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TWIG, A COMPUTER CODE FOR THE CALCULATION OF TWO-DIMENSIONAL, IDEAL GAS FLOW IN POROUS MEDIA

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November 30, 1972

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ABSTRACT

Two-dimensional flow of an ideal gas in a porous solid is described from the viewpoint of containing the gas generated in a nuclear device cavity. The flow is assumed to be isothermal and obey Darcy's Law. The governing equations are solved numerically using an explicit finite differencing scheme. From this, the pressure response in the pores and the propagation of the cavity gas is predicted. Features of the solution scheme include treatments of spatial variations in permeability and porosity, and models for the cavity pressure decay.

NOMENCLATURE

$\vec{A}, A_1, A_2$	Local area vector and directional components.
$\bar{A}_1, \bar{A}_2$	Dimensionless components of $\vec{A}$.
ds_1	Arc length in general curvilinear coordinates.
e	Specific internal energy for the gas.
e_s	Specific internal energy for the solid.
$\vec{e}_1, \vec{e}_2$	Unit vectors in general curvilinear coordinates.
g_1, g_2	General curvilinear coordinates.
h	Specific enthalpy of the gas.
$\hat{K}$	Dimensionless permeability tensor.
$\hat{K}'$	Permeability tensor.
K_0	Largest permeability encountered
$K_{11} = K_1$	Principal element of permeability tensor in λ_1 direction.
$K_{22} = K_3$	Principal element of permeability tensor in λ_2 direction.
$K_{12}, K_{21} = K_2$	Off diagonal elements of permeability tensor.
L	Vertical depth of burial.
M_1	Dimensionless initial mass in cavity.
M_2	Dimensionless current mass in cavity.
M_{out}	Total dimensionless mass which has escaped from cavity.
$\dot{M}$	Dimensionless mass flow rate from cavity nodes.
$\dot{M}_{total}$	Total dimensionless mass flow rate from cavity.
m_1	Initial cavity mass.
m_2	Current cavity mass.
$\dot{m}$	Mass flow rate from a boundary node.

N	Ratio of initial cavity pressure to undisturbed pore pressure.
P	Dimensionless pressure $\frac{P' - P_0}{P_1 - P_0}$.
P_0	Undisturbed pore pressure.
P_1	Initial cavity pressure.
P'	Gas pressure.
$\bar{P}$	Transformed dimensionless pressure $P + \frac{1}{N-1}$.
R	Gas constant.
$\vec{r}, r_1, r_2$	Position vector and components.
T'	Gas temperature.
t	Time.
$\vec{U}, U_1, U_2$	Darcy flow velocity and components.
U_{P_1}, U_{P_2}	Dimensionless velocity components of tracer particles.
V	Cavity volume.
X_1, X_2	λ_1 direction interpolation lengths.
Y_1, Y_2	λ_2 direction interpolation lengths.
ϵ	Gas filled porosity.
ϵ_0	Largest porosity encountered.
Δ	Finite change in a variable.
λ_1, λ_2	Dimensionless coordinates.
$\lambda_{1p}, \lambda_{2p}$	Coordinates of kinematic tracer particles.
μ	Gas viscosity.
π	3.1416
ρ	Gas density.
ρ_s	Solid density.
τ	Dimensionless time.
ξ_1, ξ_2	Metric coefficients in generalized curvilinear coordinates.

∇ Gradient operator.
 $\nabla \cdot$ Divergence operator.

SUBSCRIPTS

i λ_1 location in finite difference grid.
 j λ_2 location in finite difference grid.
 kk Final time step of interest.
 k Current time step.
 N, S, E, W Values at nodes surrounding a cell.
 NE, SE, NW, SW Interpolated values at cell boundaries.

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k Current time step.

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INTRODUCTION

In the underground testing of nuclear devices, two basic time regimes concern the containment engineer. Early time containment problems are associated with slowing down and stopping the flow due to the large energy release of the device. Late time containment problems are associated with the response of the cavity surroundings to the pressure within the cavity after it has stopped growing.

A particular late time phenomena is the flow of the cavity gas through the pores in the surrounding earth. It is this problem which is addressed here.

This report consists of: the application of restrictive assumptions to the conservation equations for mass, momentum and energy; formulation of these equations in generalized curvilinear coordinates; nondimensionalization of the governing equations; and the development of a finite difference solution scheme for the governing equations. This solution scheme is used in a computer code called TWIG.

A one-dimensional treatment of this problem has already been developed by Morrison^[1] which treats the flow in the stemming column. Treatment here is extended to two-dimensions with calculational schemes to account for variations in permeability and the location of the radioactive material at any time.

RESTRICTIVE ASSUMPTIONS1. Ideal Gas

Gases within the cavity are initially a mixture of rock vapor, steam and non-condensable gases^[2]. Condensation of rock vapor and steam serves to fill the pores of the surrounding media and reduce the area available for gas flow. If the cavity gas is assumed to be all non-condensable, results of calculations made will represent limiting values for the pressure response through the pores and the location of the radioactive material at any given instant. In the following, the non-condensable cavity gas is assumed to be ideal and to obey the ideal gas equation of state,

$$P' = \rho R T' \quad , \quad (1)$$

where P' is the gas pressure, T' the gas temperature, ρ the gas density, and R is the gas constant for the gas considered.

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Support for the argument in the preceding paragraph lies in one-dimensional calculations carried out by Morrison^[1,3]. When results for flow with condensation taking place were compared with those for an ideal gas, it was found that arrival times, for the interface between the radioactive and clean gas, were reduced by a factor of two.

2. Isothermal Flow

Heat transfer between the gas and the porous solid is estimated to take place very rapidly. A simple one-dimensional calculation on an average grain of 10mm diameter subjected to a flow of gas at approximately 1710°K (typical cavity temperature^[4]) shows the temperature response of the soil to the gas to be very rapid. As a result, 90% of the energy carried by the gas will be deposited within a few seconds. Since this time is small compared to the times related to the pressure history in the pores, the flow may be assumed to be nearly isothermal. In view of the fact that a large quantity of soil is available in comparison to the mass of the gas, the temperature may be assumed to be nearly that of the initial temperature in the surrounding media. Obviously, this assumption is not valid at locations very close to the cavity where large temperature gradients exist.

3. Low Reynolds Number

Flow through the porous media is dependent upon the pore size and the inter-connection between pores. At the end of the period in which cavity growth takes place, locations slightly removed from the cavity are subject to gas flow in which the kinetic energy of the fluid has been severely dissipated. This occurs as a result of the small flow area available and the tortuosity of the inter-connecting channels. Therefore, the Reynolds number, based on the pore size, should be small. It is assumed that the Reynolds number is of the order of unity.

4. Permeability and Porosity

Permeability may be thought of as the effective cross sectional area available for flow in a porous solid. It is a tensor quantity in which the principal elements are assumed to be oriented in the vertical and horizontal directions. The absence of sufficient data in most cases requires that the permeability be assumed as isotropic. In general, permeability is a function of pressure and therefore an implicit function of time. For calculations made with this program,

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the permeability is assumed to be a known function of position and to be unaffected by the pressure.

Porosity is essentially the fraction of the total volume occupied by interconnected void space. It is a scalar function of position and is assumed to be known. It is also a function of pressure in the sense that disruption of the grains in the porous solid gives rise to variations in porosity. This has been ignored and the porosities are assumed to remain constant with respect to time.

5. Two-Dimensional Flow

The computer code TWIG is written to provide the user with the option of working in the three basic coordinate systems, cartesian, cylindrical or spherical. Within these systems the flow is assumed to be two-dimensional.

In cartesian coordinates the flow is in the x and z direction as illustrated in Fig. 1. This coordinate system is useful in defining systems which are not axisymmetric or in which ground layers are not parallel to the surface.

Axisymmetric flow defines a surface and volume of revolution for the cavity and the stemming column and, as shown in Fig. 2, more realistically represents the configurations of both of these. Here the r and z axes are used and, as will be seen later, the differential equations are identical to those in cartesian coordinates.

Spherical coordinates have been included in the code and are as shown in Fig. 3. This formulation is not of much utility in problems where the ground is stratified and the permeability and porosity vary accordingly. Care should also be taken when using this formulation to transform the permeability tensor so that the new elements are defined in the spherical coordinate system.

6. Fixed Boundaries

Motion of the ground due to the elastic or plastic deformation caused by the pressure in the pores has been excluded.

Values of pressure which have been stipulated at the ground surface and at distances removed from the cavity are assumed to remain constant and to be equal

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to the initial pressure in the pore space. The hydrostatic head of air in the pores has been neglected. At the ground surface, the implication of this assumption is, that the atmosphere acts as an infinite mass sink and dissipates the flow immediately.

The collapse of the cavity is associated with times later than those of interest to the porous flow problem so the cavity boundary is assumed to remain intact and at a fixed position.

7. Cavity Pressure Decay

Measurements reported by Olsen^[4] show the cavity pressure decay with time can be represented by an exponential

$$P = 36.7 e^{-0.36t} + 7.8 \quad (2)$$

where P is in bars and t is in minutes. This equation is valid between the termination of cavity growth and the time of cavity collapse.

The pressure decay shown above is not used in TWIG. Instead, mass is explicitly conserved. The mass which has flowed from the cavity during the time interval from zero to the current time of interest is used to calculate the mass remaining in the cavity and the corresponding cavity pressure. The cavity temperature is assumed to remain constant consistent with the assumption of isothermal flow made above. When the cavity pressure is reduced to the undisturbed pore pressure, flow stops and the problem is terminated.

BASIC EQUATIONS

1. Introduction

The equations governing the flow may be written consistent with the assumptions of the previous section by considering the basic equations for conservation of mass, momentum, and energy.

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2. Conservation of Mass

This equation applies to an Eulerian control volume consisting of the gas and the porous solid. Since the properties of the porous solid do not change, the results apply for the gas occupying the void space of the control volume. Conservation of mass is then written as,

$$\epsilon \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{U} = 0, \quad (3)$$

where ϵ is the porosity, ρ the gas density, t the time, and $\nabla \cdot$ the divergence operator. The velocity $\vec{U}$ is defined to be the "apparent fluid velocity" which is numerically equal to the volume flow rate divided by the total cross sectional area of flow normal to $\vec{U}$.

3. Conservation of Momentum

Since it has been assumed that the flow within the pore space is such that the associated Reynold's number is approximately unity, the momentum equation may be replaced by an empirical equation known as Darcy's law,

$$\vec{U} = - \frac{\hat{K}'}{\mu} \cdot \nabla P', \quad (4)$$

where P' is the gas pressure, μ is the gas dynamic viscosity, $\hat{K}'$ is the permeability tensor, and ∇ is the gradient operator.

A discussion of the limitations of Darcy's Law may be found in Schiedegger^[5]. The reader should particularly note the absence of a time dependent term for momentum dissipation. This absence is a result of an order of magnitude analysis which implies that the momentum change with respect to time is small compared to the inertial and surface forces on the control volume.

4. Conservation of Energy

Since the flow has been assumed to be isothermal, this equation is superfluous, and is included only for completeness.

$$(1-\epsilon) \frac{\partial(\rho_s e_s)}{\partial t} + \frac{\epsilon \partial(\rho e)}{\partial t} + \nabla \cdot (\rho h \vec{U}) = 0 \quad (5)$$

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where the volume not occupied by the gas has been assumed to be occupied by the solid. Variables associated with the porous solid are subscripted with an s. In Eq. 5, e is the specific internal energy and h is the specific enthalpy of the gas.

For a solid and an ideal gas, Δe and Δh are proportional to the change in temperature. The change in temperature ΔT is zero so that Eq. 5 is identically zero.

5. Equation of State

Since the gas has been assumed to be ideal, the pressure, density and temperature are related through the ideal gas equation of state, Eq. 1.

$$P' = \rho RT' . \quad (1)$$

GENERALIZED COORDINATES

To simplify the coding of TWIG, the equations are written in terms of generalized curvilinear coordinates. This represents a simplification only in the two-dimensional case for which the formulation in cartesian x, z coordinates is identical to that in cylindrical r, z coordinates. In the spherical case the complete formulation requires the addition of a single term to those in the above coordinate systems.

Consider the arc length ds_1 shown in Fig. 4. This arc length may be defined in terms of the coordinate increment dg_1 and a metric coefficient ξ_1 as,

$$ds_1 = \xi_1 dg_1 . \quad (6)$$

consistent with this definition, the divergence of a vector $\vec{A}$ in two-dimensions is

$$\nabla \cdot \vec{A} = \frac{1}{\xi_1 \xi_2} \left[\frac{\partial (\xi_2 A_1)}{\partial g_1} + \frac{\partial (\xi_1 A_2)}{\partial g_2} \right] , \quad (7)$$

and the gradient of a scalar B is

$$\nabla B = \frac{\vec{e}_1}{\xi_1} \frac{\partial B}{\partial g_1} + \frac{\vec{e}_2}{\xi_2} \frac{\partial B}{\partial g_2} , \quad (8)$$

where $\vec{e}_1$ and $\vec{e}_2$ are unit vectors in the coordinate system.

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A summary of the metric coefficients for the three basic coordinate systems is shown in Table 1. A complete development of the definitions given in Eq. 6, 7, and 8 may be found in Band^[6].

NON-DIMENSIONAL FORM OF EQUATIONS

Motivation for writing the governing equations using nondimensional variables lies in the self scaling provided. This provides the user with a means to easily check the validity of his results since upper and lower bounds for all variables are 1 and 0 respectively.

A unitless pressure is defined as

$$P = \frac{P' - P_0}{P_1 - P_0} \quad (9)$$

where P_0 is the initial pressure in the pores and P_1 is the initial pressure in the cavity.

Permeability is scaled by a reference permeability K_0 which is defined as, the largest encountered in the problem.

$$\bar{K} = \frac{K'}{K_0} \quad (10)$$

Lengths are scaled by L , the vertical depth of burial.

$$\lambda_1 = \frac{\xi_2 g_2}{L} \quad (11)$$

$$\lambda_2 = \frac{\xi_2 g_2}{L} \quad (12)$$

Even though the porosity is already a dimensionless quantity, it is scaled by ϵ_0 , the largest porosity encountered.

$$\bar{\epsilon} = \frac{\epsilon}{\epsilon_0} \quad (13)$$

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Using the new variables, defined above, in the governing equations results in a natural scaling of the time so that a dimensionless time τ is defined as,

$$\tau = \frac{K_0 t (P_1 - P_0)}{\mu \epsilon_0 L^2} \quad (14)$$

Conservation of mass, Eq. 3 is now written in two-dimensional generalized coordinates,

$$\epsilon \frac{\partial \rho}{\partial \tau} + \frac{1}{\xi_1 \xi_2} \left[\frac{\partial (\xi_2 \rho U_1)}{\partial \eta_1} + \frac{\partial (\xi_1 \rho U_2)}{\partial \eta_2} \right] = 0 \quad (15)$$

In a similar fashion, Darcy's Law, Eq. 4 becomes,

$$\vec{U} = - \frac{\vec{K}'}{\mu} \cdot \left[\frac{\vec{e}_1}{\xi_1} \frac{\partial P'}{\partial \eta_1} + \frac{\vec{e}_2}{\xi_2} \frac{\partial P'}{\partial \eta_2} \right] \quad (16)$$

which has the components,

$$U_1 = - \frac{K'_{11}}{\mu \xi_1} \frac{\partial P'}{\partial \eta_1} - \frac{K'_{12}}{\mu \xi_2} \frac{\partial P'}{\partial \eta_2} \quad (17)$$

$$U_2 = - \frac{K'_{21}}{\mu \xi_1} \frac{\partial P'}{\partial \eta_1} - \frac{K'_{22}}{\mu \xi_2} \frac{\partial P'}{\partial \eta_2} \quad (18)$$

The gas viscosity μ is a function of temperature and, by virtue of the isothermal assumption made earlier, is constant. Combination of this fact with Darcy's Law, the equation for conservation of mass, and the dimensionless variables, results in

$$\frac{\partial \rho}{\partial \tau} = \frac{1}{\xi_1 \xi_2} \frac{\epsilon_0}{\epsilon} \left\{ \xi_1 \frac{\partial}{\partial \lambda_1} \left[\xi_2 \rho \left[K_{11} \frac{\partial P}{\partial \lambda_1} + K_{12} \frac{\partial P}{\partial \lambda_2} \right] \right] \right. \\ \left. + \xi_2 \frac{\partial}{\partial \lambda_2} \left[\xi_1 \rho \left[K_{21} \frac{\partial P}{\partial \lambda_1} + K_{22} \frac{\partial P}{\partial \lambda_2} \right] \right] \right\} \quad (19)$$

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The density may now be replaced with P'/RT' from Eq. 1 and a new pressure variable defined as,

$$\bar{P} = P + \frac{1}{N-1} \quad , \quad (20)$$

where N is the ratio of P_1 over P_0 .

Substitution of (20) and (1) into (19) followed by some manipulation results in the differential equation which is to be solved,

$$\begin{aligned} \frac{\partial \bar{P}}{\partial \tau} = \frac{1}{\xi_1 \xi_2} \frac{\epsilon_0}{\epsilon} \left\{ \xi_1 \frac{\partial}{\partial \lambda_1} \left[\xi_2 \bar{P} \left[K_{11} \frac{\partial \bar{P}}{\partial \lambda_1} + K_{12} \frac{\partial \bar{P}}{\partial \lambda_2} \right] \right] \right. \\ \left. + \xi_2 \frac{\partial}{\partial \lambda_2} \left[\xi_1 \bar{P} \left[K_{21} \frac{\partial \bar{P}}{\partial \lambda_1} + K_{22} \frac{\partial \bar{P}}{\partial \lambda_2} \right] \right] \right\} \quad (21) \end{aligned}$$

BOUNDARY AND ASSOCIATED CONDITIONS

1. General

Equation (21) is a non-linear differential equation in one dependent variable $\bar{P}$ and three independent variables λ_1 , λ_2 and t . It is first order in t requiring an initial condition for solution and it is second order in λ_1 and λ_2 requiring two conditions on each of these to obtain a solution.

2. Boundary Values

Conditions at problem boundaries may be specified by declaring; $\bar{P}$ to be a constant or a known function of t , or; $\frac{\partial \bar{P}}{\partial \lambda_i}$ to be a constant or a known function of t .

At the cavity boundary, the pressure is dependent upon the mass flow from the cavity. This will be developed in a later section, however, the cavity pressure is typically,

$$P' = P_1(t) \quad ,$$

or

$$\bar{P} = \bar{P}(t).$$

(22)

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At the ground surface, the gas being pushed out of the pores exhausts into an essentially infinite mass sink so that,

$$P' = P_0 \text{ at } \lambda_2 = 1 ,$$

$$\text{or } \bar{P} = \frac{1}{N-1} \text{ at } \lambda_2 = 1 . \quad (23)$$

Far from the pressure disturbance at the cavity, the pores are assumed to remain at the initial pore pressure,

$$P' \rightarrow P_0 \text{ as } \lambda_1 \rightarrow \infty ,$$

$$\text{or } \bar{P} \rightarrow \frac{1}{N-1} \text{ as } \lambda_1 \rightarrow \infty . \quad (24)$$

3. Axisymmetric Conditions

In the case of cylindrical or spherical coordinates, the center line of the stemming column is an axis of symmetry at which the pressure gradient must be zero, so

$$\frac{\partial P'}{\partial \lambda_1} = 0 \text{ at } \lambda_1 = 0 ,$$

or

$$\frac{\partial \bar{P}}{\partial \lambda_1} = 0 \text{ at } \lambda_1 = 0 \quad (25)$$

4. Initial Conditions

As input to the problem, the pressure $\bar{P}$ must be specified at every point at $t = 0$. This is commonly a step function where the pressure $\bar{P}$ is $N/N-1$ at and within the cavity boundary and $1/N-1$ everywhere else.

FINITE DIFFERENCE EQUATIONS

1. Introduction

The non-linearity of Eq. 21 precludes the development of an analytical solution for the general problem. Therefore, a numerical solution is required. This is carried out by developing a recursion relationship for $\bar{P}$ at time step $K+1$ as a function of $\bar{P}$ at the previous time step K .

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The finite difference formulation of Eq. 21 will be based on a cell centered node system like that shown in Fig. 5. Thermodynamic properties throughout each cell are assumed to be equal to those at the node points. Properties at the cell boundaries are assumed to be equal to the average of those properties at nodes adjacent to those cell boundaries. Derivatives of $\bar{P}$ are calculated using a first order central differencing scheme at all points interior to the boundaries and axes of symmetry.

2. Derivatives

In the definitions developed below, superscripts k refer to time step, subscript i refers to the λ_1 location and subscript j refers to the λ_2 location.

The first derivative of $\bar{P}$ with respect to dimensionless time τ is,

$$\frac{\partial \bar{P}}{\partial \tau} \approx \frac{\bar{P}_{ij}^{k+1} - \bar{P}_{ij}^k}{\Delta \tau} \quad (26)$$

The first derivative of $\bar{P}$ with respect to λ_1 is,

$$\frac{\partial \bar{P}}{\partial \lambda_1} \approx \frac{\bar{P}_{i+1,j}^k - \bar{P}_{i-1,j}^k}{\lambda_{i+1} - \lambda_{i-1}} \quad (27)$$

The second derivative of $\bar{P}$ with respect to λ_1 is written as,

$$\frac{\partial^2 \bar{P}}{\partial \lambda_1^2} = \frac{\frac{\bar{P}_{i+1,j} - \bar{P}_{ij}}{\lambda_{i+1} - \lambda_i} - \frac{\bar{P}_{ij} - \bar{P}_{i-1,j}}{\lambda_i - \lambda_{i-1}}}{\frac{\lambda_{i+1} - \lambda_{i-1}}{2}} \quad (28)$$

Similar expressions may be written for $\frac{\partial \bar{P}}{\partial \lambda_2}$ and $\frac{\partial^2 \bar{P}}{\partial \lambda_2^2}$ by incrementing and decrementing j instead of i in Eq. 27 and Eq. 28.

Expanding Eq. 21 results in a derivative $\frac{1}{\xi_2} \frac{\partial \xi_2}{\partial \lambda_1}$. The magnitude of this derivative is zero except when a spherical coordinate system is used. In this case,

$$\frac{1}{\xi_2} \frac{\partial \xi_2}{\partial \lambda_1} = \frac{1}{\lambda_1} \quad (29)$$

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The term in which this derivative appears is,

$$\frac{\bar{p}}{\epsilon_2} K_{11} \frac{\partial \bar{p}}{\partial \lambda_1} \frac{\partial \epsilon_2}{\partial \lambda_1} \approx \frac{\bar{p}_{ij}^k K_{1ij} (\bar{p}_{i+1,j}^k - \bar{p}_{i-1,j}^k)}{\lambda_i (\lambda_{i+1} - \lambda_{i-1})} \quad (30)$$

To simplify notation, $\Delta \lambda_1$ and $\Delta \lambda_2$ are now defined as,

$$\Delta \lambda_1 = \lambda_{i+1} - \lambda_{i-1}, \quad (31)$$

and

$$\Delta \lambda_2 = \lambda_{j+1} - \lambda_{j-1}. \quad (32)$$

3. Recursion Relation for $\bar{p}$

It is assumed that the permeability tensor is diagonal so that $K_{11} = K_{1ij}$, $K_{22} = K_{3ij}$ and $K_{12} = K_{21} = 0$. The reader should note carefully that spherical coordinate formulations are of little utility in using TWIG for cases in which the permeability tensor is not isotropic.

Substitution of the finite difference expressions into Eq. 21 results in a recursion relation for $\bar{p}$,

$$\begin{aligned} \bar{p}_{ij}^{k+1} = & \bar{p}_{ij}^k + \Delta \tau \frac{\epsilon_0}{\epsilon_{ij}} \left[\bar{p}_{ij}^k \frac{4K_{1ij}}{\Delta \lambda_1^2} (\bar{p}_{i+1,j}^k - 2\bar{p}_{ij}^k + \bar{p}_{i-1,j}^k) \right. \\ & + \frac{\bar{p}_{ij}^k}{\Delta \lambda_1^2} (\bar{p}_{i+1,j}^k - \bar{p}_{i-1,j}^k) (K_{1i+1,j} - K_{1i-1,j}) + \frac{K_{1ij}}{\Delta \lambda_1^2} (\bar{p}_{i+1,j}^k - \bar{p}_{i-1,j}^k)^2 \\ & + \frac{\bar{p}_{ij}^k 4K_{3ij}}{\Delta \lambda_2^2} (\bar{p}_{i,j+1}^k - 2\bar{p}_{ij}^k + \bar{p}_{i,j-1}^k) + \frac{\bar{p}_{ij}^k}{\Delta \lambda_2^2} (\bar{p}_{i,j+1}^k - \bar{p}_{i,j-1}^k) (K_{3i,j+1} - K_{3i,j-1}) \\ & \left. + \frac{K_{3ij}}{\Delta \lambda_2^2} (\bar{p}_{i,j+1}^k - \bar{p}_{i,j-1}^k)^2 + \frac{\bar{p}_{ij}^k K_{1ij}}{\lambda_i \Delta \lambda_1} (\bar{p}_{i+1,j}^k - \bar{p}_{i-1,j}^k) \right] \quad (33) \end{aligned}$$

The last term in Eq. 33 is zero except when spherical coordinates are used.

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4. Mass Flow from the Cavity

The mass flow from the cavity is important in two respects. Firstly, it is the mechanism by which the mass within the cavity and hence the cavity pressure is reduced. Cavity pressure decay due to cooling of the cavity gas has been neglected. Secondly, the mass flow combined with the cavity pressure decay, sets bounds on the time that the problem is to run. When the cavity pressure is no longer sufficient to drive the gas, further calculation has no meaning.

The mass flow rate from the cavity may be written as,

$$\dot{m}_{\text{total}} = \int_A \rho \vec{U} \cdot d\vec{A} \quad , \quad (34)$$

where $d\vec{A}$ is the outward normal vector associated with an elemental area dA .

From each of the boundary nodes, we have

$$\dot{m} = \rho \vec{U} \cdot \vec{A} \quad , \quad (35)$$

where the local area $\vec{A}$ is dependent on the coordinate system used. Consider points a, b, c, d and e in Fig. 6 which represents one quarter of a cavity. In cartesian coordinates, a unit depth is assumed, and in cylindrical coordinates, Fig. 6 represents the profile of a body of revolution. Table 2 shows a summary of areas A_1 and A_2 for the points a through e in both coordinate systems. Areas which are indicated to be 0 are of no importance since flow is not permitted along a boundary.

Expanding Eq. 35 in two-dimensions we have

$$\dot{m} = \rho [U_1 A_1 + U_2 A_2] \quad , \quad (36)$$

with the velocity components

$$U_1 = - \frac{K_1 K_0 (P_1 - P_0)}{\mu L} \frac{\partial P}{\partial \lambda_1} \quad , \quad (37)$$

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and

$$U_2 = - \frac{K_3 K_0}{\mu L} (P_1 - P_0) \frac{\partial P}{\partial \lambda_2} \quad (38)$$

Substituting the equation of state, Eq. 1 and Eqs. 37 and 38 into 36 results in an expression for the mass flow rate,

$$\dot{m} = - \frac{(P_1 - P_0)^2}{RT' \mu} K_0 L \left[P + \frac{1}{N-1} \right] \left[K_1 \bar{A}_1 \frac{\partial P}{\partial \lambda_1} + K_3 \bar{A}_2 \frac{\partial P}{\partial \lambda_2} \right] \quad (39)$$

where $\bar{A}_1 = A_1/L^2$ and $\bar{A}_2 = A_2/L^2$.

A dimensionless mass flow rate $\dot{M}$ can now be written, by using the definition of $\bar{P} = P + \frac{1}{N-1}$, as

$$\dot{M} = \frac{\dot{m} RT' \mu}{(P_1 - P_0)^2 K_0 L} = - \bar{P} \left[K_1 \bar{A}_1 \frac{\partial \bar{P}}{\partial \lambda_1} + K_3 \bar{A}_2 \frac{\partial \bar{P}}{\partial \lambda_2} \right] \quad (40)$$

The mass which has departed from the cavity in a time period may now be calculated by adding all of the $\dot{M}$ at all of the boundary nodes

$\dot{M}_{total} = \sum_{\text{boundary}} \dot{M}$ then integrating with respect to time to get,

$$M_{out} = \int_0^T \dot{M}_{total} d\tau \quad (41)$$

5. Boundary and Associated Conditions

5.1 Cavity Pressure Decay

The first problem addressed in this section is the decay of the cavity pressure. Conservation of mass requires that the mass remaining in the cavity at any time must be equal to the original mass minus the mass which has escaped up to that time. Initially,

$$m_1 = \rho_1 V = \frac{P_1 V}{RT'} \quad (42)$$

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which in dimensionless form is,

$$M_1 = \frac{P_1 V}{(P_1 - P_0) L^3 \epsilon_0} = \frac{N V}{(N-1) L^3 \epsilon_0} \quad (43)$$

At a particular time of interest, say kk , the mass within the cavity of volume V is,

$$m_2 = \rho_2 V = \frac{P'_{kk} V}{RT'} \quad (44)$$

which in dimensionless form is

$$M_2 = \frac{P'_{kk} V}{(P_1 - P_0) L^3 \epsilon_0} \quad (45)$$

Conservation of mass requires that

$$M_2 = M_1 - \int_0^t \dot{M}_{total} dt \quad (46)$$

which after the use of Eq. 41, 43, and 45 and some manipulation results in an equation which describes the cavity pressure decay as,

$$\bar{P}_{kk} = \frac{N}{N-1} \left[1 - \frac{(N-1) L^3 \epsilon_0}{NV} \sum_{k=1}^{kk} \dot{M}_{k total} \Delta \tau \right] \quad (47)$$

where the integral of Eq. 41 has been written in finite difference form as a summation.

5.2 Axisymmetric Conditions

At axes of symmetry, the pressure gradient is required to be zero. In finite difference form this is expressed as,

$$\frac{\bar{P}_{i+1,j} - \bar{P}_{ij}}{\lambda_{i+1} - \lambda_i} = 0 \quad (48)$$

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Therefore, at the axes,

$$\bar{p}_{ij} = \bar{p}_{i+1,j} \quad (49)$$

This condition is subject to inaccuracy depending upon the distances between adjacent nodes. Higher order expressions are available which include the effects of points farther removed from the boundary however, inclusion of these expressions led to instabilities in the calculation process.

5.3 Undisturbed Boundaries

At distances far from the cavity and at the ground surface, the pressure is equal to that in the pores so that for all time steps,

$$\bar{p}_{ij} = \frac{1}{N-1} \quad (50)$$

6. Location of Radioactive Interface

The location of the interface between radioactive gas and uncontaminated gas is found by starting kinematic tracer particles at the cavity boundary at time zero and allowing them to move with the velocity of the fluid. For a single time step, the particles, which by definition have no mass, are assumed to travel in a straight line in the direction of the velocity vector. The distance traveled during one time step locates the particle for the start of the next time step. A trace of all of the particles represents the location of the radioactive interface at that instant.

The gas velocity and hence the particle velocity is known at $t = \tau = 0$ from Darcy's Law. From the velocity, the position of a particle can be found by integration. Note carefully that Darcy's Law defines the velocity as the volume flow per unit cross-sectional area. The area available for gas flow is approximately the porosity times this so that the tracer particle velocities are equal to the Darcy velocities divided by the local porosity.

The position vector $\vec{r}$ is defined in terms of the velocity,

$$\frac{d\vec{r}}{dt} = \vec{U} \quad (51)$$

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where $\vec{r}$ has the components

$$r_1 = \xi_1 g_1 = L \lambda_{1p} \quad (52)$$

and

$$r_2 = \xi_2 g_2 = L \lambda_{2p} \quad (53)$$

By integrating Eq. 51 for one time step Δt , the change in the position vector is,

$$\Delta \vec{r} = \int_{t_1}^{t_2} \vec{U} dt = \vec{U} \Delta t \quad (54)$$

yielding nondimensional components of

$$\Delta \lambda_{1p} = U_1 \frac{\Delta t}{L} \quad (55)$$

$$\Delta \lambda_{2p} = U_2 \frac{\Delta t}{L} \quad (56)$$

Darcy's Law gives the velocity in terms of pressure as,

$$\vec{U} = - \frac{\vec{K}'}{\mu} \cdot \nabla P' \quad (57)$$

which has the components

$$U_1 = - \frac{K_1 K_0}{\mu L} (P_1 - P_0) \frac{\partial \bar{P}}{\partial \lambda_1} \quad (58)$$

and

$$U_2 = - \frac{K_3 K_0}{\mu L} (P_1 - P_0) \frac{\partial \bar{P}}{\partial \lambda_2} \quad (59)$$

Substitution of 58, 59 and the definition for τ into 55 and 56 gives the coordinate change for the particle in finite difference form

$$\Delta \lambda_{1p} = \frac{\Delta \tau}{\Delta \lambda_1} \epsilon_0 K_{1ij} (P_{i+1,j} - P_{i-1,j}) \quad (60)$$

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and

$$\Delta \lambda_{2p} = - \frac{\Delta \tau}{\Delta \lambda_2} \epsilon_0 K_{3ij} (P_{i,j+1} - P_{i,j-1}) \quad (61)$$

The location of the particle at each time step is then calculated as

$$\lambda_{1p}^{k+1} = \lambda_{1p}^k + \Delta \lambda_{1p} \quad (62)$$

and

$$\lambda_{2p}^{k+1} = \lambda_{2p}^k + \Delta \lambda_{2p} \quad (63)$$

In general, the location of a particle is interior to a cell rather than at a node point. In this case, interpolation is necessary to evaluate the gas velocity at the particle location. To do this, consider the particle in Fig. 7 interior to the nodes. Using linear interpolation, the velocities of interest are,

$$U_{E_1} = U_{NE_1} \frac{Y_1}{Y_1 + Y_2} + U_{SE_1} \frac{Y_2}{Y_1 + Y_2} \quad (64)$$

$$U_{S_2} = U_{SE_2} \frac{X_1}{X_1 + X_2} + U_{SW_2} \frac{X_2}{X_1 + X_2} \quad (65)$$

$$U_{W_1} = U_{SW_1} \frac{Y_2}{Y_1 + Y_2} + U_{NW_1} \frac{Y_1}{Y_1 + Y_2} \quad (66)$$

$$U_{N_2} = U_{NW_2} \frac{X_2}{X_1 + X_2} + U_{NE_2} \frac{X_1}{X_1 + X_2} \quad (67)$$

where the notation used is defined in Fig. 7.

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Interpolating again, the particle velocity components are,

$$\bar{U}_{P_1} = \left[U_{E_1} \frac{X_1}{X_1 + X_2} + U_{W_1} \frac{X_2}{X_1 + X_2} \right] \frac{\mu L}{K_1 K_0 (P_1 - P_0) \epsilon} \quad (68)$$

and

$$\bar{U}_{P_2} = \left[U_{N_1} \frac{Y_1}{Y_1 + Y_2} + U_{S_1} \frac{Y_2}{Y_1 + Y_2} \right] \frac{\mu L}{K_3 K_0 (P_1 - P_0) \epsilon} \quad (69)$$

In Eq. 68 and 69, K_1 , K_3 and ϵ are interpolated properties.

These velocities are then used to compute

$$\Delta \lambda_1 = \bar{U}_{P_1} \epsilon_0 \Delta \tau \quad (70)$$

and

$$\Delta \lambda_2 = \bar{U}_{P_2} \epsilon_0 \Delta \tau \quad (71)$$

7. Stability and Limitations

7.1 Stability Criteria

Stability criteria used in TWIG's computational scheme are based on the magnitude of the maximum time step. Since the equation is non-linear the stability criteria can only be inferred from a linear form of the equation [7]. The inferred criteria are,

$$\frac{\bar{P}_{ij} K_0 \Delta \tau}{\Delta \lambda^2} < 1/2 \quad (72)$$

In this case, the upper bound on $\bar{P}$ is unity so that if the time step is calculated such that

$$\Delta \tau < \frac{\Delta \lambda^2}{2K_0} \quad (73)$$

the equations should represent a stable calculational scheme. In carrying out calculations, it was found that for values of N greater than 10, the system was stable for

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$$\Delta\tau \leq \frac{\Delta\lambda^2}{2} \quad (74)$$

when N became less than 10 this was no longer the case so that the denominator in the right hand side of the inequality had to be increased.

The stability criteria used for calculations with N less than 10 were found to be

$$\Delta\tau \leq \frac{\Delta\lambda^2}{8} \quad (75)$$

The use of Eq. 74 or Eq. 75 represents some savings in computation time since the maximum permeabilities encountered are often the order of 50 which would make the $\Delta\tau$ calculated from Eq. 73 rather small in comparison.

7.2 Limitations

In addition to the assumptions made, the user of TWIG should take some care when setting up a problem with a non-uniform grid. Large aspect ratios reduce the validity of the assumption that the properties throughout a cell are well represented by those at the node point interior to the cell. This is of course left to the discretion of the user.

DESCRIPTION OF COMPUTER CODE TWIG

1. Introduction

The primary purpose of TWIG is to evaluate the pressure at each of a series of node points within a porous region for a particular instant in time.

This is accomplished solving the explicit substitution formula (33) developed in the preceding sections.

Secondary calculations which are made include the total mass flow rate from the cavity, and the velocity and location of kinematic tracer particles describing the radioactive interface at any time, and the cavity pressure decay with respect to time.

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DATE November 30, 19722. Operational Modes

Several options are available for the modes of operation of TWIG.

These include:

1. One or two-dimensions.
2. Constant or variable permeability.
3. Constant or variable porosity.
4. Anisotropic or isotropic permeability.
5. Cartesian, cylindrical or spherical coordinate systems.
6. Uniform or non uniform grid spacing.
7. Complicated boundary configurations.

3. Output Options

Graphical output is generated by TWIG in the form of

1. Three-dimensional plots of the pressure versus the two space coordinates.
2. Contour plots of the pressure on the two-dimensional space frame.
3. Traces of the radioactive interface on the two-dimensional space frame.

Printed output consists of tabulations of the pressure at each point, the total mass flow from the cavity, and the coordinates of the kinematic tracer particles.

4. Input Parameters to TWIG

All of the input parameters used by TWIG are listed in Table 3 with descriptive comments. These input parameters make possible many options. The selection of these options depends on the user's interests, available data, and the particular problem under consideration. To best illustrate the input parameters, an example problem is included here with an example of typical results.

Figure 8 shows the zoning for a particular problem in cylindrical coordinates. Both the r and the z axes have been selected as axes of symmetry.

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Included in the figure are scaling parameters, a variety of boundary conditions, variations in permeability and porosity and a complex boundary configuration. Table 4 is the input deck required for this configuration following the order and format given in Table 3.

A three-dimensional plot of the pressure surface is shown in Fig. 9 and again for a later time in Fig. 10. Corresponding contours are shown in Fig. 11 and Fig. 12. Numbers on the contour lines represent values of 0.8, 0.6, 0.4, 0.2 and 0.01 of the initial normalized cavity pressure. Also shown on Fig. 11 and Fig. 12 are the current locations and ten prior locations of the kinematic tracer particles which were started at the cavity boundary. The dotted line in Figures 11 and 12 is the current location of the radioactive clean gas interface.

5. Subroutine Descriptions

5.1 General

In the following text, each of the subroutines incorporated in TWIG is briefly described to give the user a basis for making modifications if desired. Figure 13 is a diagram of the subroutine levels, their relation to each other and their calling sequence.

5.2 MAIN

The main program serves three major purposes. First, all input data is read and processed by MAIN. Second, all of the major calculations made in the solution scheme are carried out by MAIN. These include, the change in the pressure, the mass flow from the cavity, the cavity pressure decay and the propagation of the kinematic tracer particles. Third, MAIN acts as a controller to set up a restart option, call OUTP to generate output, and unload all generated tapes and output buffers.

5.3 OUTP

Subroutine OUTP writes all output on unit 3. The time, mass flow and particle locations are tabulated as well as the normalized pressure P for each node point.

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When plotting is requested, OUTP calls T3D to set it up.

5.4 T3D

This subroutine calls DD80ID to initialize the DD80 and produce title pages for output. Following this call, additional data are read to label the three-dimensional pressure plots.

T3D generates the grid specified by the user, locates positions of tracer particles and plots a trace of the last particle locations as the radioactive interface. BACNTR is called for contour plotting.

5.5 PLOT3D

A complete description of this subroutine may be found in Reference [8], along with the description of its associated subroutines, MAP3D, LABEL, BASE and SIDE.

5.6 BACNTR

Subroutine BACNTR and its associated subroutines B7PLOT, B7BSET, and B8PLOT are modifications of the LRLL1B contour plotting routines RCONTR, Q7PLOT, Q7QSET, and Q8PLOT respectively. The user is referred to Reference [9] for a complete description of these subroutines. BACNTR provides labeled contour lines and RCONTR does not.

5.7 LRLL1B and CLIB SUBROUTINES

Subroutines which appear in the listing of the program belonging to the LRLL1B and CLIB subroutine libraries are described in References [10] and [11].

AQUISITION OF TWIG

The current source version of TWIG may be obtained by using ELF and typing
RDS .093650:TWIG:FORT

A controllee may be obtained for the 7600 or 6600 by typing

RDS .093650:TWIG:76BIN

RDS .093650:TWIG:66BIN

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TABLE 1 SUMMARY OF METRIC COEFFICIENTS

SYSTEM	COORDINATES	METRIC COEFFICIENTS
CARTESIAN	$g_1 = x$ $g_2 = y$ $g_3 = z$	$\xi_1 = 1$ $\xi_2 = 1$ $\xi_3 = 1$
CYLINDRICAL	$g_1 = r$ $g_2 = z$ $g_3 = \theta$	$\xi_1 = 1$ $\xi_2 = 1$ $\xi_3 = r$
SPHERICAL	$g_1 = r$ $g_2 = \theta$ $g_3 = \phi$	$\xi_1 = 1$ $\xi_2 = r$ $\xi_3 = r \sin \theta$

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TABLE 2

ELEMENTAL AREAS ASSOCIATED WITH FIG. 6

Point	Cartesian		Cylindrical	
	A_1/L^2	A_2/L^2	A_1/L^2	A_2/L^2
a	0	$\frac{\lambda_{i+1}}{2}$	0	$\frac{\pi}{4} (\lambda_{i+1})^2$
b	0	$\frac{\lambda_{i+1} - \lambda_{i-1}}{2}$	0	$\frac{\pi}{4} [(\lambda_{i+1} + \lambda_i)^2 - (\lambda_i + \lambda_{i-1})^2]$
c	$\frac{\lambda_j - \lambda_{j-1}}{2}$	$\frac{\lambda_i - \lambda_{i-1}}{2}$	$\pi(\lambda_j - \lambda_{j-1}) \lambda_i$	$\pi[\lambda_i^2 - \frac{(\lambda_i + \lambda_{i-1})^2}{4}]$
d	$\frac{\lambda_{j+1} - \lambda_{j-1}}{2}$	0	$\pi(\lambda_{j+1} - \lambda_{j-1}) \lambda_i$	0
e	$\frac{\lambda_{j+1}}{2}$	0	$\pi \lambda_{j+1} \lambda_i$	0

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TABLE 3
INPUT DATA REQUIRED FOR TWIG

CARD	VARIABLE	TYPE	FORMAT	DESCRIPTION
1.	ATITLE	Alphameric	10A6	Job title, up to 60 characters.
2.	SCALE	Logical	I10	0 if uniform grid desired 1 if non uniform
	PLTIT	Logical	I10	0 if no plots are desired 1 if plots are desired.
	IDBUG	Logical	I10	0 results in no debugging print is required, 1 results in voluminous output.
3.	EN	Real	F10.4	Cavity pressure in atmospheres divided by atmospheric pressure in atmospheres.
	VOL	Real	F10.4	Cavity volume in FT ³ .
	DCB	Real	F10.4	Depth of burial in FT.
4.	TWOD	Logical	I10	0 if one-dimensional problem, 1 if two-dimensional.
	PERMK	Logical	I10	0 results in variable permeability calculation, 1 results in constant permeability.
	POR	Logical	I10	0 results in variable porosity calculation, 1 in constant porosity.
	RPHI	Logical	I10	Declares spherical coordinate system is to be used.
	IMAX	Integer	I10	Maximum number of I nodes. X or R direction.
	JMAX	Integer	I10	Maximum number of J nodes. Y, Z or ϕ direction.
	KMAX	Integer	I10	Maximum number of time steps.
	RAD1	Real	F10.4	Normalized cavity radius R/L used only for spherical coordinate system calculations.
5.	RI	Real	F10.4	Scaling parameter equal to the fraction of total space to be assigned to the following I nodes.
	I1	Integer	I10	Lower limit for RI
	I2	Integer	I10	Upper limit for RI

NOTE: This card is required only if scale = 0 on card #2. It must be followed by scaling cards until I2 is equal to IMAX. All I lines must be included. This permits variable scaling throughout the zoning system.

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CARD	VARIABLE	TYPE	FORMAT	DESCRIPTION
6.	RJ	Real	F10.4	Scaling parameter equal to the fraction of the total J space to be assigned to the following J nodes.
	J1	Integer	I10	Lower limit for RJ
	J2	Integer	I10	Upper limit for RJ

NOTE: This card may or may not be #6 depending on the number of I scaling cards used. However, the remarks in #5 also apply. Values of J1 and J2 must run from 1 to JMAX.

7.	IM	Integer	I4	Minimum I line for type N class boundary
	IX	Integer	I4	Maximum I line for type N class boundary
	JM	Integer	I4	Minimum J line for type N class boundary
	JX	Integer	I4	Maximum J line for type N class boundary

NOTE: Class of boundaries are as follows

- N = 1 Cavity boundary condition. This is programmed as a constant or may be requested as a function of time.
- N = 2 Free surface boundary where pressures are equal to ambient conditions.
- N = 3 Symmetry boundary where pressure derivative in X or R direction is zero.
- N = 4 Long distance boundary where pressure approaches ambient conditions.
- N = 5 Symmetry boundary where pressure derivative in Y, Z or ϕ direction is zero.

All data cards for type 1 boundaries must be followed by a card with 9999 in columns 1 through 4. This is then followed by cards defining type 2 boundaries then a 9999 card until all types, 1 through 5, have been declared and delimited with 9999 cards.

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CARD	VARIABLE	TYPE	FORMAT	DESCRIPTION
8.	NPART	Integer	I10	ID number of tracer particle
	A1	Real	F10.4	λ_1 location of tracer particle.
	A2	Real	F10.4	λ_2 location of tracer particle.
NOTE: This card permits the input of the initial locations of tracer particles in the grid system. Care should be taken to insure that points are sequential around the cavity boundary. These cards are delimited with 9999 in columns 7 through 10.				
9.	IM IX	Integer	2I10	I limits on permeability and porosity zone.
	JM JX	Integer	2I10	J limits on permeability and porosity zone.
	PER1 PER2	Real	2F10.4	Directional permeabilities, for I and J zone specified above, in Darcies.
	EP	Real	F10.4	Porosity for I and J zone.
NOTE: The range of IM, IX, JM and JX must cover all nodal points. The default option for a constant permeability calculation is a constant porosity calculation, however, a constant porosity calculation may be made with variable permeabilities. Porosities of zero are not permitted as input. Permeabilities of zero are permitted as input.				
These data cards are excluded if PERMK $\neq$ 0 on card #4.				
Permeability, porosity data are delimited with a card with 9999 in columns 7 through 10.				
10.	AXX AXZ	Alphanumeric	4A6	Titles for the R, X and Z axes respectively, for use with 3-D plot. 2,6 character words each.
11.	HEX	Alphanumeric	10A6	Horizontal title for 3-D plot. 60 characters.
12.	HEY	Alphanumeric	10A6	Vertical title for 3-D plot. 60 characters.
13.	PHI	Real	F10.4	Angle at which negative X axis is to be drawn for 3-D plot.

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<u>CARD</u>	<u>VARIABLE</u>	<u>TYPE</u>	<u>FORMAT</u>	<u>DESCRIPTION</u>
14.	XS,YS,ZS	Real	3F10.4	Relative sizes of maximum X,Y,Z dimensions on 3-D plot.

NOTE: Cards 10 through 14 are not required if PLTIT = 0 on card 2.

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TABLE 4

DATA DECK FOR EXAMPLE PROBLEM

Small numbers refer to card column. Comments in parentheses are only for clarification.

1
TWIG, EXAMPLE, PROBLEM

	10	20	30				
	1	1	0				
1	11	21					
45.	16362.5	800.					
	10	20	30	40	49	59	67 71
	1	0	0	0	25	25	1000 1.
1		20	29				
0.0625		1	10				
1		19	29				
0.9375		10	25				
1		20	29				
0.0625		1	10				
1		19	29				
0.9375		10	25				
	4	8	12	15			
	1	4	1	10			
	4	8	12	16			
5	6	1	9				
	4	8	12	16			
7	7	1	8				
	4	8	12	16			
8	8	1	7				
	4	8	12	16			
9	9	1	6				
	3	7	12	16			
10	10	1	4				
1							
9999							
	4	7	11	15			
1	1	25	25	25			
1							
9999							
	4	8	11	15			
1	1	11	24				
1							
9999							
	3	7	12	15			
1	25	25	2	24			
1							
9999							
	3	7	12	16			
1	11	25	1	1			
1							
9999							

(Scaling in r direction)

(Scaling in z direction)

(Cavity boundary)

(Free surface)

(Vertical axis of symmetry)

(Long distance boundary)

(Horizontal axis of symmetry)

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$$\begin{matrix} 10 & 12 & & 22 \\ 1 & 0.063 & & 0.007 \end{matrix}$$

$$\begin{matrix} 10 & 12 & & 22 \\ 2 & 0.063 & & 0.014 \end{matrix}$$

$$\begin{matrix} 10 & 12 & & 22 \\ 3 & 0.063 & & 0.021 \end{matrix}$$

$$\begin{matrix} 10 & 12 & & 22 \\ 4 & 0.056 & & 0.028 \end{matrix}$$

$$\begin{matrix} 10 & 12 & & 22 \\ 5 & 0.056 & & 0.035 \end{matrix}$$

$$\begin{matrix} 10 & 12 & & 22 \\ 6 & 0.049 & & 0.042 \end{matrix}$$

$$\begin{matrix} 10 & 12 & & 22 \\ 7 & 0.042 & & 0.049 \end{matrix}$$

$$\begin{matrix} 10 & 12 & & 22 \\ 8 & 0.035 & & 0.056 \end{matrix}$$

$$\begin{matrix} 10 & 12 & & 22 \\ 9 & 0.028 & & 0.056 \end{matrix}$$

$$\begin{matrix} 9 & 12 & & 22 \\ 10 & 0.021 & & 0.063 \end{matrix}$$

$$\begin{matrix} 9 & 12 & & 22 \\ 11 & 0.014 & & 0.063 \end{matrix}$$

$$\begin{matrix} 9 & 12 & & 22 \\ 12 & 0.007 & & 0.063 \end{matrix}$$

(Tracer particle locations at time zero
on cavity boundary)

$$\begin{matrix} 7 \\ 9999 \end{matrix}$$

$$\begin{matrix} 10 & 19 & 30 \\ 1 & 25 & 1 \end{matrix}$$

$$\begin{matrix} 10 & 19 & 29 \\ 1 & 25 & 12 \end{matrix}$$

$$\begin{matrix} 10 & 19 & 29 \\ 1 & 25 & 16 \end{matrix}$$

$$\begin{matrix} 39 & 42 \\ 11 & 2. \end{matrix}$$

$$\begin{matrix} 39 & 42 \\ 15 & 10. \end{matrix}$$

$$\begin{matrix} 39 & 42 \\ 25 & 50. \end{matrix}$$

$$\begin{matrix} 52 \\ 2. \end{matrix}$$

$$\begin{matrix} 52 \\ 10. \end{matrix}$$

$$\begin{matrix} 52 \\ 50. \end{matrix}$$

$$\begin{matrix} 62 \\ 0.3 \end{matrix}$$

$$\begin{matrix} 62 \\ 0.21 \end{matrix}$$

$$\begin{matrix} 62 \\ 0.15 \end{matrix}$$

(Permeability and
Porosity zones)

$$\begin{matrix} 7 \\ 9999 \end{matrix}$$

$$\begin{matrix} 2 \\ R_AXIS \end{matrix}$$

$$\begin{matrix} 26 \\ Z_AXIS \end{matrix}$$

$$\begin{matrix} 2 \\ EXAMPLE_PROBLEM_PRESSURE_SURFACE \end{matrix}$$

$$\begin{matrix} 2 \\ NORMALIZED_PRESSURE \end{matrix}$$

(Plotting data for labels)

$$\begin{matrix} 2 & 12 & 22 & 32 \\ 45. & 1. & 1. & 1. \end{matrix}$$

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FIG. 1 - X-Z Coordinate System for use with TWIG

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FIG. 2 - Cylindrical Coordinate System used by TWIG

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FIG. 3 - Spherical Coordinate System used by TWIG

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FIG. 4 - Generalized Curvilinear Coordinate System.

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FIG. 5 - Cell and Node System used by TWIG for Finite Differencing of Equations

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FIG. 6 - Points Defining Flow Areas Corresponding to Table 2

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FIG. 7 - Interpolation System to Find the Velocity of a Tracer Particle Interior to a Cell

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FIG. 8 - Zoning for an Example Problem for TWIG

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FIG. 9 - Pressure Surface for TWIG Example Problem at $t = 3400$ sec
Axes are in Fractions of $DOB \times 10$

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FIG. 10 - Pressure Surface for TWIG Example Problem at $t = 6500$ sec
Axes are in Fractions of $DOB \times 10$

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FIG. 11 - Pressure Contours and Radioactive Interface Location
Corresponding to Fig. 9. Axes are in fractions of DOB

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FIG. 12 - Pressure Contours and Radioactive Interface Location
Corresponding to Fig. 10. Axes are in fractions of DOB.

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FIG. 13 - Subroutine Tree for TWIG

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