on Systematic Bacteriology.

6.1.2 Biochemistry

While the acidogenic bacteria can produce a wide variety of metabolic products, those used by the methanogenic bacteria are limited to hydrogen, carbon dioxide, formic acid, and, perhaps, methanol and acetic acid (Mah et al., 1977; Zeikus, 1977).

Hydrogen gas is a common product of anaerobic fermentation. Bacteria that make it are able to accomplish a more complete "oxidation" of their organic substrates and thereby obtain more energy from them (as adenosine

triphosphate, ATP). There are two basic ways to form hydrogen, the so-called "clostridial" and "coliform" systems (Gray and Gest, 1965). In the former system, pyruvic acid is oxidized to acetic acid, carbon dioxide and hydrogen. The oxidations occur with the pyruvate bound to the coenzyme thiamine pyrophosphate, and the electrons are transferred to hydrogen via ferredoxin and hydrogenase. In the latter system, the electrons attached to ferredoxin are first used to reduce biotin-bound carbon dioxide to formic acid. The formic acid is then oxidized to carbon dioxide and hydrogen by the hydrogenase enzyme. Both systems are inhibited by accumulated hydrogen, and this inhibition forces the bacteria to revert to non-hydrogen-forming fermentations, such as the homolactic.

All the methanogenic bacteria can reproduce autotrophically using carbon dioxide as the sole carbon source and obtaining energy from the reaction of hydrogen and carbon dioxide (Mah et al., 1977; Zeikus, 1977). In these cases, methane is a product of the energy metabolism of the microbes (Zeikus, 1977):

$$G = -33 \text{ Kcal} \quad (69)$$

Methanosarcina sarcina is the only methanogen believed to produce methane from acetate in pure culture (Mah et al., 1977). Radio tracer studies indicate that the methyl moiety of the acetate is converted intact directly to methane, but the conversion is very slow and may require hydrogen (Mah, Smith, and Baresi, 1978; Zeikus, 1977). The energy yield is small, which may explain the slow rate of conversion (Zeikus, 1977):

$$G = -8.6 \text{ Kcal} \quad (70)$$

6.2 UNINHIBITED KINETICS

It is generally believed that the methanogenic bacteria reproduce much more slowly than the acidogenic bacteria, so that the overall kinetics of methane formation are those of the methanogens. Simple mass balances on any arbitrary culture configuration yield the following equations (Kirsch and Sykes, 1971):

$$\mu = \theta_c^{-1} + k_d \quad (71)$$

$$X\theta_h = \frac{Y\theta_c(S_i - S_e)}{1 + K_d\theta_c} \quad (72)$$

where:

- μ = the specific reproduction rate of the methanogens (per day),
- θ_h = the hydraulic detention time of the culture vessel (days),
- K_d = the specific decay rate of the methanogens (per day),
- X = the concentration of the methanogens in the culture vessel (g cells/m³),
- Y = the growth yield of the methanogens (g cells/g substrate),
- θ_c = the cell retention time (days),
- S_i = the concentration of substrate in the influent flow (g substrate/m³), and
- S_e = the concentration of substrate in the culture vessel effluent (g substrate/m³).

The specific reproduction rate is thought to be, among other variables, a function of the ambient substrate concentration:

$$\mu = \frac{\mu_m S_e}{K + S_e} \quad (73)$$

where:

- μ_m = the maximum specific reproduction rate of the methanogens (per day), and
- K = the Monod half-velocity constant (g substrate/m³).

Some empirical determinations of the various parameters in these equations are cited in Table 6.1. It is presumed that no inhibitors were present in these experiments. It should be noted that K_d for growth on hydrogen plus carbon dioxide has the wrong sign.

6.3 ENVIRONMENTAL EFFECTS

The literature indicates that the dominant environmental variables affecting landfill methane production are moisture, oxygen, temperature, and nutrients.

6.3.1 Moisture

Interregional comparisons of landfills and lysimeter studies indicate that gas and leachate generation rates are strongly influenced by the amount of water in the landfill (DeWalle and Chian, 1978; Eliassen, 1942; Farquhar and Rovers, 1973; Leckie, Pacey, and Halvadakis, 1979; Rovers and Farquhar, 1973). The required moisture content for optimum methane production appears to be about 50-100% of the dry weight of the waste. Moisture levels much above field capacity cause increased leachate production.

These observations are consistent with the known effects of drying upon bacterial survival (Pirt, 1975). Bacterial growth rates are influenced by the activity of water in the growth medium, because water activity affects the energy required to transport nutrients into the bacterial cell. The optimum water activity for bacterial growth is about 0.95 to 0.98 (dimensionless), and maximum specific reproduction rates decrease linearly and rapidly as the water activity decreases below that level.

The water activity in any system is equal to the relative humidity of the gas phase. Thus, the effects of moisture upon bacterial growth can be approximated by a function of the following form:

$$\mu_m = \mu_{mo}[1 - K_h(H_o - H)] \quad (74)$$

where:

μ_{mo} = the maximum specific reproduction rate under optimum conditions (per day),

K_h = an empirical coefficient (reciprocal percent humidity),

H_o = the optimum relative humidity (percent), and

H = the ambient relative humidity (percent).

Landfill humidity can be affected by gas pumping. In some cases, high gas pumping rates may dry the fill and inhibit methane formation. Therefore, any valid kinetic model of methane formation must include subroutines for landfill moisture and temperature so that the relative humidity of the fill can be predicted.

6.3.2 Oxygen and Temperature

The available evidence indicates that newly placed solid wastes decompose aerobically as long as oxygen is available (Fungaroli and Steiner, 1971; Rovers and Farquhar, 1973), and that during the aerobic phase the fill may attain temperatures as high as 60° to 80°C (Eliassen, 1942; Farquhar and Rovers, 1973; Fungaroli and Steiner, 1971). During this initial phase, no methane and little leachate are formed.

Oxygen is known to be very poisonous to acidogenic and methanogenic bacteria, but the concentration at which its toxic effects begin has not been established (Kirsch and Sykes, 1971). However, data from landfill and

Table 6.1 Parameter Values for Methanogen Growth on Hydrogen and Carbon Dioxide and on Acetic Acid

Parameter	Hydrogen ^a	Acetate ^b
μ	1.06 ^c	0.324 ^c
K	569.00 ^d	154.00 ^e
Y	0.34 ^f	0.00408
K_d	-0.009 ^c	0.019 ^c

^aShea et al., 1968.

^bLawrence and McCarty, 1967.

^cPer day.

^dmm Hg of H.

^emg acetate/L.

^fmg cells/mg H.

δ mg cells/mg acetate.

lysimeter studies suggest the toxic effects of oxygen begin around a few percent oxygen by volume in the gas phase (anon., 1969; Farquhar and Rovers, 1973; Fungaroli and Steiner, 1971; Rovers and Farquhar, 1973).

The optimum temperature for methane production is known to be about 35° to 40°C, but high rates of methane formation occur at temperatures as high as 55° to 60°C (Miorin et al., 1977; Pfeffer, 1974; van den Berg, 1977). This suggests that the temperatures attained during the aerobic phase may be inhibitory. On the other hand, in the older, deeper regions of the fill, the temperature is likely to be controlled by the surrounding soil and water. Deep ground temperatures in the northern states are usually less than 15° to 20°C, so methane production in the deeper, older regions may be temperature-limited.

There are no formulae in the literature for the relationships among landfill gas production, oxygen, and temperature. However, arguing by analogy with other biological processes, the following formulae may be suggested:

$$\mu_m = \mu_{mo} \frac{K}{K_o + P_o} \quad (75)$$

$$\mu_m = \mu_{mo} \theta^{T-35}$$

where:

K_o = an empirical constant (atm of O_2),

P_o = the partial pressure of oxygen (atm), and

θ = an empirical constant.

Excessive gas pumping will draw atmospheric oxygen into the fill. This will quench methane production in two ways: (1) by the intrinsic toxicity of oxygen to the methanogens and acidogens, and (2) by the increased temperature due to aerobic decay. The oxygen entering the fill may also react with the methane present, causing fires and explosions.

6.3.3 Nutrients

The materials placed in landfills usually contain large amounts of carbon (about 40-50%) and small amounts of nitrogen (less than 1%) and other nutrients (Golueke and McGauhey, 1967). The optimum level of nitrogen in the feed of anaerobic digesters is 5-10% by weight (Sanders and Bloodgood, 1965; Sievers and Brune, 1978). This nitrogen must be converted to ammonia before the methanogens can use it (Bryant et al., 1971). The methanogenic bacteria are also known to have rather high iron requirements (Hoban and van den Berg, 1979; Patel, Khan, and Roth, 1978; Taylor and Pirt, 1977). High concentrations of other minerals may also be required (Mah, Smith and Baresi, 1978). The mineral requirements reported in these recent studies are so high that it is likely that the early kinetic studies on methanogens employed iron-limited cultures.

Nutrient deficiencies can be made good either by nutrient additions to the solid wastes or by leachate recycling. Leachate recycling systems may be required to prevent groundwater contamination anyway, so the latter option may be the preferred solution to nutrient deficiencies. However, there is no evidence that landfill gas production is limited by nutrient deficiencies.

6.4 ANALYTICAL REPRESENTATION OF GAS GENERATION RATE

Moisture, oxygen, and temperature are the most easily controlled landfill variables. They may be manipulated by adjustments to infiltration, gas recovery, and leachate recycling. For both infiltration and gas pumping there are intermediate levels that are optimum: water and gas fluxes that are substantially different from these optima lead to lowered gas generation rates.

The available literature suggests that landfill gas production is most sensitive to moisture and oxygen. Leachate analyses show acetic acid levels that are too high to be kinetically limiting, and these acid concentrations may be controllable via moisture and oxygen. Therefore, as a first approximation, the rate of methane production is taken to be proportional to each of the corrections indicated above for moisture, oxygen, and temperature, i.e.,

$$r = r_{mo} [1 - K_h (H_o - H)] \left(\frac{K_o}{K_o + P_o} \right) \theta^{T-35} \quad (76)$$

where:

r = the observed rate of methane production (m^3 CH/ m^3 fill/day), and

r_{mo} = the maximum rate of methane production under optimum conditions (m^3 CH/ m^3 fill/day).

7 CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK

Computer simulation offers an economical and effective way to examine alternatives in the design and operation of methane recovery installations at landfills. By providing a means for predicting oxygen draw that might detrimentally affect methane production, the approach described in this paper should result in considerable financial savings in field operations.

7.1 DEVELOPMENT OF INTERACTIVE GRAPHICS CAPABILITIES

In the Puente Hills site study, as more realistic geometries were incorporated into the computer program, the generation of input data cards occupied an increasingly large proportion of the total project time. It was felt that, for computer-assisted design and operation to have a significant impact on landfill methane recovery, the computer programs would have to be made available in a more user-oriented format.

Therefore, an interactive graphics alternative was proposed to allow the user considerable flexibility in providing input to the program. In addition, it would format program output in a much more useful way than possible under previous batch modes of operation.

Preliminary work was undertaken on a Tektronix 4014 computer interactive graphics terminal to investigate the feasibility of this approach. A typical result is shown in Fig. 7.1, which illustrates where the methane concentration exceeds 5% around a hypothetical landfill. However, the 4014 has serious limitations. First, the device has essentially no local intelligence and thus depends entirely upon the host machine for its computational power. Because much of the conditioning of input and output data can be done with a small amount of intelligence, the use of host machine time for such simple tasks is highly inefficient.

Fig. 7.1 Sample Output from Computer Graphics Terminal
(showing area where methane concentration
exceeds 5%)

The second limitation of the 4014 for the present study is its lack of dynamic graphics capability. Such a capability is important because it would permit proposed design configurations to be modified quite easily. For example, the designer may want to use a specific configuration for methane recovery wells; the number and locations of the wells could be optimized by the computer. Dynamic graphics capability facilitates moving and adding wells quickly and avoids the necessity of inputting large amounts of data for each well. Based on the success of the preliminary studies with the 4014, a proposal was submitted for the purchase of a Tektronix 4054 dynamic graphics terminal with expanded local intelligence.

7.2 DEVELOPMENT OF HYBRID NUMERICAL METHODS TO TREAT EXTRACTION WELLS

Additional recommendations for further work include expansion of the computer programs to more realistically simulate important details of the field configurations for methane recovery systems. Because of the complexity of the well configurations in commercial recovery systems, the computer programs must be modified to achieve more effective resolution in specifying the geometry at the well point. This, in turn, requires that the basic numerical methods employed in the programs be modified to introduce hybrid solution elements in the vicinity of the wells. Although the hybrid approach is conceptually borrowed from finite element techniques, it retains the structural simplicity of the finite difference formulation.

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APPENDIX A
CODE IV LISTING

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C PROGRAM AXISYMMETRIC FLOW WITH PENETRATING VENTS AND
C CONCENTRATION & PRESSURE GRADIENTS 2-DIMENSIONAL
C PROGRAMMED BY I.S.RAI
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONE/Q,DTHET,POUT(4),CK1,CK2,CK3,CK4,EMDA,QMAX,
1 ML,NL,NCMP,MF,NF,MM,NP,MP,NHIST,IAX,IIN,IOUT,IPUMP,IBARR,ITR
DIMENSION HED(10)
COMMON A(20000),IA(8)
MTOT=20000
CALL ERRSET(208,256,-1,1)
10 READ(5,40) MF,NF,ML,NL,MP,NP,NCMP,NHIST,IIN,IOUT,IPUMP,IBARR,ITR
IF(MF.EQ.0) GO TO 30
IAX=8
FL=ML-1
FF=MF-1
R1=FL/FF
FL=NL-1
FF=NF-1
R2=FL/FF
READ(5,50) HED
WRITE(6,70) HED,R1,R2
IF(1BARR.NE.0) ML=ML+1
WRITE(6,60) MF,NF,ML,NL,MP,NP,NCMP,NHIST
NNCMP=NCMP*NCMP
MN=ML*NL
MNC=MN*NCMP
MM=MAXO(ML,NL)
M1=1
M2=M1+MNC
M3=M2+MNC
M4=M3+MNC
M5=M4+MN
M6=M5+MNC*NCMP
M7=M6+MNC
M8=M7+NCMP
M9=M8+NCMP
M10=M9+MM
M11=M10+MM
M12=M11+MM
M13=M12+MM
M14=M13+MM
M15=M14+MM
M16=M15+MM
M17=M16+NCMP
M18=M17+NCMP
M19=M18+NCMP
M20=M19+NNCMP
M21=M20+NNCMP
M22=M21+NNCMP
M23=M22+NNCMP
M24=M23+NNCMP
M25=M24+NCMP
M26=M25+ML
M27=M26+NCMP*NHIST
MLAST=M27+NHIST
WRITE(6,90) MLAST
IF(MLAST.LT.MTOT) GO TO 20
JJ=MLAST-MTOT-1
WRITE(6,80) JJ
GO TO 30
20 CALL SOLV(A(M1),A(M2),A(M3),A(M4),A(M5),A(M6),A(M7),A(M8),A(M9),
1 A(M10),A(M11),A(M12),A(M13),A(M14),A(M15),A(M16),A(M17),A(M18),A(M1
29),A(M20),A(M21),A(M22),A(M23),A(M24),A(M25),A(M26),A(M27),A(M1))
GO TO 10
30 STOP
C
C
C
40 FORMAT(16I5)
50 FORMAT(10A8)
60 FORMAT(50H-NUMBER OF MESH POINTS UPTO END OF FILL
1,15/50H NUMBER OF MESH POINTS UPTO DEPTH OF FILL,15/50H N
2UMBER OF MESH POINTS UPTO END OF LAND,15/50H NUMBER OF
3MESH POINTS UPTO DEPTH OF LAND,15/
4 50H NUMBER OF MESH POINTS UPTO V

```



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5ENT LOCATION ,15/30H NUMBER OF MESH POINTS UPTO DEPTH OF V
6ENT ,15/
7 30H TOTAL NUMBER OF GAS COMPONENTS ,15/30
8H NO. OF POINTS ON FILL COMPOSITION HISTORY CURVE ,15/
70 FORMAT (1H1,10A8,' RS/RF =',F5.2,' DS/DF =',F5.2)
80 FORMAT ('-REQUIRED CORE EXCEEDS MTOT BY ',110)
90 FORMAT ('OMTOT REQUIRED FOR THIS PROBLEM = ',110)
END
SUBROUTINE PRBDIC (PH,PS,PP,P,DD,DP,QO,DTAUE)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONE/Q,DTHT,POUT(4),CK1,CK2,CK3,CK4,EMDA,QMAX,
1 ML,NL,NCMP,MF,NF,MM,NP,MP,NHIST,IAX,IIN,IOUT,IPUMP,IBARR,ITR
DIMENSION PN(ML,NL,NCMP),PS(ML,NL,NCMP),PP(ML,NL,NCMP),
1 P(ML,NL),DD(ML,NL,NCMP,NCMP),DP(ML,NL,NCMP),QO(NCMP)
ML1=ML-1
DO 180 L=1,NCMP
PNOUT=POUT(L)
DO 180 I=IAX,ML1
IP=I+1
IM=I-1
FI1=2*I-2
FIIP=(FI1+1.000)/FI1
FIIM=(FI1-1.000)/FI1
DO 180 J=1,NL
JP=J+1
JM=J-1
IF (1.EQ.ML1.AND.J.GT.NP) GO TO 180
IF (1.LE.MP.OR.J.GT.NP) GO TO 4
FI1=FI1-2.000
FIIP=(FI1+1.000)/FI1
FIIM=(FI1-1.000)/FI1
4 FIJ=0.000
DO 50 M=1,NCMP
DIJK=DD(I,J,L,M)
PSIJK=PS(I,J,M)
IF (1.EQ.IAX) GO TO 10
IF (J.GT.NP) GO TO 8
IF (1.EQ.MP) GO TO 12
IF (1.EQ.MP+1) GO TO 10
8 DPRIM=(DD(IP,J,L,M)-DD(IM,J,L,M))*0.25
PPRIM=PS(IP,J,M)-PS(IM,J,M)
FIJ=FIJ+DPRIM*PPRIM+(FIIP*PS(IP,J,M)-2.000*PSIJK+FIIM*PS(IM,J,M))
1 *DIJK
GO TO 20
10 FIJ=FIJ+2.000*DIJK*(PS(IP,J,M)-PSIJK)
GO TO 20
12 FIJ=FIJ+2.000*DIJK*(PS(IM,J,M)-PSIJK)
20 IF (J.EQ.1) GO TO 30
IF (J.EQ.NL) GO TO 40
IF (J.EQ.NP.AND.1.GT.MP) GO TO 32
IF (J.EQ.NP+1.AND.1.GE.MP) GO TO 34
DPRIM=(DD(I,JP,L,M)-DD(I,JM,L,M))*0.2500
PPRIM=PS(I,JP,M)-PS(I,JM,M)
FIJ=FIJ+DPRIM*PPRIM+(PS(I,JP,M)-2.000*PSIJK+PS(I,JM,M))*DIJK
GO TO 50
30 FIJ=FIJ+2.000*DIJK*(PS(I,JP,M)-PSIJK)
GO TO 50
32 DPRIM=(DD(IM,JP,L,M)-DD(IM,JM,L,M))*0.2500
PPRIM=PS(IM,JP,M)-PS(IM,JM,M)
FIJ=FIJ+DPRIM*PPRIM+(PS(IM,JP,M)-2.000*PSIJK+PS(IM,JM,M))*DIJK
GO TO 50
34 IF (1.GT.MP) GO TO 36
DPRIM=(2.000*DD(I,JP,L,M)-DD(I,JM,L,M)-DD(IP,JM,L,M))*0.062500
PPRIM=2.000*PS(I,JP,M)-PS(I,JM,M)-PS(IP,JM,M)
FIJ=FIJ+DPRIM*PPRIM+(PS(I,JP,M)-2.000*PSIJK+(PS(I,JM,M)+
. PS(IP,JM,M))*0.5000)*DIJK
GO TO 50
36 DPRIM=(DD(I,JP,L,M)-DD(IP,JM,L,M))*0.2500
PPRIM=PS(I,JP,M)-PS(IP,JM,M)
FIJ=FIJ+DPRIM*PPRIM+(PS(I,JP,M)-2.000*PSIJK+PS(IP,JM,M))*DIJK
GO TO 50
40 IF (NL.EQ.NP+1.AND.1.GE.MP) GO TO 42
FIJ=FIJ+2.000*DIJK*(PS(I,JM,M)-PSIJK)
GO TO 50
42 IF (1.GT.MP) GO TO 44

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      FIJ=FIJ+DIJK*(PS(I,JM,M)+PS(IP,JM,M)-2.000*PSIJK)
      GO TO 50
44  FIJ=FIJ+DIJK*.2,000*(PS(IP,JM,M)-PSIJK)
50  CONTINUE
      PSIJK=PS(I,J,L)
      DPIJK=DP(I,J,L)
      PIJK=P(I,J)
      IF(I.EQ.IAX) GO TO 90
      IF(J.GT.NP) GO TO 88
      IF(I.EQ.MP) GO TO 92
      IF(I.EQ.MP+1) GO TO 90
88  DPRIM=(DP(IP,J,L)-DP(IM,J,L))*0.2500
      PPRIM=P(IP,J)-P(IM,J)
      FIJ=FIJ+DPRIM*PPRIM+(P(IP,J)*FIIP-2.000*PIJK+P(IM,J)*FIIM)*
      . DPIJK
      GO TO 100
90  FIJ=FIJ+2.000*DPIJK*(P(IP,J)-PIJK)
      GO TO 100
92  FIJ=FIJ+2.000*DPIJK*(P(IM,J)-PIJK)
100 IF(J.EQ.1) GO TO 110
      IF(J.EQ.NL) GO TO 120
      IF(J.EQ.NP.AND.I.GT.MP) GO TO 112
      IF(J.EQ.NP+1.AND.I.GE.MP) GO TO 114
      DPRIM=(DP(I,JP,L)-DP(I,JM,L))*0.2500
      PPRIM=P(I,JP)-P(I,JM)
      FIJ=FIJ+DPRIM*PPRIM+(P(I,JP)-2.000*PIJK+P(I,JM))*DPIJK
      GO TO 130
110 FIJ=FIJ+2.000*DPIJK*(P(I,JP)-PIJK)+CK1*(PNOUT-PSIJK)
      IF(I.NE.MP) GO TO 130
      FIJ=FIJ+(PNOUT-PSIJK)*(CK2-CK1)
      GO TO 130
120 IF(NL.EQ.NP+1.AND.I.GE.MP) GO TO 122
      FIJ=FIJ+2.000*DPIJK*(P(I,JM)-PIJK)
      GO TO 130
122 IF(I.GT.MP) GO TO 124
      FIJ=FIJ+DPIJK*(P(I,JM)+P(IP,JM)-2.000*PIJK)
      GO TO 130
124 FIJ=FIJ+2.000*DPIJK*(P(IP,JM)-PIJK)
      GO TO 130
112 DPRIM=(DP(IM,JP,L)-DP(I,JM,L))*0.2500
      PPRIM=P(IM,JP)-P(I,JM)
      FIJ=FIJ+DPRIM*PPRIM+DPIJK*(P(IM,JP)-2.000*PIJK+P(I,JM))
      GO TO 130
114 IF(I.GT.MP) GO TO 116
      DPRIM=(2.000*DP(I,JP,L)-DP(I,JM,L)-DP(IP,JM,L))*0.062500
      PPRIM=2.000*P(I,JP)-P(I,JM)-P(IP,JM)
      FIJ=FIJ+DPRIM*PPRIM+DPIJK*((P(I,JM)+P(IP,JM))*0.500-2.000*PIJK
      . +P(I,JP))
      GO TO 130
116 DPRIM=(DP(I,JP,L)-DP(IP,JM,L))*0.2500
      PPRIM=P(I,JP)-P(IP,JM)
      FIJ=FIJ+DPRIM*PPRIM+DPIJK*(P(IP,JM)-2.000*PIJK+P(I,JP))
130 CONTINUE
      IF(J.EQ.1.OR.I.NE.MP.OR.J.GT.NP) GO TO 162
      IF(IPUMP.EQ.2) GO TO 140
      IF(L.NE.NCMP) GO TO 162
      FIJ=FIJ+Q
      GO TO 162
140 FIJ=FIJ-Q*PSIJK
162 CONTINUE
      IF(I.GT.MF.OR.J.GT.NF) GO TO 165
      FIJ=FIJ+QO(L)
165 FIJ=FIJ*EMDA+PS(I,J,L)
      PP(I,J,L)=FIJ
170 CONTINUE
180 CONTINUE
      DO 210 I=IAX,ML1
      DO 210 J=1,NL
      PIJK=0.0
      DO 190 N=1,NCMP
      PSIJK=PP(I,J,N)
      PS(I,J,N)=PSIJK
      PN(I,J,N)=PSIJK
190 PIJK=PIJK+PSIJK
200 P(I,J)=PIJK

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210 CONTINUE
DO 355 I=1,ML
  IF (I.EQ.MP) GO TO 355
  PIJK=1.000/P(I,1)
  P(I,1)=1.000
DO 354 L=1,NCMP
  PS(I,1,L)=PIJK
  PP(I,1,L)=PS(I,1,L)
  PN(I,J,N)=PS(I,1,L)
354 PS(I,1,L)=PS(I,1,L)
355 CONTINUE
  IF(QMAX.NE.0.) GO TO 357
  IF(ITR.EQ.0) GO TO 357
DO 356 J=1,NP
  PIJK=1.000/P(MP,J)
  P(MP,J)=1.000
DO 356 L=1,NCMP
  PS(I,1,L)=P(MP,J,L)*PIJK
  PP(MP,J,L)=PS(I,1,L)
  PN(I,J,N)=PS(I,1,L)
356 PS(MP,J,L)=PS(I,1,L)
357 CONTINUE
RETURN
END
SUBROUTINE CORBCT (PN,PS,PP,P,DP,DD,A,B,C,F,CPRIM,BETA,GAMMA,QO,
  DTAUE)
  IMPLICIT REAL*8 (A-H,O-Z)
  COMMON/ONE/Q,DTHET,POUT(4),CK1,CK2,CK3,CK4,EMDA,QMAX,
1  ML,NL,NCMP,MF,NF,MM,NP,MP,NHIST,IAX,IIN,IOUT,IPUMP,IBARR,ITR
  DIMENSION PN(ML,NL,NCMP),PS(ML,NL,NCMP),PP(ML,NL,NCMP),
1  P(ML,NL),DD(ML,NL,NCMP),DP(ML,NL,NCMP),QO(NCMP),
2  A(MM),B(MM),C(MM),F(MM),BETA(MM),GAMMA(MM),CPRIM(MM)
  ML=ML-1
DO 210 L=1,NCMP
  MAX=ML
  PNOUT=POUT(L)
DO 210 J=1,NL
  JP=J+1
  JM=J-1
  MIN=IAX
  IF (J.GT.NP) MAX=ML-2
DO 180 I=1,MAX
  FII=2*I-2
  IF (I.LE.MP.OR.J.GT.NP) GO TO 4
  FII=FII-2.0
4  FIJ=0.000
  FIIP=(FII+1.000)/FII
  FIIM=(FII-1.000)/FII
  IP=I+1
  IM=I-1
DO 50 M=1,NCMP
  IF(L.EQ.M) GO TO 50
  DIJK=DD(I,J,L,M)
  PS(I,J,M)=PS(I,J,M)
  IF(I.EQ.IAX) GO TO 10
  IF (J.GT.NP) GO TO 8
  IF (I.EQ.MP) GO TO 12
  IF (I.EQ.MP+1) GO TO 10
8  DPRIM= (DD(IP,J,L,M)-DD(IM,J,L,M))*0.25
  PPRIM= PS(IP,J,M)-PS(IM,J,M)
  FIJ=FIJ+DPRIM*PPRIM+(FIIP*PS(IP,J,M)-2.000*PS(I,J,M)+FIIM*PS(IM,J,M))
  *DIJK
  GO TO 20
10  FIJ=FIJ+2.000*DIJK*(PS(IP,J,M)-PS(I,J,M))
  GO TO 20
12  FIJ=FIJ+2.000*DIJK*(PS(IM,J,M)-PS(I,J,M))
20  IF(J.EQ.1) GO TO 30
  IF(J.EQ.NL) GO TO 40
  IF (J.EQ.NP.AND.I.GT.MP) GO TO 32
  IF (J.EQ.NP+1.AND.I.GE.MP) GO TO 34
  DPRIM=(DD(I,JP,L,M)-DD(I,JM,L,M))*0.2500
  PPRIM=PS(I,JP,M)-PS(I,JM,M)
  FIJ=FIJ+DPRIM*PPRIM+(PS(I,JP,M)-2.000*PS(I,J,M)+PS(I,JM,M))*DIJK
  GO TO 30
30  FIJ=FIJ+2.000*DIJK*(PS(I,JP,M)-PS(I,J,M))

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GO TO 50
32 DPRIM=(DD(IM,JP,L,M)-DD(I,JM,L,M))*0.2500
PPRIM=PS(IM,JP,M)-PS(I,JM,M)
FIJ=FIJ+DPRIM*PPRIM+(PS(IM,JP,M)-2.000*PS(IJK)+PS(I,JM,M))*DIJK
GO TO 50
34 IF (I.GT.MP) GO TO 36
DPRIM=(2.000*DD(I,JP,L,M)-DD(I,JM,L,M)-DD(IP,JM,L,M))*0.062500
PPRIM=2.000*PS(I,JP,M)-PS(I,JM,M)-PS(IP,JM,M)
FIJ=FIJ+DPRIM*PPRIM+(PS(I,JP,M)-2.000*PS(IJK)+(PS(I,JM,M)+
. PS(IP,JM,M))*0.5000)*DIJK
GO TO 50
36 DPRIM=(DD(I,JP,L,M)-DD(IP,JM,L,M))*0.2500
PPRIM=PS(I,JP,M)-PS(IP,JM,M)
FIJ=FIJ+DPRIM*PPRIM+(PS(I,JP,M)-2.000*PS(IJK)+PS(IP,JM,M))*DIJK
GO TO 50
40 IF (NL.EQ.NP+1.AND.I.GE.MP) GO TO 42
FIJ=FIJ+2.000*DIJK*(PS(I,JM,M)-PS(IJK))
GO TO 50
42 IF (I.GT.MP) GO TO 44
FIJ=FIJ+DIJK*(PS(I,JM,M)+PS(IP,JM,M)-2.000*PS(IJK))
GO TO 50
44 FIJ=FIJ+DIJK*2.000*(PS(IP,JM,M)-PS(IJK))
50 CONTINUE
DPIJK=DP(I,J,L)
PIJK=P(I,J)
PSIJK=PS(I,J,L)
PNIJK=PN(I,J,L)
DDEJK=DD(I,J,L,L)
IF(I.EQ.IAX) GO TO 90
IF(J.GT.NP) GO TO 88
IF(I.EQ.MP) GO TO 92
IF(I.EQ.MP+1) GO TO 90
88 DPRIM=(DP(IP,J,L)-DP(IM,J,L))*0.2500
DDRIM=(DD(IP,J,L,L)-DD(IM,J,L,L))*0.2500
PPRIM=P(IP,J)-P(IM,J)
PSPRIM=PS(IP,J,L)-PS(IM,J,L)
PNPRIM=PN(IP,J,L)-PN(IM,J,L)
FIJ=FIJ+DPRIM*PPRIM+DPIJK*(FIIP*P(IP,J)-2.000*PIJK+FIIM*
. P(IM,J))+DDIJK*(FIIM*PN(IM,J,L)
2. -2.000*PNIJK+FIIP*PN(IP,J,L))+DDRIM*PNPRIM)*0.500
A(I)=DDRIM-DDIJK*FIIM
C(I)=-DDRIM-DDIJK*FIIP
GO TO 100
90 FIJ=FIJ+2.000*DPIJK*(P(IP,J)-PIJK)+DDIJK*(PN(IP,J,L)-PNIJK)
C(I)=-2.000*DDIJK
A(I)=0.000
GO TO 100
92 FIJ=FIJ+2.000*DPIJK*(P(IM,J)-PIJK)+DDIJK*(PN(IM,J,L)-PNIJK)
C(I)=0.000
A(I)=-2.000*DDIJK
100 B(I)=EMDA+2.0*DDIJK
IF(J.EQ.1) GO TO 110
IF(J.EQ.NL) GO TO 120
IF(J.EQ.NP.AND.I.GT.MP) GO TO 112
IF(J.EQ.NP+1.AND.I.GE.MP) GO TO 114
DPRIM=(DP(I,JP,L)-DP(I,JM,L))*0.2500
DDRIM=(DD(I,JP,L,L)-DD(I,JM,L,L))*0.2500
PPRIM=P(I,JP)-P(I,JM)
PSPRIM=PS(I,JP,L)-PS(I,JM,L)
PNPRIM=PN(I,JP,L)-PN(I,JM,L)
FIJ=FIJ+DPRIM*PPRIM+DPIJK*(P(I,JP)-2.000*PIJK+P(I,JM))+DDRIM*
. PNPRIM+DDIJK*(PN(I,JP,L)-2.000*PNIJK+PN(I,JM,L))
GO TO 130
110 FIJ=FIJ+2.000*DPIJK*(P(I,JP)-PIJK)+2.000*DDIJK*(PN(I,JP,L)-
. PNIJK)+CK1*(PNOUT-PSIJK)
IF (I.NE.MP) GO TO 130
FIJ=FIJ+ (PNOUT-PSIJK)*(CK2-CK1)
GO TO 130
120 IF (NL.EQ.NP+1.AND.I.GE.MP) GO TO 122
FIJ=FIJ+2.000*DPIJK*(P(I,JM)-PIJK)+2.000*DDIJK*(PN(I,JM,L)-PNIJK)
GO TO 130
122 IF (I.GT.MP) GO TO 124
FIJ=FIJ+DPIJK*(P(I,JM)+P(IP,JM)-2.000*PIJK)
. +DDIJK*(PN(I,JM,L)+PN(IP,JM,L)-2.000*PNIJK)
GO TO 130

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124 FIJ=FIJ+2.000*DPIJK*(P(IP,JM)-PIJK)
    +2.000*DDIJK*(PN(IP,JM,L)-PNIJK)
    GO TO 130
112 DPRIM=(DP(IM,JP,L)-DP(I,JM,L))*0.2500
    DDRIM=(DD(IM,JP,L,L)-DD(I,JM,L,L))*0.2500
    PPRIM=P(IM,JP)-P(I,JM)
    PNPRIM=PN(IM,JP,L)-PN(I,JM,L)
    FIJ=FIJ+DPRIM*PPRIM+DPIJK*(P(IM,JP)-2.000*PIJK+P(I,JM))
    + DDRIM*PNPRIM+DDIJK*(PN(IM,JP,L)-2.000*PNIJK+PN(I,JM,L))
    GO TO 130
114 IF (I.GT.MP) GO TO 116
    DPRIM=(2.000*DP(I,JP,L)-DP(I,JM,L)-DP(IP,JM,L))*0.062500
    DDRIM=(2.000*DD(I,JP,L,L)-DD(I,JM,L,L)-DD(IP,JM,L,L))*0.062500
    PNPRIM=2.000*PN(I,JP,L)-PN(I,JM,L)-PN(IP,JM,L)
    PPRIM=2.000*P(I,JP)-P(I,JM)-P(IP,JM)
    FIJ=FIJ+DPRIM*PPRIM+DPIJK*((P(I,JM)+P(IP,JM))*0.500-2.000*PIJK
    +P(I,JP))+DDRIM*PNPRIM+DDIJK*(PN(I,JP,L)-2.000*PNIJK+0.5000*
    (PN(I,JM,L)+PN(IP,JM,L)))
    GO TO 130
116 DPRIM=(DP(I,JP,L)-DP(IP,JM,L))*0.2500
    DDRIM=(DD(I,JP,L,L)-DD(IP,JM,L,L))*0.2500
    PPRIM=P(I,JP)-P(IP,JM)
    PNPRIM=PN(I,JP,L)-PN(IP,JM,L)
    FIJ=FIJ+DPRIM*PPRIM+DPIJK*(P(IP,JM)-2.000*PIJK+P(I,JP))
    +DDRIM*PNPRIM+DDIJK*(PN(I,JP,L)-2.000*PNIJK+PN(IP,JM,L))
130 CONTINUE
    IF (J.EQ.1.OR.I.NE.MP.OR.J.GT.NP) GO TO 162
    IF (IPUMP.EQ.2) GO TO 140
    IF (L.NE.NCMP) GO TO 162
    FIJ=FIJ+Q
    GO TO 162
140 FIJ=FIJ-Q*PSIJK
162 CONTINUE
    FIJ=FIJ*2.000+EMDA*PNIJK
    IF (I.GT.MF.OR.J.GT.NF) GO TO 175
    FIJ=FIJ+QO(L)*2.000
175 F(I)=FIJ
180 CONTINUE
190 F(MAX)=F(MAX)-C(MAX)*POUT(L)
    CALL TRIDAG (MIN,MAX,A,B,C,F,CPRIM,BETA,GAMMA,MM)
    DO 200 I=MIN,MAX
200 PP(I,J,L)=CPRIM(I)
210 CONTINUE
    DO 220 I=IAX,MAX
    DO 220 J=1,NL
    DO 220 L=1,NCMP
220 PS(I,J,L)=PP(I,J,L)
    MAX=NL
    DO 290 L=1,NCMP
    DO 290 II=IAX,ML1
    MIN=1
    I=11
    DO 260 J=1,NL
    IF (I.GT.IP.AND.J.GT.NP) I=I1-1
    IP=I+1
    IM=I-1
    DDIJK=DD(I,J,L,L)
    PNIJK=PN(I,J,L)
    BJ=2.000*DDIJK
    FIJ=EMDA*PS(I,J,L)+BJ*PNIJK
    B(J)=EMDA+BJ
    JP=J+1
    JM=J-1
    IF (J.EQ.1) GO TO 230
    IF (J.EQ.NL) GO TO 240
    IF (J.EQ.NP.AND.I.GT.MP) GO TO 232
    IF (J.EQ.NP+1.AND.I.GE.MP) GO TO 234
    DDRIM=(DD(I,JP,L,L)-DD(I,JM,L,L))*0.2500
    A(J)=DDRIM-DDIJK
    C(J)=-DDRIM-DDIJK
    F(J)=FIJ+A(J)*PN(I,JM,L)+C(J)*PN(I,JP,L)
    GO TO 260
232 DDRIM=(DD(IM,JP,L,L)-DD(I,JM,L,L))*0.2500
    A(J)=DDRIM-DDIJK
    C(J)=-DDRIM-DDIJK

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F(J)=F1J+A(J)*PN(I,JM,L)+C(J)*PN(I,JP,L)
GO TO 260
234 IF (I.GT.MP) GO TO 236
DDRIM=(2.000*DD(I,JP,L,L)-DD(I,JM,L,L)-DD(IP,JM,L,L))*0.125D0
A(J)=DDRIM-DD1JK
C(J)=-DDRIM-DD1JK
F(J)=F1J+A(J)*(PN(I,JM,L)+PN(IP,JM,L))*0.5D0+C(J)*PN(I,JP,L)
GO TO 260
236 DDRIM=(DD(I,JP,L,L)-DD(IP,JM,L,L))*0.25D0
A(J)=DDRIM-DD1JK
C(J)=-DDRIM-DD1JK
F(J)=F1J+A(J)*PN(IP,JM,L)+C(J)*PN(I,JP,L)
GO TO 260
230 C(J)=-BJ
F(J)=F1J-BJ*PN(I,JP,L)
GO TO 260
240 A(J)=-BJ
IF (NL.EQ.NP+1.AND.I.GE.MP) GO TO 242
F(J)=F1J-BJ*PN(I,JM,L)
GO TO 260
242 IF (I.GT.MP) GO TO 244
F(J)=F1J-BJ*(PN(I,JM,L)+PN(IP,JM,L))*0.5D0
GO TO 260
244 F(J)=F1J-BJ*PN(IP,JM,L)
260 CONTINUE
CALL TRIDAG (MIN,MAX,A,B,C,F,CPRIM,BETA,GAMMA,MM)
DO 280 J=MIN,MAX
I=1
IF (I.GT.MP.AND.J.GT.NP) I=11-1
280 PP(I,J,L)=CPRIM(J)
290 CONTINUE
RETURN
END
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)=B(IF)
GAMMA(IF)=D(IF)/BETA(IF)
IF (IF.EQ.L) GO TO 30
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)
GO TO 40
30 V(L)=GAMMA(L)
40 RETURN
END
SUBROUTINE PREDIC (PN,PS,PP,P,DD,DP,QO,DTAUE)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONE/Q,DTNET,POUT(4),CK1,CK2,CK3,CK4,EMDA,QMAX,
1 ML,NL,NCMP,MF,NF,MM,NP,MP,NHIST,IAX,IIN,IOUT,IPUMP,IBARR,ITR
DIMENSION PN(ML,NL,NCMP),PS(ML,NL,NCMP),PP(ML,NL,NCMP),
1 P(ML,NL),DD(ML,NL,NCMP,NCMP),DP(ML,NL,NCMP),QO(NCMP)
ML1=ML-1
DO 180 L=1,NCMP
PNOUT=POUT(L)
DO 180 I=1,AX,ML1
IP=I+1
IM=I-1
FII=2*I-2
FIIP=(FII+1.0D0)/FII
FIIM=(FII-1.0D0)/FII
DO 180 J=1,NL
FIJ=0.0D0
DO 50 M=1,NCMP
DIJK=DD(I,J,L,M)
PS1JK=PS(I,J,M)
IF (I.EQ.IAX) GO TO 10
DPRIM=(DD(I+1,J,L,M)-DD(I-1,J,L,M))*0.25
PPRIM=PS(I+1,J,M)-PS(I-1,J,M)

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      FIJ=FIJ+OPRIM*PPRIM+(FIIP*PS(I+1,J,M)-2.000*PSIJK+FIIM*PS(I-1,J,M)
1      )*DIJK
      GO TO 20
10     FIJ=FIJ+2.000*DIJK*(PS(I+1,J,M)-PSIJK)
      GO TO 20
12     FIJ=FIJ+2.000*DIJK*(PS(IM,J,M)-PSIJK)
20     IF(J.EQ.1) GO TO 30
      IF(J.EQ.NL) GO TO 40
      DPRIM=(DD(I,J+1,L,M)-DD(I,J-1,L,M))*0.25
      PPRIM=PS(I,J+1,M)-PS(I,J-1,M)
      FIJ=FIJ+OPRIM*PPRIM+(PS(I,J+1,M)-2.000*PSIJK+PS(I,J-1,M))*DIJK
      GO TO 50
30     FIJ=FIJ+2.000*DIJK*(PS(I,J+1,M)-PSIJK)
      GO TO 50
40     FIJ=FIJ+2.000*DIJK*(PS(I,J-1,M)-PSIJK)
50     CONTINUE
      PSIJK=PS(I,J,L)
      DPIJK=DP(I,J,L)
      PIJK=P(I,J)
      IF(I.EQ.IAX) GO TO 90
      DPRIM=(DP(I+1,J,L)-DP(I-1,J,L))*0.2500
      PPRIM=P(I+1,J)-P(I-1,J)
      FIJ=FIJ+OPRIM*PPRIM+(P(I+1,J)*FIIP-2.000*PIJK+P(I-1,J)*FIIM)*
      . DPIJK
      GO TO 100
90     FIJ=FIJ+2.000*DPIJK*(P(I+1,J)-PIJK)
      GO TO 100
92     FIJ=FIJ+2.000*DPIJK*(P(IM,J)-PIJK)
100    IF(J.EQ.1) GO TO 110
      IF(J.EQ.NL) GO TO 120
      DPRIM=(DP(I,J+1,L)-DP(I,J-1,L))*0.2500
      PPRIM=P(I,J+1)-P(I,J-1)
      FIJ=FIJ+OPRIM*PPRIM+(P(I,J+1)-2.000*PIJK+P(I,J-1))*DPIJK
      GO TO 130
110    FIJ=FIJ+2.000*DPIJK*(P(I,J+1)-PIJK)
      IF(NCMP.EQ.1) CK=CK3
      IF(NCMP.EQ.2) CK=CK2
      IF(NCMP.EQ.3) CK=CK4
      FIJ=FIJ+CK*(PNOUT-PSIJK)
      IF(I.NE.MP) GO TO 130
      FIJ=FIJ+      (PNOUT-PSIJK)*(CK2-CK1)
      GO TO 130
120    FIJ=FIJ+2.000*DPIJK*(P(I,J-1)-PIJK)
130    CONTINUE
      IF(J.EQ.1.OR.1.NE.MP.OR.J.GT.NP) GO TO 162
      IF(IPUMP.EQ.2) GO TO 140
      IF(L.NE.NCMP) GO TO 162
      FIJ=FIJ+Q
      GO TO 162
140    FIJ=FIJ-Q*PSIJK
162    CONTINUE
      IF      (I.GT.MF.OR.J.GT.NF) GO TO 165
      FIJ=FIJ+QO(L)
165    FIJ=FIJ*EMDA+PS(I,J,L)
      PP(I,J,L)=FIJ
170    CONTINUE
180    CONTINUE
      DO 210 I=IAX,ML1
      DO 210 J=1,NL
      PIJK=0.0
      DO 190 N=1,NCMP
      PSIJK=PP(I,J,N)
      PN(I,J,N)=PSIJK
      PS(I,J,N)=PSIJK
190    PIJK=PIJK+PSIJK
200    P(I,J)=PIJK
210    CONTINUE
      DO 355 I=IAX,ML1
      IF(I.EQ.MP) GO TO 355
      PIJK=1.000/P(I,1)
      P(I,1)=1.000
      DO 354 L=1,NCMP
      PSIJK=PS(I,1,L)*PIJK
      PN(I,1,L)=PSIJK
      PP(I,1,L)=PSIJK

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354: PS(I,1,L)=PSIJK
355: CONTINUE
      IF(QMAX.NE.0.) GO TO 357
      IF(ITR.EQ.0)GO TO 357
      DO 356 J=1,NP
      PIJK=1.000/P(MP,J)
      P(MP,J)=1.000
      DO 356 L=1,NCMP
      PSIJK =PS(MP,J,L)*PIJK
      PN(MP,J,L)=PSIJK
      PP(MP,J,L)=PSIJK
356: PS(MP,J,L)=PSIJK
357: CONTINUE
      RETURN
      END
      SUBROUTINE CORECT (PN,PS,PP,P,DP,DD,A,B,C,F,CPRIM,BETA,GAMMA,QO,
      . DTAUE)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ONE/Q,DTHET,POUT(4),CK1,CK2,CK3,CK4,EMDA,QMAX,
      1 ML,NL,NCMP,MF,NF,MM,NP,MP,NHIST,IAX,IIN,IOUT,IPUMP,IBARR,ITR
      DIMENSION PN(ML,NL,NCMP),PS(ML,NL,NCMP),PP(ML,NL,NCMP),
      1 P(ML,NL),DD(ML,NL,NCMP),DP(ML,NL,NCMP),QO(NCMP),
      2 A(MM),B(MM),C(MM),F(MM),BETA(MM),GAMMA(MM),CPRIM(MM)
      ML1=ML-1
      MAX=ML1
      DO 210 L=1,NCMP
      PNOUT=POUT(L)
      DO 210 J=1,NL
      MIN=IAX
      DO 180 I=IAX,ML1
      FI1=2*I-2
      FIIP=(FI1+1.000)/FI1
      FIIM=(FI1-1.000)/FI1
      FIJ=0.000
      DO 50 M=1,NCMP
      IF(L.EQ.M) GO TO 50
      DIJK=DD(I,J,L,M)
      PSIJK=PS(I,J,M)
      IF(I.EQ.IAX) GO TO 10
      DPRIM=(DD(I+1,J,L,M)-DD(I-1,J,L,M))*0.25
      PPRIM=PS(I+1,J,M)-PS(I-1,J,M)
      FIJ=FIJ+(DPRIM*PPRIM+(FIIP*PS(I+1,J,M)-2.000*PSIJK+FIIM*PS(I-1,J,M)
      1 ))*DIJK)
      GO TO 20
10: FIJ=FIJ+2.0*DIJK*(PS(I+1,J,M)-PSIJK)
20: IF(J.EQ.1) GO TO 30
      IF(J.EQ.NL) GO TO 40
      DPRIM=(DD(I,J+1,L,M)-DD(I,J-1,L,M))*0.25
      PPRIM=PS(I,J+1,M)-PS(I,J-1,M)
      FIJ=FIJ+DPRIM*PPRIM+(PS(I,J+1,M)-2.000*PSIJK+PS(I,J-1,M))*DIJK
      GO TO 50
30: FIJ=FIJ+2.000*DIJK*(PS(I,J+1,M)-PSIJK)
      GO TO 50
40: FIJ=FIJ+2.000*DIJK*(PS(I,J-1,M)-PSIJK)
50: CONTINUE
      DPIJK=DP(I,J,L)
      PIJK=P(I,J)
      PSIJK=PS(I,J,L)
      PNIJK=PN(I,J,L)
      DDIJK=DD(I,J,L,L)
      IF(I.EQ.IAX) GO TO 90
      DPRIM=(DP(I+1,J,L)-DP(I-1,J,L))*0.2500
      DDRIM=(DD(I+1,J,L,L)-DD(I-1,J,L,L))*0.2500
      PSPRIM=PS(I+1,J,L)-PS(I-1,J,L)
      PPRIM=P(I+1,J)-P(I-1,J)
      PNPRIM=PN(I+1,J,L)-PN(I-1,J,L)
      FIJ=FIJ+DPRIM*PPRIM+DPIJK*(FIIP*P(I+1,J)-2.000*PIJK+FIIM*
      . P(I-1,J))+(DDIJK*(FIIM*PN(I-1,J,L)
      2 -2.000*PNIJK+FIIP*PN(I+1,J,L))+DDRIM*PNPRIM)*0.500
      A(I)=DDRIM-DDIJK*FIIM
      B(I)=EMDA+2.0*DDIJK
      C(I)=-DDRIM-DDIJK*FIIP
      GO TO 100
90: FIJ=FIJ+2.000*DPIJK*(P(I+1,J)-PIJK)
      IN(I+1,J,L)=PNIJK
      +DDIJK*(P

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```

      B(I)=EMDA+2.000*DDIJK
      C(I)=-2.000*DDIJK
100  IF(J.EQ.1) GO TO 110
      IF(J.EQ.NL) GO TO 120
      DPRIM=(DP(I,J+1,L)-DP(I,J-1,L))*0.2500
      DDRIM=(DD(I,J+1,L,L)-DD(I,J-1,L,L))*0.2500
      PSPRIM=PS(I,J+1,L)-PS(I,J-1,L)
      PPRIM=P(I,J+1)-P(I,J-1)
      PNPRIM=PN(I,J+1,L)-PN(I,J-1,L)
      FIJ=FIJ+OPRIM*PPRIM+DPIJK*(P(I,J+1)
1      +P(I,J-1)
      )+DDRIM*PNPRIM+DDIJK*(PN(I,J+1,L)-2
2.000*PNIJK+PN(I,J-1,L))
      GO TO 130
110  FIJ=FIJ+2.000*DPIJK*(P(I,J+1)-PIJK) + 2.000*DDIJK*(P
1N(I,J+1,L)-PNIJK)
      IF(NCMP.EQ.1) CK=CK3
      IF(NCMP.EQ.2) CK=CK2
      IF(NCMP.EQ.3) CK=CK4
      FIJ=FIJ+CK*(PNOUT-PSIJK)
      IF (I.NE.MP) GO TO 130
      FIJ=FIJ+ (PNOUT-PSIJK)*(CK2-CK1)
      GO TO 130
120  FIJ=FIJ+2.000*DPIJK*(P(I,J-1)-PIJK) + 2.000*DDIJK*(P
1N(I,J-1,L)-PNIJK)
130  CONTINUE
      IF (J.EQ.1.OR.I.NE.MP.OR.J.GT.NP) GO TO 162
      IF (IPUMP.EQ.2) GO TO 140
      IF (L.NE.NCMP) GO TO 162
      FIJ=FIJ+Q
      GO TO 162
140  FIJ=FIJ-Q*PSIJK
162  CONTINUE
      FIJ=FIJ+2.000+EMDA*PNIJK
      IF (I.GT.MF.OR.J.GT.NF) GO TO 175
      FIJ=FIJ+QO(L)*2.000
175  F(I)=FIJ
180  CONTINUE
190  F(MAX)=F(MAX)-C(MAX)*POUT(L)
      CALL TRIDAG (MIN,MAX,A,B,C,F,CPRIM,BETA,GAMMA,MM)
      DO 200 I=MIN,MAX
200  PP(I,J,L)=CPRIM(I)
210  CONTINUE
      DO 220 I=1,AX,ML1
      DO 220 J=1,NL
      DO 220 L=1,NCMP
220  PS(I,J,L)=PP(I,J,L)
      MAX=NL
      MIN=1
      DO 290 L=1,NCMP
      DO 290 I=1,AX,ML1
      MIN=1
      DO 260 J=1,NL
      DDIJK=DD(I,J,L,L)
      PNIJK=PN(I,J,L)
      FIJ=EMDA*PS(I,J,L)
      BJ=2.000*DDIJK
      B(J)=EMDA+BJ
      IF(J.EQ.1) GO TO 230
      IF(J.EQ.NL) GO TO 240
      DDRIM=(DD(I,J+1,L,L)-DD(I,J-1,L,L))*0.2500
      A(J)=DDRIM-DDIJK
      C(J)=-DDRIM-DDIJK
      F(J)=FIJ+A(J)*PN(I,J-1,L)+BJ*PNIJK+C(J)*PN(I,J+1,L)
      GO TO 260
230  C(J)=-2.000*DDIJK
      F(J)=FIJ-2.000*DDIJK*(PN(I,J+1,L)-PNIJK)
      GO TO 260
240  A(J)=-2.000*DDIJK
      F(J)=FIJ-2.000*DDIJK*(PN(I,J-1,L)-PNIJK)
260  CONTINUE
      CALL TRIDAG (MIN,MAX,A,B,C,F,CPRIM,BETA,GAMMA,MM)
      DO 280 J=MIN,MAX
280  PP(I,J,L)=CPRIM(J)
290  CONTINUE
      RETURN

```

```

END
SUBROUTINE SOLV (PN,PS,PP,P,DD,DP,PO, PRS,A,B,C,F,CPRIM,BETA,GAMMA
1,AM,AMU,AK,DAB,PHI,BBB,AAA,AA,QO,X,QOO,TTIM,IAA)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONE/Q,DTHET,POUT(4),CK1,CK2,CK3,CK4,EMDA,QMAX,
1 ML,NL,NCMP,MF,NF,MM,NP,MP,NHIST,IAX,IIN,IOUT,IPUMP,IBARR,ITR
DIMENSION PN(ML,NL,NCMP),PS(ML,NL,NCMP),PP(ML,NL,NCMP),
1 P(ML,NL),DD(ML,NL,NCMP,NCMP),DP(ML,NL,NCMP), PO(NCMP),
2 PRS(NCMP),A(MM),B(MM),C(MM),CPRIM(MM),BETA(MM),GAMMA(MM),AM(NCMP)
3,AMU(NCMP),AK(NCMP),DAB(NCMP,NCMP),QO(NCMP),X(ML),F(MM),
4 PHI(NCMP,NCMP),BBB(NCMP,NCMP),AAA(NCMP,NCMP),AA(NCMP,NCMP),
5 QOO(NHIST,NCMP),TTIM(NHIST),IAA(NCMP),
6 R(10),FV(10)
DIMENSION PPUM(3),QPUM(3),D(3,3)
DATA STAR/1H* /
QQ(QPUM1,QPUM2,QPUM3,PPUMP)=QPUM1+QPUM2*PPUMP+QPUM3*PPUMP**2
NCMP=NCMP*NCMP
ML1=ML-1
IMIN=MAX0(MP-6,IAX)
IMAX=MIN0(MP+6,ML)
ISTOP=0
READ (5,360) Q,POUT
WRITE (6,560) Q
READ (5,360) TORT,TEMP,DX,TMAX1,DT1
READ (5,370) IFREQ,NSTEP,NPRDC
READ (5,360) CK1,CK2,CK3,CK4
READ (5,380) NRADII,(R(I),FV(I),I=1,NRADII)
WRITE (6,470) (I,I=1,NCMP)
DO 10 I=1,NHIST
READ (5,360) TTIM(I),(QOO(I,J),J=1,NCMP)
10 WRITE (6,480) TTIM(I),(QOO(I,J),J=1,NCMP)
DO 20 I=1,NCMP
READ (5,360) PO(I),PRS(I),AM(I),AMU(I)
20 DO 30 I=1,NCMP
READ (5,360) (DAB(I,J),J=1,NCMP)
READ (5,380) NPUMP,(QPUM(I),PPUM(I),I=1,NPUMP)
QMAX=QPUM(1)
IF (NPUMP.EQ.1) GO TO 32
CALL PUMP(PPUM1,QPUM,D,NPUMP)
QPUM1=QPUM(1)
QPUM2=QPUM(2)
QPUM3=QPUM(3)
GO TO 34
32 QPUM1=QPUM(1)
WRITE (6,560) QPUM1
34 PI=2.0*DARSIN(1.0D0)
E=0.0D0
RFV=0.0D0
RSQFV=0.0D0
PIBF=PI*0.25D0
DO 40 I=1,NRADII
REQ=R(I)
FVE=FV(I)
RFV=RFV+REQ*FVE
RSQFV=RSQFV+FVE*REQ**2
40 E=E+FVE
FMP=(NP-1)*(MP-1)
C
WRITE (6,390) E,TORT,TEMP,DX,TMAX1,DT1,Q,NSTEP,IFREQ,NPRDC
WRITE (6,400) CK1,CK2
WRITE (6,460) (I,POUT(I),I=1,NCMP)
WRITE (6,410) (I,R(I),FV(I),I=1,NRADII)
WRITE (6,420)
WRITE (6,430) (I, PO(I),PRS(I),AM(I),AMU(I),I=1,NCMP)
WRITE (6,440)
QQQ=QMAX
QOLD=2.0*QQQ
QF=DX**2
QFF=471.934/(E*FMP*DX)
DO 45 I=1,NHIST
DO 45 J=1,NCMP
45 QOO(I,J)=QOO(I,J)*QF
CK1=2.0D0*DX*CK1
CK2=2.0D0*DX*CK2
CK3=2.0D0*DX*CK3

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CK4=2.000*DX*CK4
DO 50 I=1,NCMP
AK(I)=9.700-05*DSQRT(TEMP/AM(I))
AMU(I)=AMU(I)*1.0D16
50 WRITE (6,450) (DAB(I,J),J=1,NCMP)
PRESF=0.000
PRESS=0.000
DO 60 I=1,NCMP
PRESS=PRESS+PRS(I)
PRESF=PRESF+PO(I)
DO 60 J=1,NCMP
DSQ=(1.0D0+DSQRT(AMU(I)/AMU(J)*DSQRT(AM(J)/AM(I))))**2
60 PHI(I,J)=DSQRT(0.125D0*AM(J)/(AM(J)+AM(I)))*DSQ
C
FACTOR=86400.000
RT=82.057*TEMP
DTU=DTI
C
C SET INITIAL CONDITIONS
C
TAU=0.000
KOUNT=0
DTMAX=0.000
DPMAX=0.000
MOUT=(ML-1)/13+1
NOUT=(NL-1AX)/13+1
NSTAR=(MF-1AX)*9/MOUT+1
KMP=(MP+MOUT-1-1AX)/MOUT*MOUT+1AX-1
DO 65 I=1,ML
65 X(I)=(I-1)*DX
IF (IBARR.EQ.0) GO TO 67
J=MP+1
DO 66 I=J,ML
66 X(I)=X(I)-DX
67 IF (IIN.EQ.1) GO TO 74
DO 70 I=1,ML
DO 70 J=1,NL
P(I,J)=PRESS
DO 70 L=1,NCMP
PN(I,J,L)=PRS(L)
PS(I,J,L)=PRS(L)
70 PP(I,J,L)=PRS(L)
DO 72 I=1,MF
DO 72 J=1,NF
P(I,J)=PRESF
DO 72 L=1,NCMP
PN(I,J,L)=PO(L)
PS(I,J,L)=PO(L)
72 PP(I,J,L)=PO(L)
GO TO 80
74 READ (5,600) (((PN(I,J,L),I=1AX,ML),J=1,NL),L=1,NCMP),
((P(I,J),I=1AX,ML),J=1,NL),TAU
DO 76 I=1AX,ML
DO 76 J=1,NL
DO 76 L=1,NCMP
PP(I,J,L)=PN(I,J,L)
76 PS(I,J,L)=PN(I,J,L)
80 CONTINUE
ICOUNT=0
WRITE (6,580)
WRITE(6,582)QQQ
DO 90 N=1,NCMP
WRITE (6,490) TAU,DTU,DTMAX,DPMAX,KOUNT,N
WRITE (6,510) (X(I),I=1AX,ML,MOUT)
WRITE (6,500) (I,I=1AX,ML,MOUT)
DO 90 J=1,NL,NOUT
IF (J.GT.NP.AND.IBARR.NE.0) GO TO 82
WRITE (6,520) X(J),(PN(I,J,N),I=1AX,ML,MOUT)
GO TO 84
82 WRITE (6,520) X(J),(PN(I,J,N),I=1AX,MP,MOUT)
(PN(I,J,N),I=KMP,ML,MOUT)
84 WRITE (6,530) J
IF(J.LE.NF) WRITE (6,540) (STAR,I=1,NSTAR)
90 CONTINUE
WRITE (6,490) TAU,DTU,DTMAX,DPMAX,KOUNT

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WRITE (6,510) (X(I),I=IAX,ML,MOUT)
WRITE (6,500) (I,I=IAX,ML,MOUT)
DO 100 J=1,NL,NOUT
  IF (J.GT.NP.AND.IBARR.NE.0) GO TO 92
  WRITE (6,520) X(J),(P(I,J),I=IAX,ML,MOUT)
  GO TO 94
92  WRITE (6,520) X(J),(P(I,J),I=IAX,MP,MOUT),(P(I,J),I=KMP,ML,MOUT)
94  WRITE (6,530) J
    IF (J.LE.NF) WRITE (6,540) (STAR,I= 1,NSTAR)
100  CONTINUE
    WRITE (6,580)
    DO 126 N=1,NCMP
      WRITE (6,490) TAU,DTU,DTMAX,DPMAX,KOUNT,N
      WRITE (6,510) (X(I),I=IMIN,IMAX)
      WRITE (6,500) (I,I=IMIN,IMAX)
      DO 126 J=1,NL,NOUT
        IF (J.GT.NP.AND.IBARR.NE.0) GO TO 112
        WRITE (6,520) X(J),(PN(I,J,N),I=IMIN,IMAX)
        GO TO 114
112  WRITE (6,520) X(J),(PN(I,J,N),I=IMIN,MP),(PN(I,J,N),I=MP,IMAX)
114  WRITE (6,530) J
126  CONTINUE
      WRITE (6,490) TAU,DTU,DTMAX,DPMAX,KOUNT
      WRITE (6,510) (X(I),I=IMIN,IMAX)
      WRITE (6,500) (I,I=IMIN,IMAX)
      DO 127 J=1,NL,NOUT
        IF (J.GT.NP.AND.IBARR.NE.0) GO TO 116
        WRITE (6,520) X(J),(P(I,J),I=IMIN,IMAX)
        GO TO 118
116  WRITE (6,520) X(J),(P(I,J),I=IMIN,MP) , (P(I,J),I=MP,IMAX)
118  WRITE (6,530) J
127  CONTINUE
C
C
C  CALCULATION OF RECOVERY AT PUMP FOR COMPONENT ONE
C  QQQ=0.000
C  DO 85 J=1,NP
C 85  QQQ=QQQ+QQ*PN(MP,J,1,1)*P(MP,J,1)
C  WRITE (6,550) QQQ
C
C  IF (ISTOP.EQ.1) RETURN
120  ICOUNT=ICOUNT+1
    KOUNT=KOUNT+1
    IF (KOUNT.GT.NSTEP.OR.TAU.GT.TMAX1) GO TO 122
    GO TO 124
C 122  ISTOP=1
122  IF (IOUT.EQ.1) WRITE (7,600)
    . ((PN(I,J,L),I=IAX,ML),J=1,NL),L=1,NCMP),
    . ((P(I,J),I=IAX,ML),J=1,NL) ,TAU
    RETURN
124  DPMAX=0.000
    DO 200 I=IAX,ML
      DO 200 J=1,NL
        DO 130 L=1,NCMP
          DO 130 M=1,NCMP
130  BBB(L,M)=0.000
          DO 160 JR=1,NRADII
            E=FV(JR)
            REQ=R(JR)
            RFV=REQ*E
            DO 140 L=1,NCMP
              AA(L,L)=TORT/(AK(L)*RFV)
            DO 140 M=1,NCMP
              IF (L.EQ.M) GO TO 140
              DABET=TORT/(DAB(L,M)*E)
              AA(L,L)=AA(L,L)+PN(I,J,M)*DABET
              AA(L,M)=-PN(I,J,L)*DABET
140  CONTINUE
          CALL INVERT (AA,MCMP,NCMP,IAA,AAA)
          DO 150 L=1,NCMP
            DO 150 M=1,NCMP
150  BBB(L,M)=BBB(L,M)+AA(L,M)
160  CONTINUE
          AMUMX=0.000
          DO 180 L=1,NCMP

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      PPHIJ=0.000
      DO 170 M=1,NCMP
170    PPHIJ=PPHIJ+PN(I,J,M)*PHI(L,M)
180    AMUMX=AMU1X+PN(I,J,L)*AMU(L)/PPHIJ
      DO 190 L=1,NCMP
      PCMU=PN(I,J,L)*RSQFV/(8.000*AMUMX*TORT)
      DPMAX1=BBB(L,L)+PCMU
      IF(DPMAX1.GT.DPMAX) DPMAX=DPMAX1
      DP(I,J,L)=PCMU
      DO 190 M=1,NCMP
190    DD(I,J,L,M)=BBB(L,M)
200    CONTINUE
      DTMAX=0.5*DX*DX/(DPMAX*FACTOR)
      DTAU=DTU*FACTOR
      EMDA=DTAU/DX**2
      DTAUE=DTAU
C      .....PREDICTOR STEP.....
      Q=QMAX
      IF (NPUMP.EQ.1) GO TO 201
      PPUMP=P(MP,2)
      IF(IPUMP.EQ.1)GO TO 202
      IF(PPUMP.GT.0.95)GO TO 204
      GO TO 203
202    IF(PPUMP.LT.1.05)GO TO 204
203    Q= QQ(QPUM1,QPUM2,QPUM3,PPUMP)
      IF(Q.LT.0.0)Q=0.0
      IF (Q.GT.QMAX) Q=QMAX
204    IF (KOUNT.LT.2) Q=QMAX*0.1
      IF (Q.GT.QOLD.AND.QOLD.GT.QMAX*0.005) Q=QOLD
      QQQ=Q
      QOLD=2.0*Q
201    Q=Q*OFF
      TAU=TAU+DTU
      CALL CFIL (QQ,QQQ,TTIM,TAU)
      IF (IBARR.EQ.0) GO TO 205
      CALL PRBDIC (PN,PS,PP,P,DD,DP,QQ,DTAUE)
      GO TO 210
205    CALL PREDIC (PN,PS,PP,P,DD,DP,QQ,DTAUE)
210    CONTINUE
C      ... PRINT CONCENTRATIONS .....
      IF(DABS(TAU-TMAX1).LT.DTU) ICOUNT=IFREQ
      IF(ICOUNT.NE.IFREQ) GO TO 120
      GO TO 80
C
C
C
360    FORMAT (8F10.0)
370    FORMAT (16I5)
380    FORMAT (15/,(2F10.0))
390    FORMAT (45H POROSITY OF SOIL (DIMENSIONLESS)      = ,F10.3/45H
1 TORTUOSITY (DIMENSIONLESS)      = ,F10.3/45H TEMPERATUR
2E (DEGREES KELVIN )      = ,F10.3/45H SPATIAL MESH SIZE (CM
3)      = ,F10.3/45H ANALYSIS PERIOD      (DAYS)
4      = ,F10.3/45H INITIAL DT      (DAYS)
5 ,F10.3/45H DISCHARGE AT PUMP (CFM)      = ,F10.3/45H
6 MAXIUM NUMBER OF STEPS      = ,110/45H NUMBER OF ST
7EPS BETWEEN PRINTOUTS      = ,110/45H NUMBER OF PREDICTOR STEPS
8      = ,110/)
400    FORMAT (' SURFACE CONDUCTIVITY OF SOIL      ',E10.3/' SURFACE CONDU
1CTIVITY OF TRENCH      ',E10.3/)
410    FORMAT (' NUMBER PORE RADIUS VOLUMETRIC FRACTION'/(17,2X,F12.2,
111X,F10.4)/)
420    FORMAT (' COMPONENTS'///' SERIAL # PRESSURE IN PRESSURE IN MOLECU
1LAR VISCOSITY '/'      FILL      SOIL      WEIGHT ')
430    FORMAT (' ',18,4F12.4)
440    FORMAT (' BULK DIFFUSION COEFFIECIENTS')
450    FORMAT (' ',8F12.4)
460    FORMAT ('OPRESSURE OUTSIDE THE BOUNDARY '/' COMPONENT PRESSURE '/'
1(110,F10.3))
470    FORMAT ('OFILL HISTORY ON FILL BOUNDARY'/'0 TIME RATE OF
1GENERATIONS FOR COMPONENTS'/10X,8I10)
480    FORMAT (' ',F10.3,8E10.3)
490    FORMAT (31H-MOLE FRACTION AT TIME (DAYS) =,F9.1,2X,13HDTAU (DAYS)
1=,F6.1,2X,14HDTMAX (DAYS) =,F6.1,2X,11HDPMAX      =,E10.3
2      /,14H STEP NUMBER =,15,20H COMPONENT NUMBER = ,15/)

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500 FORMAT (' (CM)',13I9)
510 FORMAT ('0 DISTANCE - ',1P13E9.2)
520 FORMAT ('-',1PE9.2,4X,13E9.2)
530 FORMAT (' ',13)
540 FORMAT ('+',14X,80A1)
C 550 FORMAT ('-METHANE RECOVERED (CFM) = ',E15.4)
560 FORMAT (' DISCHARGE AT VENT = ',F10.3)
580 FORMAT ('1H1)
582 FORMAT ('10MOD1SCHRG= ',E10.3)
600 FORMAT ('8E10.3)
END
SUBROUTINE CFIL (PO,POO,TIME,TAU)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONE/Q,DTHET,POUT(4),CK1,CK2,CK3,CK4,EMDA,QMAX,
1 ML,NL,NCMP,MF,NF,MM,NP,MP,NHIST,IAX,IIN,IOUT,IPUMP,IBARR,ITR
DIMENSION PO(NCMP),POO(NHIST,NCMP),TIME(NHIST)
C
C THIS SUBROUTINE COMPUTES APPLIED MOLE FRACTIONS FROM GIVEN HISTORY
C
DO 10 I=1,NHIST
IF(TAU.EQ.0.00) GO TO 20
IF(TAU-TIME(I)) 40,40,10
CONTINUE
10 DO 30 J=1,NCMP
PO(J)=POO(I,J)
GO TO 60
40 TX=(TAU-TIME(I-1))/(TIME(I)-TIME(I-1))
DO 50 J=1,NCMP
PO(J)=POO(I-1,J)+(POO(I,J)-POO(I-1,J))*TX
50 CONTINUE
60 RETURN
END
SUBROUTINE INVERT (A,MM,N,M,C)
IMPLICIT REAL*8 (A-H,O-Z)
C
C GENERAL MATRIX INVERSION SUBROUTINE
C
DIMENSION A(MM),C(MM),M(N)
C
NN=N
DO 10 I=1,NN
M(I)=-1
C
DO 140 J=1,NN
C
C LOCATE LARGEST ELEMENT
C
D=0.0
DO 70 L=1,NN
IF(M(L)) 20,20,70
20 J=L
DO 60 K=1,NN
IF(M(K)) 30,30,50
30 IF(DABS(D)-DABS(A(J))) 40,40,50
40 LD=L
KD=K
D=A(J)
50 J=J+N
60 CONTINUE
70 CONTINUE
C
C INTERCHANGE ROWS
C
TEMP=-M(LD)
M(LD)=M(KD)
M(KD)=TEMP
L=LD
K=KD
DO 80 J=1,NN
C(J)=A(L)
A(L)=A(K)
A(K)=C(J)
L=L+N
K=K+N
80
C

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C      DIVIDE COLUMN BY LARGEST ELEMENT
C
      NR=(KD-1)*N+1
      NH=NR+N-1
      DO 90 K=NR,NH
90      A(K)=A(K)/D
C
C      REDUCE REMAINING ROWS AND COLUMNS
C
      L=1
      DO 130 J=1,NN
      IF(J-KD) 110,100,110
100      L=L+N
      GO TO 130
110      DO 120 K=NR,NH
      A(L)=A(L)-C(J)*A(K)
120      L=L+1
130      CONTINUE
C
C      REDUCE ROW
C
      C(KD)=-1.0
      J=KD
      DO 140 K=1,NN
      A(J)=-C(K)/D
140      J=J+N
C
C      INTERCHANGE COLUMNS
C
      DO 170 I=1,NN
      L=0
150      L=L+1
      IF(M(L)-I) 150,160,150
160      K=(L-1)*N+1
      J=(I-1)*N+1
      M(L)=M(I)
      M(I)=I
      DO 170 L=1,NN
      TEMP=A(K)
      A(K)=A(J)
      A(J)=TEMP
      J=J+1
170      K=K+1
C
C      RETURN
C
      END
      SUBROUTINE PUMP (P,B,A,N)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(N),B(N),A(N,N)
      DO 10 I=1,N
      DO 10 J=1,N
10      A(I,J) = P(I)**(J-1)
      M=N-1
      DO 400 I=1,M
      L=I+1
      DO 400 J=L,N
      C=A(J,I)/A(I,I)
      B(J)=B(J)- C*B(I)
      DO 400 K=L,N
400      A(J,K)=A(J,K)-A(I,K)*C
      B(N)=B(N)/A(N,N)
C      BACK SUBSTITUTION
      DO 800 I=1,M
      J=N-I
      L=J+1
      DO 600 K=L,N
600      B(J)=B(J)-A(J,K)*B(K)
800      B(J)=B(J)/A(J,J)
      WRITE(6,200) (B(I),I=1,N)
200      FORMAT(10X,E20.5)
      RETURN
      END
      END OF DATA

```

APPENDIX B

CODE V LISTING

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C   PROGRAM   AXISYMMETRIC FLOW WITH PENETRATING VENTS AND
C   CONCENTRATION & PRESSURE GRADIENTS
C   PROGRAMMED BY I.S.RAI
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ONE/Q(8),DTHET,POUT(4),EMDA,
1      ML,NL,KL,NCMP,MF,NF,MN,NP(8),NP(8),NHIST,NPC
2      ,NPIPS,IAX,IAXX,IIN,IOUT,ITER,MPOR
      DIMENSION HED(10)
      COMMON A(35000),IA(8)
      MTOT=35000
10  READ (5,40) MF,NF,ML,NL,KL,NPIPS,NCMP,NHIST,IIN,IOUT,MPOR
      READ (5,45) NPC,(NP(1),MP(1),Q(1),I=1,NPC)
      IF(MF.EQ.0) GO TO 30
      IAX=2
      IAXX=6
      IF (IAXX.LT.IAX) IAXX=IAX
      DTHET=3.141592653*2.0/(NPIPS*KL)
      FL=ML-1
      FF=MF-1
      R1=FL/FF
      FL=NL-1
      FF=NF-1
      R2=FL/FF
      READ (5,50) HED
      WRITE (6,70) HED,R1,R2
      WRITE (6,60) MF,NF,ML,NL,KL,NPIPS,NCMP,NHIST,NPC
      WRITE (6,65) (1,NP(1),MP(1),Q(1),I=1,NPC)
      NNCMP=NCMP*NCMP
      MN=ML*NL*KL
      MNC=MN*NCMP
      M1=1
      M2=M1+MNC
      M3=M2+MNC
      M4=M3+MNC
      M5=M4+MNC
      M6=M5+MNC*NCMP
      M7=M6+MNC
      M8=M7+NCMP
      M9=M8+NCMP
      M16=M9+MNC
      M17=M16+NCMP
      M18=M17+NCMP
      M19=M18+NCMP
      M19A=M19+NCMP
      M20=M19A+NNCMP
      M21=M20+NNCMP
      M22=M21+NNCMP
      M23=M22+NNCMP
      M24=M23+NNCMP
      M25=M24+NCMP
      M26=M25+ML
      M27=M26+NCMP*NHIST
      M28=M27+NHIST
      M29=M28+MNC
      M30=M29+NCMP
      MLAST=M30+MN
      WRITE (6,90) MLAST
      IF(MLAST.LT.MTOT) GO TO 20
      JJ=MLAST-MTOT-1
      WRITE (6,80) JJ
      GO TO 30
20  CALL SOLV (A(M1),A(M2),A(M3),A(M4),A(M5),A(M6),A(M7),A(M8),A(M9),A
1      (M16),A(M17),A(M18),A(M19),A(M19A),A(M20),A(M21),A(M22),A(M23),A(M
2      24),A(M25),A(M26),A(M27),A(M28),A(M29),A(M30),A(M1))
      GO TO 10
30  STOP
C
C
C
40  FORMAT (16I5)
45  FORMAT (15/,(2I5,F5.0))
50  FORMAT (10A8)
60  FORMAT (50H-NUMBER OF MESH POINTS UPTO END OF FILL
1,15/50H NUMBER OF MESH POINTS UPTO DEPTH OF FILL ,15/50H N

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NUMBER OF MESH POINTS UPTO END OF LAND ,15/50H NUMBER OF
3MESH POINTS UPTO DEPTH OF LAND ,15/50H NUMBER OF MESH POIN
4TS ALONG THETA DIRECTION ,15/50H TOTAL NUMBER OF PIPES ALONG
5CIRCUMFERENCE ,15/50H TOTAL NUMBER OF GAS COMPONENTS
6 ,15/50H NO. OF POINTS ON FILL COMPOSITION HISTORY CURVE
7 ,15/50H NO. OF PIPE SETS ,15/)
65 FORMAT (' NUMBER NPIPE MPIPE Q'/(17,2X,15,3X,15,1X,F5.2)/)
70 FORMAT (1H1,10A8,' RS/RF =' ,F5.2,' DS/DF =' ,F5.2)
80 FORMAT ('-REQUIRED CORE EXCEEDS MTOT BY ' ,110)
90 FORMAT ('OMTOT REQUIRED FOR THIS PROBLEM =' ,110)
END
SUBROUTINE SOLV (PN,PS,PP,P,DD,DP,PO, PRS,DELP
1,AM,AMU,AK,CK,DAB,PHI,BBB,AAA,AA,QO,X,QOO,TTIM,GNR,GNER,IFILPT,IAA
2)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONE/Q(8),DTHET,POUT(4),EMDA,
1 ML,NL,KL,NCMP,MF,NF,MM,NP(8),MP(8),NHIST,NPC
2 ,NPIPS,IAX,IAXX,IIN,IOUT,ITER,MPOR
DIMENSION PN(ML,NL,KL,NCMP),PS(ML,NL,KL,NCMP),PP(ML,NL,KL,NCMP),
1 P(ML,NL,KL),DD(ML,NL,KL,NCMP,NCMP),DP(ML,NL,KL,NCMP), PO(NCMP),
2 PRS(NCMP),DELP(ML,NL,KL,NCMP), AM(NCMP)
3 ,AMU(NCMP),AK(NCMP),CK(NCMP),DAB(NCMP,NCMP),QO(NCMP),X(ML),
4 PHI(NCMP,NCMP),BBB(NCMP,NCMP),AAA(NCMP,NCMP),AA(NCMP,NCMP),
5 QOO(NHIST,NCMP),TTIM(NHIST),GNR(ML,NL,KL,NCMP),GNER(NCMP),IFILPT(M
6 L,NL,KL),IAA(NCMP),
7 R(10),FV(10),TIM(12),FMP(8),QQ(8),QFF(8)
DATA STAR/1H* /
NCMP=NCMP*NCMP
ML1=ML-1
IMIN=MAX0(MPOR-6,IAX)
IMAX=MINO(MPOR+6,ML)
ISTOP=0
READ (5,360) POUT
READ (5,360) TORT,TEMP,DX,TMAX1,TMAX2,DTI
READ (5,370) IFREQ,NSTEP,NPRDC
READ (5,380) NRADII,(R(1),FV(1),I=1,NRADII)
WRITE (6,470) (1,I=1,NCMP)
DO 10 I=1,NHIST
READ (5,360) TTIM(1),(QOO(1,J),J=1,NCMP)
10 WRITE (6,480) TTIM(1),(QOO(1,J),J=1,NCMP)
DO 20 I=1,NCMP
READ (5,360) PO(1),PRS(1),AM(1),AMU(1),CK(1),GNER(1)
20 DO 30 I=1,NCMP
READ (5,360) (DAB(1,J),J=1,NCMP)
30 PI=2.0*DARSIN(1.000)
E=0.00
RFV=0.000
RSQFV=0.000
PIBF=PI*0.2500
DTHET=PI/(NPIPS*(KL-1))
DO 40 I=1,NRADII
REQ=R(1)
FVE=FV(1)
RFV=RFV+REQ*FVE
RSQFV=RSQFV+FVE*REQ**2
40 E=E+FVE
DO 41 M=1,NPC
FMP(M)=NP(M)*(MP(M)-1)
41 CONTINUE
C
WRITE (6,390) E,TORT,TEMP,DX,TMAX1,DTI,NSTEP,IFREQ,NPRDC,MPOR
WRITE (6,460) (1,POUT(1),I=1,NCMP)
WRITE (6,410) (1,R(1),FV(1),I=1,NRADII)
WRITE (6,420)
WRITE (6,430) (1, PO(1),PRS(1),AM(1),AMU(1),CK(1),I=1,NCMP)
WRITE (6,440)
DO 42 M=1,NPC
QQ(M)=Q(M)/NP(M)
QFF(M)=471.934/(E*FMP(M)*DX*DTHET)
42 Q(M)=Q(M)*QFF(M)
QF=DX**2
C DO 45 I=1,NHIST
C DO 45 J=1,NCMP
C 45 QOO(1,J) =QOO(1,J)*QF
DO 47 M=1,NCMP

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      CK(M)=2.000*DX*CK(M)
447  CONTINUE
      DO 50 I=1,NOMP
      AK(I)=9.700-05*DSORT(TEMP/AM(I))
      AMU(I)=AMU(I)*1.0016
550  WRITE (6,450) (DAB(I,J),J=1,NOMP)
      PRESF=0.000
      PRESS=0.000
      DO 60 I=1,NOMP
      PRESS=PRESS+PRS(I)
      PRESF=PRESF+PO(I)
      DO 60 J=1,NOMP
      DSQ=(1.000+DSORT(AMU(I)/AMU(J)*DSORT(AM(J)/AM(I))))**2
660  PHI(I,J)=DSQRT(0.12500*AM(J)/(AM(J)+AM(I)))*DSQ
      EC
      FACTOR=86400.000
      RT=82.057*TEMP
      DTU=DT.I
      EC
      EC
      EC
      SET INITIAL CONDITIONS
      TAU=0.000
      KOUNT=0
      DTMAX=0.000
      DPMAX=0.000
      MOUT=(ML-1)/13+1
      NOUT=(NL-1AX)/13+1
      NSTAR=(MF-1AX)*9./MOUT+1
      DO 65 I=1,ML
665  X(I)=(I-1)*DX
      IF (CIN.EQ.1) GO TO 74
      DO 70 I=1,ML
      DO 70 J=1,NL
      DO 70 K=1,KL
      P(I,J,K)=PRESS
      DO 70 L=1,NOMP
      PN(I,J,K,L)=PRS(L)
      PS(I,J,K,L)=PRS(L)
770  PP(I,J,K,L)=PRS(L)
      DO 72 I=1,MF
      DO 72 J=1,NF
      DO 72 K=1,KL
      P(I,J,K)=PRESF
      DO 72 L=1,NOMP
      PN(I,J,K,L)=PO(L)
      PS(I,J,K,L)=PO(L)
772  PP(I,J,K,L)=PO(L)
      GO TO 80
74  CONTINUE
      DO 750 K=1,KL
      DO 750 J=1,NL
      READ (5,600) (IFILEPT(I,J,K),I=1AX,ML)
750  CONTINUE
      READ (5,601) TAU
      DO 754 I=1AX,ML
      DO 754 J=1,NL
      DO 754 K=1,KL
      P(I,J,K)=1.0
      IF (IFILEPT(I,J,K).EQ.1) GO TO 752
      DO 751 L=1,NOMP
      PN(I,J,K,L)=PRS(L)
      GNR(I,J,K,L)=0.0
751  CONTINUE
      GO TO 753
752  DO 753 L=1,NOMP
      PN(I,J,K,L)=PO(L)
      GNR(I,J,K,L)=GNR(L)
753  CONTINUE
754  CONTINUE
      DO 76 I=1AX,ML
      DO 76 J=1,NL
      DO 76 K=1,KL
      DO 76 L=1,NOMP
      GNR(I,J,K,L)=GNR(I,J,K,L)*OF
      PP(I,J,K,L)=PN(I,J,K,L)

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AA(L,L)=TORT/(AK(L)*RFV)
DO 140 M=1,NCMP
  IF(L.EQ.M) GO TO 140
  DABET=TORT/(DAB(L,M)*E)
  AA(L,L)=AA(L,L)+PN(I,J,K,M)*DABET
  AA(L,M)=-PN(I,J,K,L)*DABET
140 CONTINUE
  CALL INVERT (AA,NCMP,NCMP,IAA,AAA)
  DO 150 L=1,NCMP
  DO 150 M=1,NCMP
150 BBB(L,M)=BBB(L,M)+AA(L,M)
160 CONTINUE
  AMUMX=0.000
  DO 180 L=1,NCMP
  PPHIJ=0.000
  DO 170 M=1,NCMP
170 PPHIJ=PPHIJ+PN(I,J,K,M)*PHI(L,M)
180 AMUMX=AMUMX+PN(I,J,K,L)*AMU(L)/PPHIJ
  DO 190 L=1,NCMP
  PCMU=PN(I,J,K,L)*RSQFV/(8.000*AMUMX*TORT)
  DPMAX1=BBB(L,L)+PCMU
  IF(DPMAX1.GT.DPMAX) DPMAX=DPMAX1
  DP(I,J,K,L)=PCMU
  DO 190 M=1,NCMP
190 DD(I,J,K,L,M)=BBB(L,M)
200 CONTINUE
  DTMAX=0.5*DX*DX/(DPMAX*FACTOR)
  DTAU=DTU*FACTOR
  EMDA=0.500*DTAU/DX**2.
  DTAUE=DTAU
C .....PREDICTOR STEP.....
  TAU=TAU+DTU
C CALL CFIL (QO,QOO,TTIM,TAU)
C CALL PREDIC (PN,PS,PP,P,DD,DP,QO,DTAUE,DELP,CX,GNR)
C ... PRINT CONCENTRATIONS .....
  IF(DABS(TAU-TMAX1).LT.DTU) ICOUNT=IFREQ
  IF(ICOUNT.NE.IFREQ) GO TO 120
  GO TO 80

C
C
C
360 FORMAT (8E10.3)
370 FORMAT (16I5)
380 FORMAT (15/,(2F10.0))
390 FORMAT (45H POROSITY OF SOIL (DIMENSIONLESS) = ,F10.3/45H
1 TORTUOSITY (DIMENSIONLESS) = ,F10.3/45H TEMPERATUR
2E (DEGREES KELVIN ) = ,F10.3/45H SPATIAL MESH SIZE (CM
3) = ,F10.3/45H DECOMPOSITION TIME -TMAX1 (DAYS)
4 = ,F10.3/45H INITIAL DT (DAYS)
5 ,F10.3/45H MAXIMUM NUMBER OF STEPS = ,110/45H
6NUMBER OF STEPS BETWEEN PRINTOUTS = ,110/45H NUMBER OF PRE
7DICTOR STEPS = ,110/45H POINT OF MAXIMUM RESOLUTIO
8N ,110/)
400 FORMAT (' SURFACE CONDUCTIVITY AT TOP',E10.3/' SURFACE CONDUCTIVITY
1AT ',E10.3/' SURFACE CONDUCTIVITY AT ',E10.3/' SURFACE CONDUCT
2TIVITY AT ',E10.3/)
410 FORMAT (' NUMBER PORE RADIUS VOLUMETRIC FRACTION'/(17,2X,F12.2,
111X,F10.4)/)
420 FORMAT (' COMPONENTS'/' SERIAL # PRESSURE IN PRESSURE IN MOLECU
1LAR VISCOSITY CONVECTION COEFF. '/' FILL
2SOIL WEIGHT ')
430 FORMAT (' ',18,4F12.4,1E10.3)
440 FORMAT (' BULK DIFFUSION COEFFECIENTS')
450 FORMAT (' ',8F12.4)
460 FORMAT ('OPRESSURE OUTSIDE THE BOUNDARY '/' COMPONENT PRESSURE '/'
1(110,F10.3))
470 FORMAT ('OFILL HISTORY ON FILL BOUNDARY'/'0 TIME RATE OF
1GENERATIONS FOR COMPONENTS'/10X,8110)
480 FORMAT (' ',F10.3,8E10.3)
490 FORMAT (31H-MOLE FRACTION AT TIME (DAYS) =,F9.1,2X,13HDTAU (DAYS)
1=,F6.1,2X,14HDTMAX (DAYS) =,F6.1,2X,11HDPMAX =,E10.3,2X,8H THE
2TA =,F8.2 /,14H STEP NUMBER =,15,20H COMPONENT NUMBER = ,15/)
500 FORMAT (' (CM) ',13I9)
510 FORMAT ('0 DISTANCE ',1P13E9.2)
520 FORMAT ('-',1PE9.2,4X,13F9.2)

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530 FORMAT (' ',13)
540 FORMAT ('+',14X,80A1)
C 550 FORMAT ('-METHANE RECOVERED (CFM) = ',E15.4)
560 FORMAT (' DISCHARGE AT VENT = ',F10.3)
580 FORMAT (1H1)
600 FORMAT (8011)
601 FORMAT (8E10.3)
END
SUBROUTINE CFIL (PO,POO,TIME,TAU)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONE/Q,DTHET,POUT(4),CK1,CK2,CK3,CK4,EMDA,
1 ML,NL,KL,NCMP,MF,NF,MM,NP,MP,NHIST
2 ,NPIPS,IAX,IAXX,IIN,IOUT,ITER
DIMENSION PO(NCMP),POO(NHIST,NCMP),TIME(NHIST)
C
C THIS SUBROUTINE COMPUTES APPLIED MOLE FRACTIONS FROM GIVEN HISTORY
C
DO 10 I=1,NHIST
IF(TAU.EQ.0.D0) GO TO 20
IF(TAU-TIME(I)) 40,40,10
10 CONTINUE
20 DO 30 J=1,NCMP
PO(J)=POO(I,J)
GO TO 60
40 TX=(TAU-TIME(I-1))/(TIME(I)-TIME(I-1))
DO 50 J=1,NCMP
PO(J)=POO(I-1,J)+(POO(I,J)-POO(I-1,J))*TX
50 CONTINUE
60 RETURN
END
SUBROUTINE INVERT (A,MM,N,M,C)
IMPLICIT REAL*8 (A-H,O-Z)
C
C GENERAL MATRIX INVERSION SUBROUTINE
C
DIMENSION A(MM),C(MM),M(N)
C
NN=N
DO 10 I=1,NN
M(I)=-1
10
C
DO 140 I=1,NN
C
C LOCATE LARGEST ELEMENT
C
D=0.0
DO 70 L=1,NN
IF(M(L)) 20,20,70
20 J=L
DO 60 K=1,NN
IF(M(K)) 30,30,50
30 IF(DABS(D)-DABS(A(J))) 40,40,50
40 LD=L
KD=K
D=A(J)
50 J=J+N
60 CONTINUE
70 CONTINUE
C
C INTERCHANGE ROWS.
C
TEMP=-M(LD)
M(LD)=M(KD)
M(KD)=TEMP
L=LD
K=KD
DO 80 J=1,NN
C(J)=A(L)
A(L)=A(K)
A(K)=C(J)
L=L+N
80 K=K+N
C
C DIVIDE COLUMN BY LARGEST ELEMENT
C

```

```

NR=(KD-1)*N+1
NH=NR+N-1
DO 90 K=NR,NH
90 A(K)=A(K)/D
C
C REDUCE REMAINING ROWS AND COLUMNS
C
L=1
DO 130 J=1,NN
IF(J-KD) 110,100,110
100 L=L+N
GO TO 130
110 DO 120 K=NR,NH
A(L)=A(L)-C(J)*A(K)
120 L=L+1
130 CONTINUE
C
C REDUCE ROW
C
C(KD)=-1.0
J=KD
DO 140 K=1,NN
A(J)=-C(K)/D
140 J=J+N
C
C INTERCHANGE COLUMNS
C
DO 170 I=1,NN
L=0
150 L=L+1
IF(M(L)-I) 150,160,150
160 K=(L-1)*N+1
J=(I-1)*N+1
M(L)=M(I)
M(I)=I
DO 170 L=1,NN
TEMP=A(K)
A(K)=A(J)
A(J)=TEMP
J=J+1
170 K=K+1
C
C RETURN
C
END
SUBROUTINE PREDIC (PN,PS,PP,P,DD,DP,QO,DTAUE,DELP,CK,GNR)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/ONE/Q(8),DTHET,POUT(4),EMDA,
1 ML,NL,KL,NCMP,MF,NF,MM,NP(8),MP(8),NHIST,NPC
2 ,NPIPS,IAX,IAXX,IIN,IOUT,ITER,MPOR
DIMENSION PN(ML,NL,KL,NCMP),PS(ML,NL,KL,NCMP),PP(ML,NL,KL,NCMP),
1 P(ML,NL,KL),DD(ML,NL,KL,NCMP,NCMP),DP(ML,NL,KL,NCMP),QO(NCMP)
2 ,DELP(ML,NL,KL,NCMP),CK(NCMP),GNR(ML,NL,KL,NCMP)
ITER=10
ML1=ML-1
DO 180 L=1,NCMP
PNOUT=POUT(L)
DO 170 I=IAX,ML1
FII=2*I-2
FII1P=(FII+1.000)/FII
FII1M=(FII-1.000)/FII
FISQ=1.000/((I-1)*DTHET)**2
DO 170 J=1,NL
DO 170 K=1,KL
ITR=1
FIJ=0.000
DO 80 M=1,NCMP
DIJK=DD(I,J,K,L,M)
PSIJK=PS(I,J,K,M)
IF(I.EQ.IAX) GO TO 10
DPRIM=(DD(I+1,J,K,L,M)-DD(I-1,J,K,L,M))*0.25
PPRIM=PS(I+1,J,K,M)-PS(I-1,J,K,M)
FIJ=FIJ+DPRIM*PPRIM+(FII1P*PS(I+1,J,K,M)-2.000*PSIJK+FII1M*PS(I-1,J,
1K,M))*DIJK
GO TO 20

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10 FIJ=FIJ+2.000*DIJK*(PS(I+1,J,K,M)-PS(IJK)
20 IF(J.EQ.1) GO TO 30
   IF(J.EQ.NL) GO TO 40
   DPRIM=(DD(I,J+1,K,L,M)-DD(I,J-1,K,L,M))*0.25
   PPRIM=PS(I,J+1,K,M)-PS(I,J-1,K,M)
   FIJ=FIJ+DPRIM*PPRIM+(PS(I,J+1,K,M)-2.000*PS(IJK)+PS(I,J-1,K,M))*DIJ
   GO TO 50
30 FIJ=FIJ+2.000*DIJK*(PS(I,J+1,K,M)-PS(IJK)
   GO TO 50
40 FIJ=FIJ+2.000*DIJK*(PS(I,J-1,K,M)-PS(IJK)
50 CONTINUE
   IF(I.LT.IAXX) GO TO 80
   IF(K.EQ.1) GO TO 60
   IF(K.EQ.KL) GO TO 70
   DPRIM=(DD(I,J,K+1,L,M)-DD(I,J,K-1,L,M))*0.25
   PPRIM=PS(I,J,K+1,M)-PS(I,J,K-1,M)
   FIJ=FIJ+(DPRIM*PPRIM+(PS(I,J,K+1,M)-2.000*PS(IJK)+PS(I,J,K-1,M))*DIJ
   (K)*FISQ
   GO TO 80
60 FIJ=FIJ+2.000*DIJK*FISQ*(PS(I,J,K+1,M)-PS(IJK)
   GO TO 80
70 FIJ=FIJ+2.000*DIJK*FISQ*(PS(I,J,K-1,M)-PS(IJK)
80 CONTINUE
   PS(IJK)=PS(I,J,K,L)
   DPIJK=DP(I,J,K,L)
   PIJK=P(I,J,K)
   IF(I.EQ.IAXX) GO TO 90
   DPRIM=(DP(I+1,J,K,L)-DP(I-1,J,K,L))*0.2500
   PPRIM=P(I+1,J,K)-P(I-1,J,K)
   FIJ=FIJ+DPRIM*PPRIM+(P(I+1,J,K)*FIIP-2.000*PIJK+P(I-1,J,K)*FIIM)*
   DPIJK
   GO TO 100
90 FIJ=FIJ+2.000*DPIJK*(P(I+1,J,K)-PIJK)
100 IF(J.EQ.1) GO TO 110
   IF(J.EQ.NL) GO TO 120
   DPRIM=(DP(I,J+1,K,L)-DP(I,J-1,K,L))*0.2500
   PPRIM=P(I,J+1,K)-P(I,J-1,K)
   FIJ=FIJ+DPRIM*PPRIM+(P(I,J+1,K)-2.000*PIJK+P(I,J-1,K))*DPIJK
   GO TO 130
110 FIJ=FIJ+2.000*DPIJK*(P(I,J+1,K)-PIJK)+CK(L)*(PNOUT-PS(IJK)
   GO TO 130
120 FIJ=FIJ+2.000*DPIJK*(P(I,J-1,K)-PIJK)
130 CONTINUE
   IF(I.LT.IAXX) GO TO 160
   IF(K.EQ.1) GO TO 140
   IF(K.EQ.KL) GO TO 150
   DPRIM=(DP(I,J,K+1,L)-DP(I,J,K-1,L))*0.2500
   PPRIM=P(I,J,K+1)-P(I,J,K-1)
   FIJ=FIJ+(DPRIM*PPRIM+(P(I,J,K+1)-2.000*PIJK+P(I,J,K-1))*DPIJK)*FIS
   IQ
   GO TO 160
140 FIJ=FIJ+2.000*DPIJK*FISQ*(P(I,J,K+1)-PIJK)
   GO TO 160
150 FIJ=FIJ+2.000*DPIJK*FISQ*(P(I,J,K-1)-PIJK)
160 CONTINUE
   IF(K.NE.1) GO TO 162
   IF(J.EQ.1) GO TO 162
   DO 161 M=1,NPC
   IF(I.EQ.MP(M).AND.J.LT.NP(M)) FIJ=FIJ-Q(M)*PS(IJK)
161 CONTINUE
162 CONTINUE
   IF (I.GT.MF.OR.J.GT.NF) GO TO 165
   FIJ=FIJ+GNR(I,J,K,L)
165 FIJ=FIJ*EMDA
   DELP(I,J,K,L)=FIJ
   PP(I,J,K,L)=FIJ
   IF (FIJ.LT.1.00-05) GO TO 170
   DO 168 IT=1,ITER
   FIJ=EMDA*FIJ
   DELP(I,J,K,L)=PP(I,J,K,L)+FIJ
   IF (FIJ.LT.1.00-05) GO TO 170
168 CONTINUE
   IF (IT.GT.2) WRITE (6,*) IT,I,J,K,L,FIJ
170 CONTINUE
180 CONTINUE

```

```

DO 172 I=1,AX,ML1
DO 172 J=1,NL
DO 172 K=1,KL
DO 172 N=1,NCMP
172 PS(I,J,K,N)=DELP(I,J,K,N)
DO 210 I=1,AX,ML1
DO 210 J=1,NL
DO 200 K=1,KL
PIJK=0.0
DO 190 N=1,NCMP
PSIJK=PS(I,J,K,N) +PN(I,J,K,N)
PN(I,J,K,N)=PSIJK
PS(I,J,K,N)=PSIJK
190 PIJK=PIJK+PSIJK
200 P(I,J,K)=PIJK
210 CONTINUE
DO 354 I=1,AX,ML1
DO 354 K=1,KL
PIJK=1.000/P(I,1,K)
P(I,1,K)=1.000
DO 354 L=1,NCMP
PSIJK=PS(I,1,K,L)*PIJK
PS(I,1,K,L)=PSIJK
354 PN(I,1,K,L)=PSIJK
RETURN
END
END OF DATA

```

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