User's Manual for the MIGRAT Pre- and Postprocessor

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ABSTRACT

MIGRAT is a state-of-the-art computer code that numerically solves Richard's equation for the migration of moisture in the unsaturated zone and the advective diffusion equation for the associated movement of contaminants. This code utilizes the integral form of these governing equations. This formulation allows the use of polygonal computational cells which can provide an accurate representation of the modeled region. The penalty for this realism is the extensive input data necessary for model applications. In order to render the MIGRAT code more suitable for routine applications, an interactive preprocessor has been developed which allows a user to enter input data rapidly and in a more convenient format. The preprocessor is designed for use on a personal computer to allow the user to develop, modify, and display input data prior to its transmission to a mainframe for MIGRAT execution. Model output can be captured by the personal computer for display utilizing the preprocessor's graphics software.

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1. INTRODUCTION

MIGRAT is a state-of-the-art computer code for simulating the movement
of moisture and two contaminants in the unsaturated zone. The code was
constructed from the TRUST code (Ref. 1), which solves Richard's equation
(Ref. 2) for the movement of moisture, by adding ORNL-developed subroutines
that solve the advective diffusion equation for up to two retarded and
decaying contaminants. As a result of this code's capability to model
realistic geologic and geohydrologic systems, the quantity of input data
required to drive the model is extensive, and the steps necessary to convert
these data from the typically available format into the format required by
the code are both tedious and error prone. Furthermore, errors which can
occur in the preparation of input may be so subtle that they may not become
apparent until the final stages of the code's execution.

The realism and versatility of the MIGRAT code make it a potentially
valuable tool for a variety of applications including subsurface pathways
analysis, evaluation of waste disposal design options, and efficacy of
remedial actions. However, the magnitude of effort required to use the model
renders it an impractical tool for most potential users. To remedy this
situation, with support by the U.S. Nuclear Regulatory Commission, ORNL has
developed a personal computer-based pre- and postprocessor system designed to
allow MIGRAT to be implemented by a broader cross section of users.

The motivation for the development of a personal computer based system
of pre- and postprocessor software was threefold: (1) to allow the
development of model input and graphical presentation of model input and
output independent of the mainframe computer required to execute the MIGRAT
code, (2) to greatly reduce the extent of data which must be provided by the
user, and (3) to allow the user to enter data in a form which is more
convenient than that required by the MIGRAT code. Items (2) and (3) were
developed in a manner that allows the rapid entry of data.

It should be noted that the MIGRAT code is general and, consequently,
capable of accommodating a broad class of problems dealing with the migration
of moisture and contaminants in the unsaturated zone. This flexibility gives
rise to the need for extensive and complex input data. Any attempt to
streamline the entry of input data can result in restrictions which would
reduce the applicability of the computer code. Thus, the development of a

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preprocessor represents a compromise where the increased efficiency of data entry is offset by a loss of generality of the computer code. The MIGRAT preprocessor was developed with the objective of making the data input as simple as possible while minimizing the loss of generality of the MIGRAT code; however, some loss of generality is inevitable. Where appropriate in this report, limiting assumptions in the preprocessor are identified and described so as to allow a user to evaluate the implications of each assumption for a given problem.

Tests of the preprocessor indicate that this software reduces the time required to prepare the input data files associated with a problem of moderate complexity. The approximately six weeks of preparation time required by a user who is familiar with the input-output requirements of the code can be reduced to one day, or less, for the occasional user of the code.

Most of the time required for the development of data is associated with cell geometry and cell configuration. To allow accurate representation of local stratigraphy, disposal unit design, etc., MIGRAT utilizes cells of arbitrary shape. Not only does this feature require far more information to define each computation cell, as compared with other schemes utilizing rectangular cells, but the manner in which each cell is connected to all adjacent cells must be provided as input data. In order to relieve the user of this burden, a significant part of the MIGRAT preprocessor is devoted to simplifying the generation of cell geometry data. This simplification is successfully accomplished with a scheme which automatically generates 3-, 4-, or 5-sided computation cells based on an overlay of a user-specified rectangular grid system with a series of user-specified interfacial curves. The information necessary to generate a grid system is entered interactively at the personal computer (PC) by the user through a sequence of prompts. Using the entered information, the preprocessor software creates an input data file containing all cell geometry and connectivity information necessary for the MIGRAT code.

A second tedious task in the preparation of MIGRAT input data is the entering of a number of attributes, such as material type (clay, sandstone) and initial conditions on a cell-by-cell basis. This aspect of input data preparation has been greatly streamlined through the use of a layer concept. The interface lines segregate the grid into regions possessing constant attributes. Thus, the cells in the region bounded by adjacent interface

lines all have identical attributes. This identity allows attributes to be entered on a layer-by-layer basis rather than a cell-by-cell basis. A considerable saving of time results considering the fact that a typical application could involve only 10 layers but in excess of 500 cells.

The following section describes the methodologies employed in the preprocessor. Section 3 provides summary descriptions of the MIGRAT input data and format, highlighting input parameters which are influenced by the use of the preprocessor. Section 4 illustrates the execution of the preprocessor and, where appropriate, provides printouts of interactive sessions. Section 5 discusses communications between mainframe and PC, MIGRAT control data, and editing files for problem restart. The final section provides annotated results of a test run of the MIGRAT code.

2. THE MIGRAT PREPROCESSOR

2.1 OVERVIEW

Input to the MIGRAT code can be divided into the following four categories:

1. geometric data such as the shape and location of each computational cell and the relationship between each cell and every adjacent cell;
2. attributes such as material type (e.g., sandstone, clay) and initial and boundary conditions that must be specified for each grid cell;
3. properties such as conductivity and retardation that vary with material and are functions of pressure, contaminant concentration, etc.;
4. constants, such as a reference density for water, and computational control parameters.

These data categories are listed in descending order of effort required for a typical application. The MIGRAT preprocessor focuses on simplifying the input for the first two classes (i.e., geometric information and attributes of each cell) because this would have the greatest effect on the level of effort required to develop MIGRAT input data.

The approach adopted in the preprocessor for minimizing the input of geometric data and cell properties defines the computational system as an overlay of a layered structure with a nonuniform rectangular grid system. This approach considerably reduces the amount of user-specified input data by (1) defining each layer to be composed of cells with constant attributes in order that attribute data may be entered by layer rather than by cell, and (2) allowing accurate physical representation of the modeled region through the use of nonrectangular cells created by the intersection of the layer interfaces with the rectangular grid cells. In the layer concept (Fig. 2.1), each layer has properties that are different from those of other layers. For example, the region between the lines labeled -2 and 2 is comprised of sandstone. However, an unconfined aquifer occupies the lower portion of this region. Consequently, the line labeled 1 is drawn to correspond to the initial elevation of the water table. The result is two layers, each having

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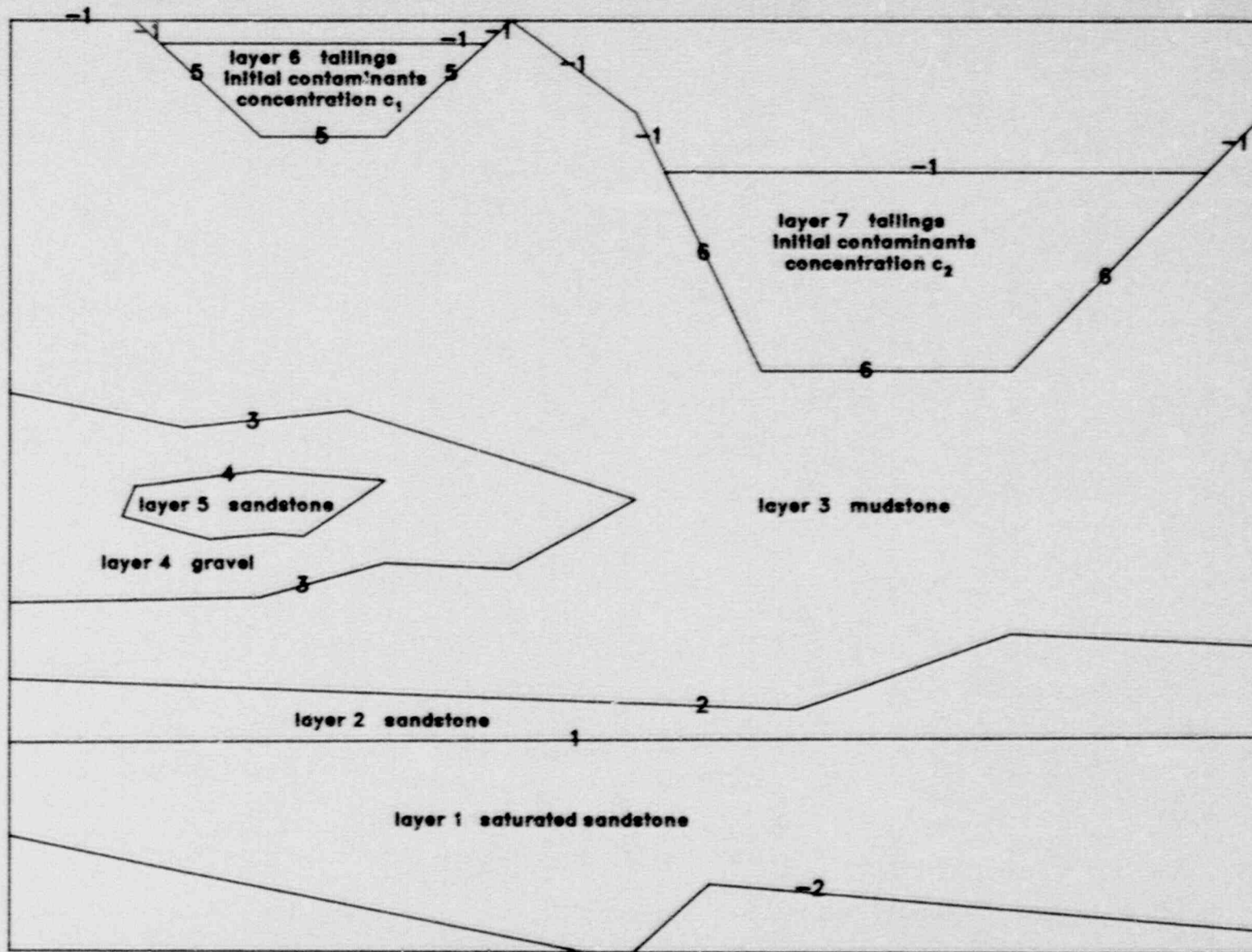
Fig. 2.1. Annotated drawing of the modeled region showing layers defined by the numbered interfacial lines.

homogeneous attributes. Layers 1 and 2 have the same physical properties except for the initial moisture content.

In order to simplify the generation of geometric input data which is performed by the preprocessor, the following constraints are imposed on the interfacial lines which define the layers.

1. Interfacial line numbers -2 and -1 are reserved for lower and upper boundaries, respectively, of the modeled region;

2. Interfacial lines are comprised of sequences of line segments having constant slope (The endpoints of each line segment must correspond to vertical grid lines and no vertical line segments are allowed.);

3. Interfacial lines must be closed, such as line 4 (Fig. 2.1), or have endpoints at upper, lower, or lateral boundaries, such as lines -2, -1, 1, 2, and 3 (Fig. 2.1), or have endpoints at another interfacial line, such as lines 5 and 6 (Fig. 2.1).

The reasons for imposing the first two constraints are given in the subsequent discussion. The reason for the third constraint is that the boundary of every layer must be closed.

The creation of the system of layers is the first step in the development of the computational grid. The next step is the development of a rectangular grid system which is superimposed on the interfacial lines. This grid system, while flexible, is not arbitrary and must satisfy certain constraints. In order to understand the necessity for these constraints as well as those imposed on the interfacial lines, it is useful to examine the geometric input data required by the MIGRAT code.

2.2 GEOMETRIC INPUT DATA REQUIREMENTS

The MIGRAT code allows a physically realistic representation of the modeled region by allowing the region to be composed of computational cells, where each cell can have an arbitrary number of sides. The code requires geometric input data that characterizes each computational cell and characterizes relationships among cells. Each computational cell is characterized by (1) a unique integer identification number, (2) its area, and (3) the vertical coordinate of the centroid. The relationships among

computation cells are illustrated in Fig. 2.2. Figure 2.2a depicts a set of six computational cells. Input must be developed to quantify the relationship between a given cell and all other cells with which it shares a side. Referring to Fig. 2.2a, it is apparent that this cell shares its sides with the five cells numbered 2 through 6. The information required to define connections involving cell 1 are tabulated below.

Cell i	Cell j	d_{ij}	d_{ji}	ℓ_{ij}
1	2	d_{12}	d_{21}	ℓ_{12}
1	3	d_{13}	d_{31}	ℓ_{13}
1	4	d_{14}	d_{41}	ℓ_{14}
1	5	d_{15}	d_{51}	ℓ_{15}
1	6	d_{16}	d_{61}	ℓ_{16}

The entries in the columns headed cell i and cell j are the cell identifier numbers of the two cells whose connections are being described. The d_{ij} entry is the distance along the line connecting the nodes (centroids) of cells i and j from the node of cell i to the side of cell i that is common to cell j. As illustrated in Fig. 2.2b for cells 1 and 2, d_{12} is the length of the portion of the line connecting node 1 and node 2 between node 1 and the point where this line intersects the line segment AA'. Similarly, d_{21} is the distance along the same line from node 2 to the intersection with AA'. The ℓ_{12} entry, depicted in Fig. 2.2c as the dashed line, is the length of the side common to cells i and j when projected onto the line normal to the line connecting the centroids of cells i and j.

It is clear from the foregoing discussion that the preparation and entry of the cell connection data for all the cells in the modeled region represent a significant effort, which is the penalty associated with the flexibility of a system composed of arbitrary grid cells. At the other extreme is the rectangular grid system that offers relatively poor physical representation of the modeled region but requires no externally specified cell connection data. All computational grid systems require cell connection information comparable to that tabulated above. With such information for a rectangular grid system that has cells identified by a two-dimensional index (I,J), it is obvious that cell (I,J) is connected to cells (I±1,J) and (I,J±1). Thus, there is no need for the explicit entry of this information into a code.
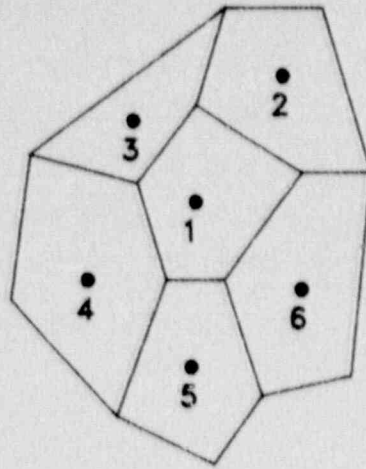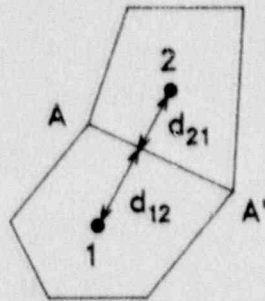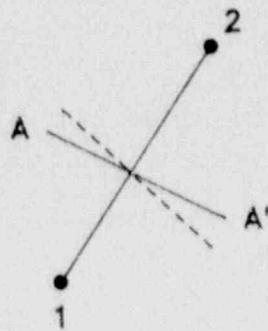
Fig. 2.2. Illustration of MIGRAT grid geometrics depicting (a) 6 computational grid cells; (b) the lengths from node 1 and node 2 to the common cell side, d_{12} and d_{21}, respectively; and (c) ℓ_{12} the normal projection of the length of the common cell side.

In developing the MIGRAT preprocessor, it was desirable to utilize a more restricted grid system that can utilize some of the simplicities of a rectangular grid system while maintaining as much accuracy in physical representation as possible. This attempt led to the concept of a system of layers overlaying a rectangular grid. A grid system was produced that is fundamentally rectangular but has additional cells that can be three-, four-, or five-sided when a rectangular cell is split by a segment of an interfacial (layer) line. The concept is illustrated in Fig. 2.3 and shows a single interfacial line (labeled 2) separating layers 1 and 2 superimposed on a simple rectangular grid. The original 5 x 5 grid with 25 rectangular cells becomes a system of 32 cells (with 12 nonrectangular cells) as a result of the interfacial line splitting the rectangular cells (1,5), (2,4), (3,4), (3,3), (4,3), (5,3), and (5,4). In order to simplify the computations performed by the preprocessor in generating the geometric input data, the following types of split grid cells are excluded (see Fig. 2.4):

1. cells with interfacial line segments which change slope in the interior of a cell (Fig. 2.4a), and
2. cells which are split by more than one interfacial line segment associated with either the same (Fig. 2.4b) or different (Fig. 2.4c) interfacial lines.

The motivation for these restrictions is to limit cells to no more than five sides and to ensure that the most complex cells can be decomposed into two rectangles and a right triangle (as shown in Fig. 2.5). The first restriction requires that interfacial line segments change slope only on a boundary of a rectangular cell. To simplify the entry of user-provided data and to avoid inadvertent violations of this restriction, interfacial line segments are further constrained to change slope only on vertical grid lines. This constraint is one of convenience, and its purpose is illustrated by Fig. 2.6. It is necessary for the user to input the coordinates which define the location (x',z') where an interfacial line changes slope (Fig. 2.6a). Should the value of x' be entered with either more or less precision than the value of the vertical grid line on which it lies, the situation depicted in Fig. 2.6b could result, and is in violation of the restriction. To prevent the occurrence of this situation, the preprocessor does not request the
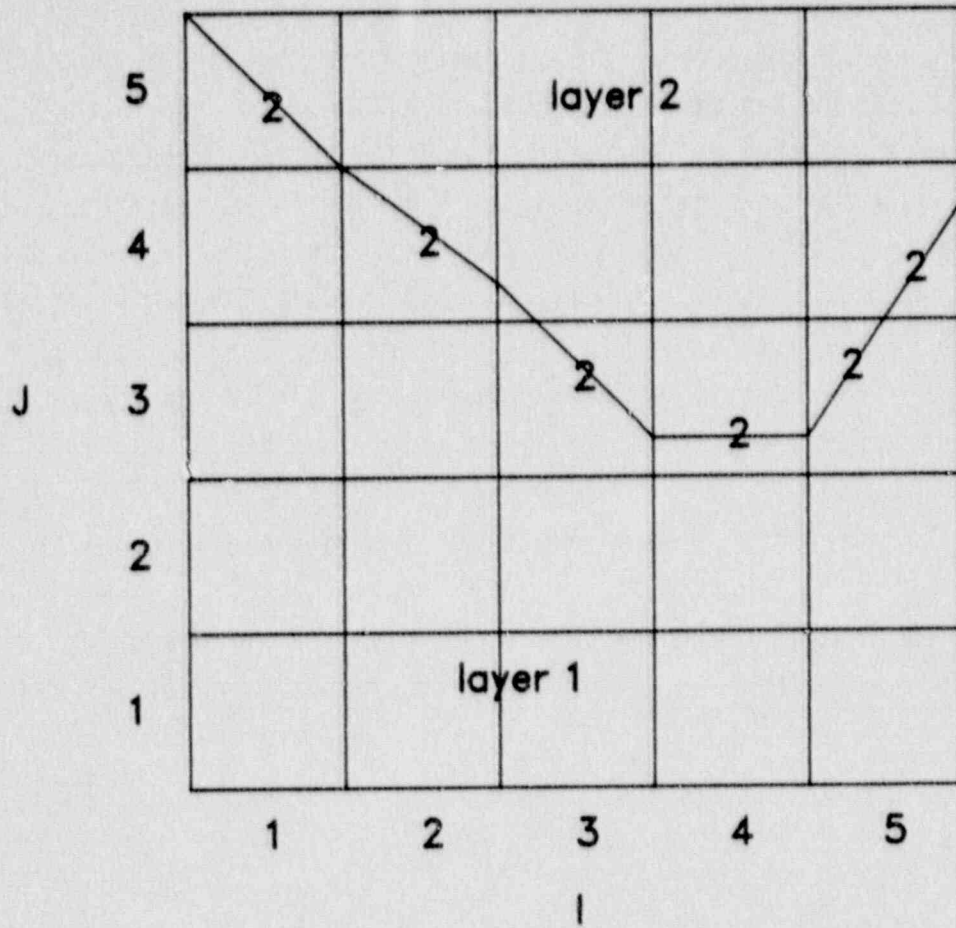
Fig. 2.3. An example of the cell structure and two layer system created by overlaying a rectangular grid system with a single interfacial line.
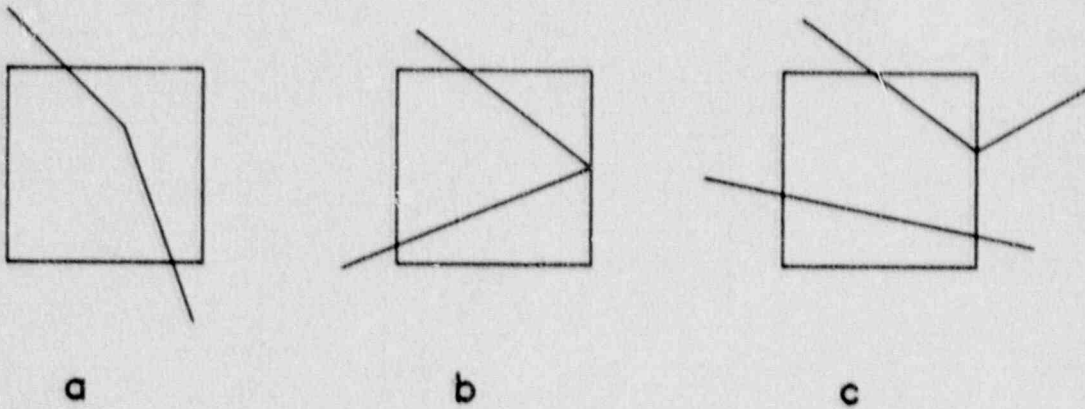
Fig. 2.4. Examples of the three types of split grid cells which violate the grid generation conditions in the preprocessor.
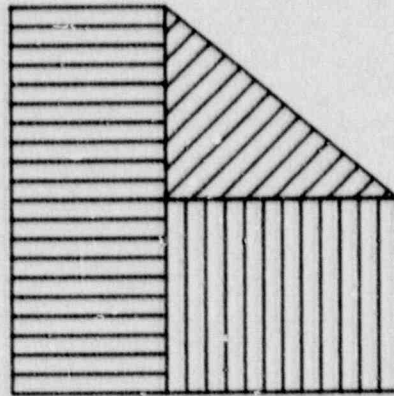
Fig. 2.5. An example of the decomposition of a five-sided grid cell into two rectangles and a right triangle.
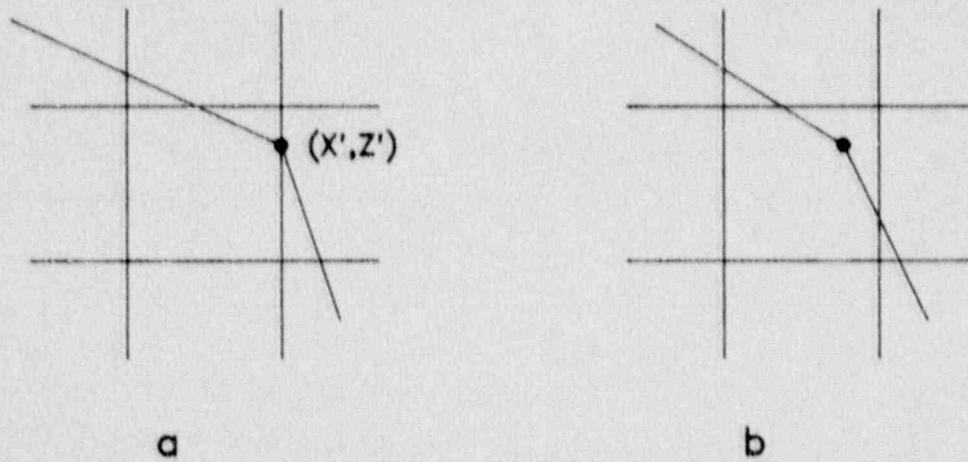
Fig. 2.6. (a) An example of a proper interfacial line segment slope change and (b) a slope-change point which violates a condition of the preprocessor as a result of imprecision in data entry.

coordinate pair but, rather, the index of the vertical grid line on which the slope change occurs and the elevation of this point, z'. This ensures compliance with the restriction.

It should be noted here that the restrictions imposed on the grid do not significantly reduce the accuracy of the physical representation. While a computational cell with a shape illustrated in Fig. 2.7a cannot be constructed by the preprocessor, the same shape can be generated using two cells as shown in Fig. 2.7b. As also illustrated by Fig. 2.7, additional computational cells are required to represent more complex shapes.

2.3 GRID CONSTRUCTION

With an understanding of the restrictions on the grid geometry, it is appropriate to return the discussion to the construction of the grid system. After creating a layer map from a set of interfacial lines (Fig. 2.1), the first step is to construct a vertical line through every slope change point on every interfacial line (Fig. 2.8). To do this will satisfy the requirement that all interfacial line slope changes occur on vertical grid lines. Horizontal grid lines can be selected in a manner which ensures that no rectangular grid cell is split by more than one line segment. This requires (1) that there is at least one horizontal grid line between each interfacial line and (2) that a horizontal grid line must pass through every point where an interfacial line "turns back" (Fig. 2.9a) or where two interfacial lines meet (Fig. 2.9b). Figure 2.10 shows an overlay of the interfacial lines defining the layer and the minimum rectangular grid system. Additional horizontal and vertical grid lines may be added arbitrarily by the user.

As previously noted, creating a grid with accurate physical representation can produce a large number of computational grid cells. In static regions (areas where moisture content and contaminant concentrations do not deviate significantly from the initial conditions), these additional grid cells are unnecessary. Consequently, the user is advised to simplify interfacial lines in these regions so as to minimize the number of split cells. On the other hand, in dynamic regions (areas expected to have significant gradients in moisture content and contaminant concentrations),
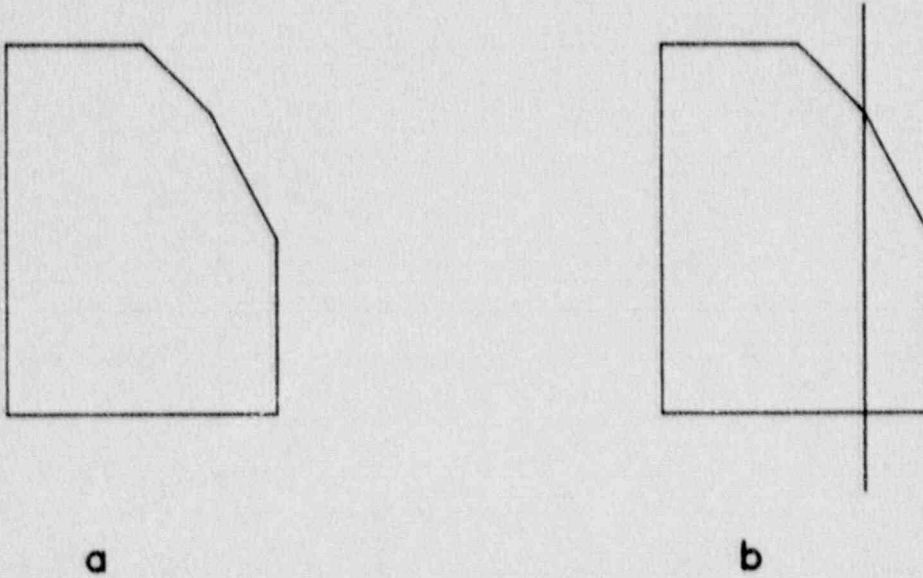
Fig. 2.7. (a) An example of a single grid cell which cannot be generated by the preprocessor and (b) an identical two-cell representation which can be achieved with the preprocessor.
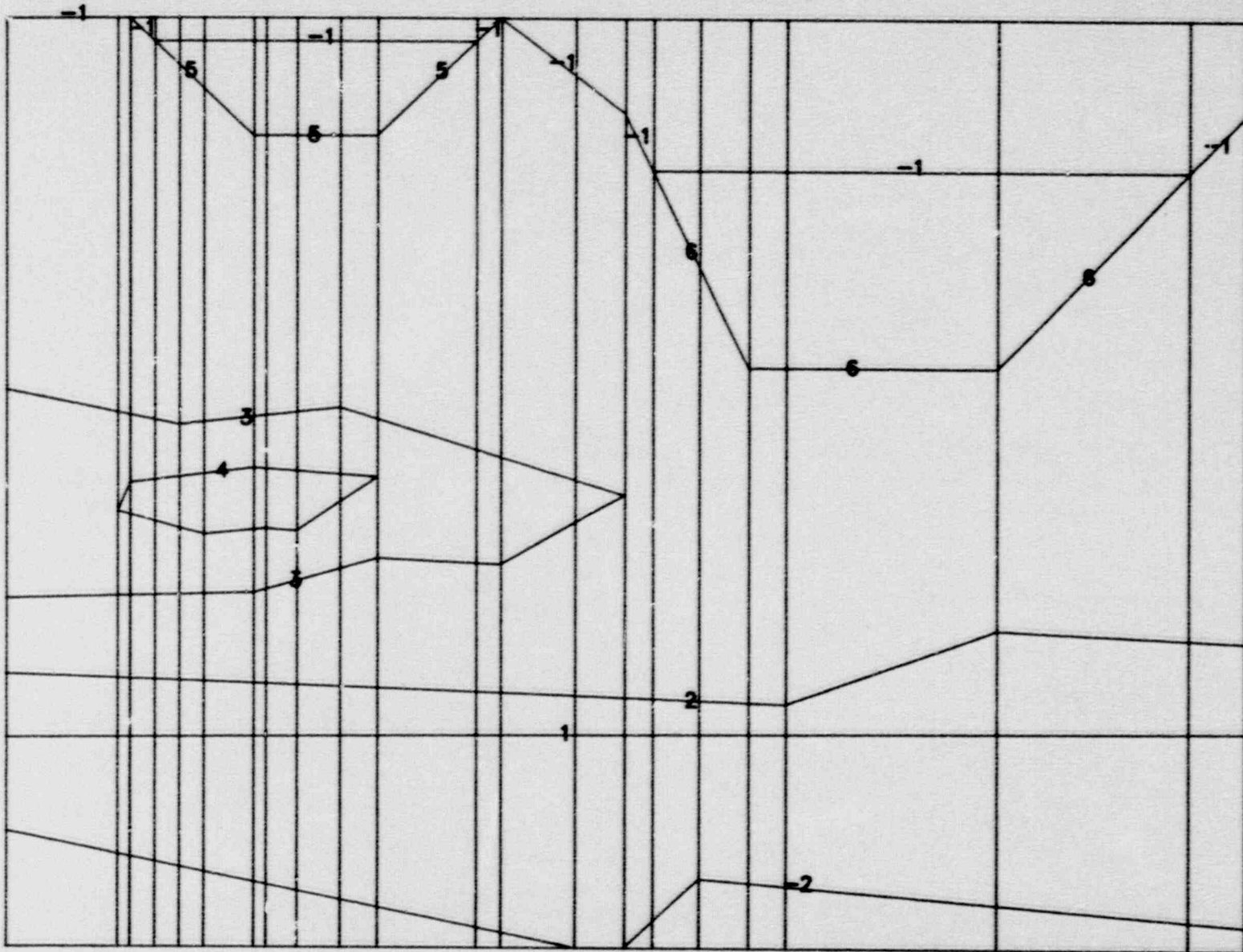
Fig. 2.8. The minimum vertical grid lines for the layer structure shown in Fig. 2.1 as required to satisfy the constraints of the preprocessor.
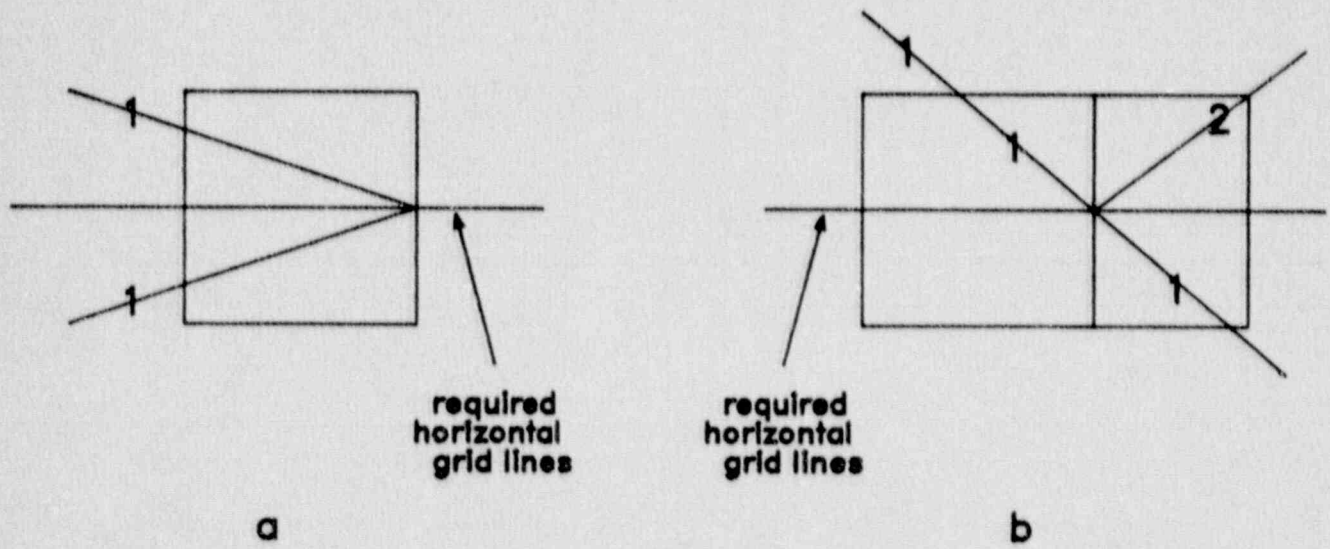
Fig. 2.9. Illustrations of the two situations that require horizontal grid lines to satisfy the preprocessor constraints.

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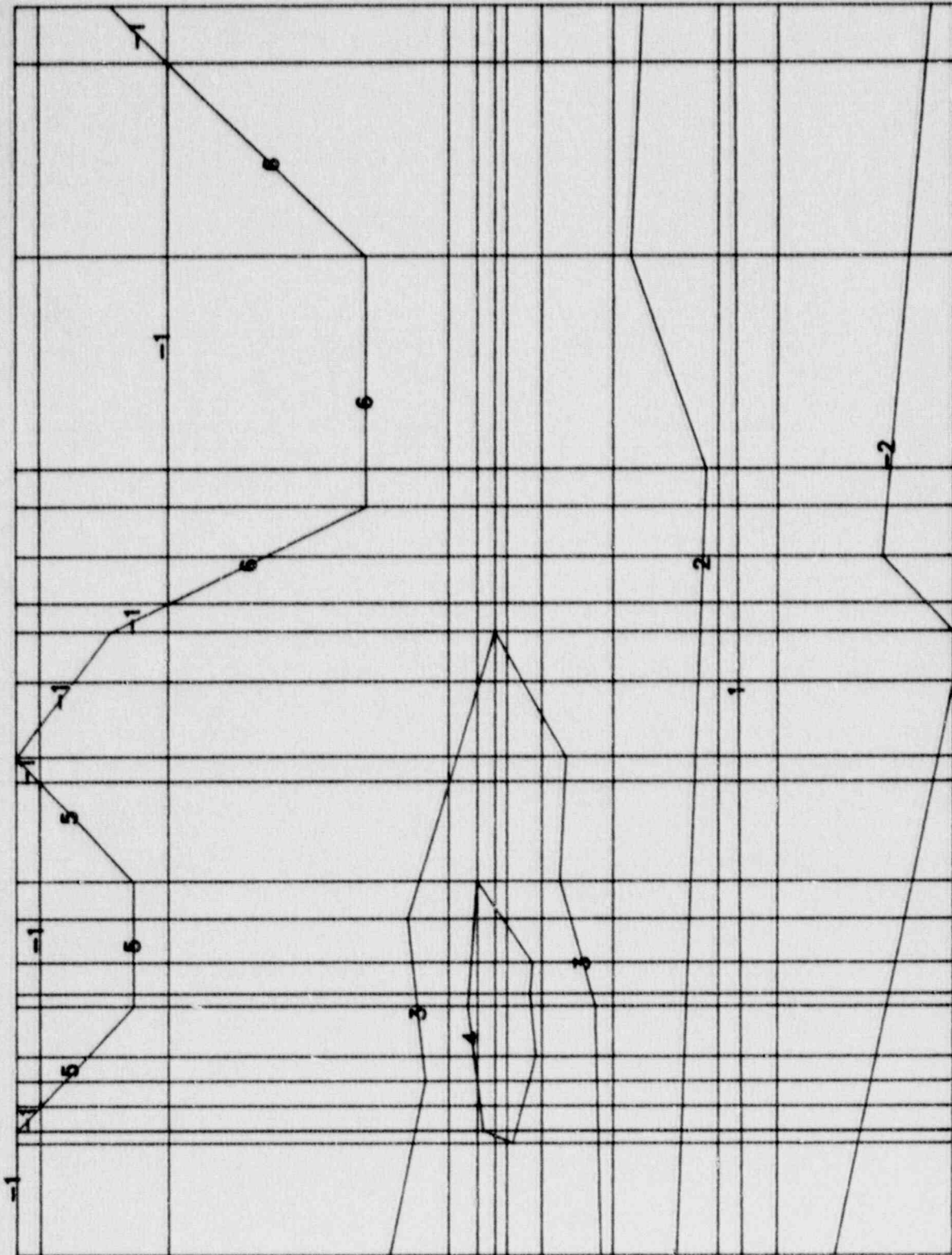
Fig. 2.10. The full grid system for the layer structure shown in Fig. 2.1 based on the minimum requirements for the rectangular grid.

the user is advised to add horizontal and vertical grid lines to create a fine grid structure to accurately resolve gradients in such regions.

2.4 GENERATION OF GEOMETRIC INPUT

The preprocessor software generates all the geometric input data required by the MIGRAT code from the user-specified interfacial lines and rectangular grid. The first step in this procedure is the identification of all split cells. This is accomplished in the preprocessor by scanning every rectangular grid and identifying every grid cell which is split by an interfacial line. For every rectangular grid cell (I,J), a flag, $IS(I,J)$, is set to indicate that the cell is either not split, $IS(I,J) = 0$, or split, $IS(I,J) \neq 0$. For split cells, the value of IS is set equal to the number of the interfacial line which splits that cell (Fig. 2.11a). For rectangular cells in which an interfacial line lies on a horizontal cell boundary, it is assumed that the interfacial line segment belongs to the cell above (Fig. 2.11b). This assumption is necessary for the construction of the layer map which will be described later. Two coordinate pairs - $X_1(I,J)$, $Z_1(I,J)$ and $X_2(I,J)$, $Z_2(I,J)$ - define the points where the interfacial line intersects the rectangular cell boundary (Fig. 2.11c).

With this information, the preprocessor begins the generation of data which characterize each computational cell and the connections between cells. A node number NODE is assigned to each cell by vertically sweeping the rectangular grid from left to right. A test is performed to determine if the -2 interfacial boundary (the lower boundary) is crossed. No node number is assigned until this boundary is crossed. The node number 1 is assigned to the first cell above the -2 line on the first grid column on the left, and node numbers are incremented by 1 for each cell above. When a split cell is encountered, two successive node numbers are assigned with the lower number assigned to the cell in the lower portion. When the -1 interfacial line is encountered, the vertical sweep of the column is terminated, and the procedure begins from the bottom of the next column to the right. Figure 2.12 is a sample grid with node numbers assigned to illustrate the node number assignment. In this grid, note that split cells such as (1,3) have two assigned node numbers, since two computational cells have been created by
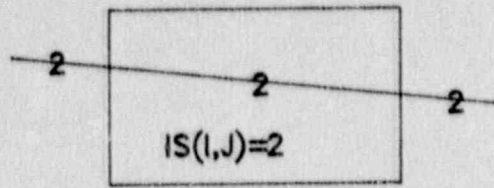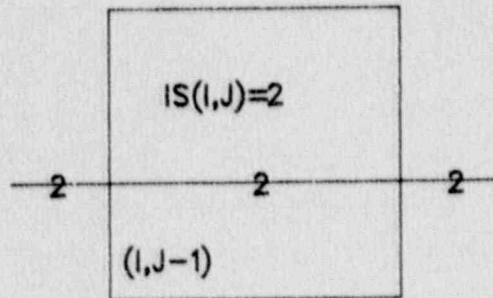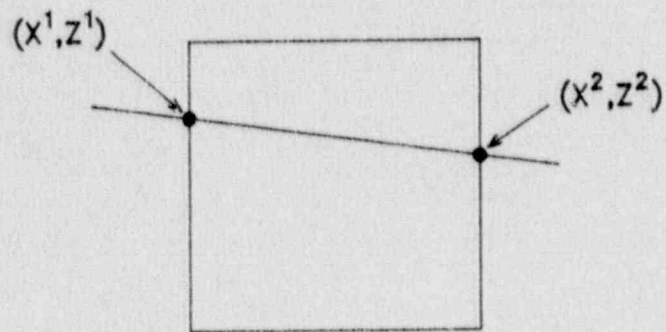
Fig. 2.11. Illustrations of (a and b) the assignment of split cell identifier indexing and (c) the points of intersections of a rectangular grid cell with an interfacial line.
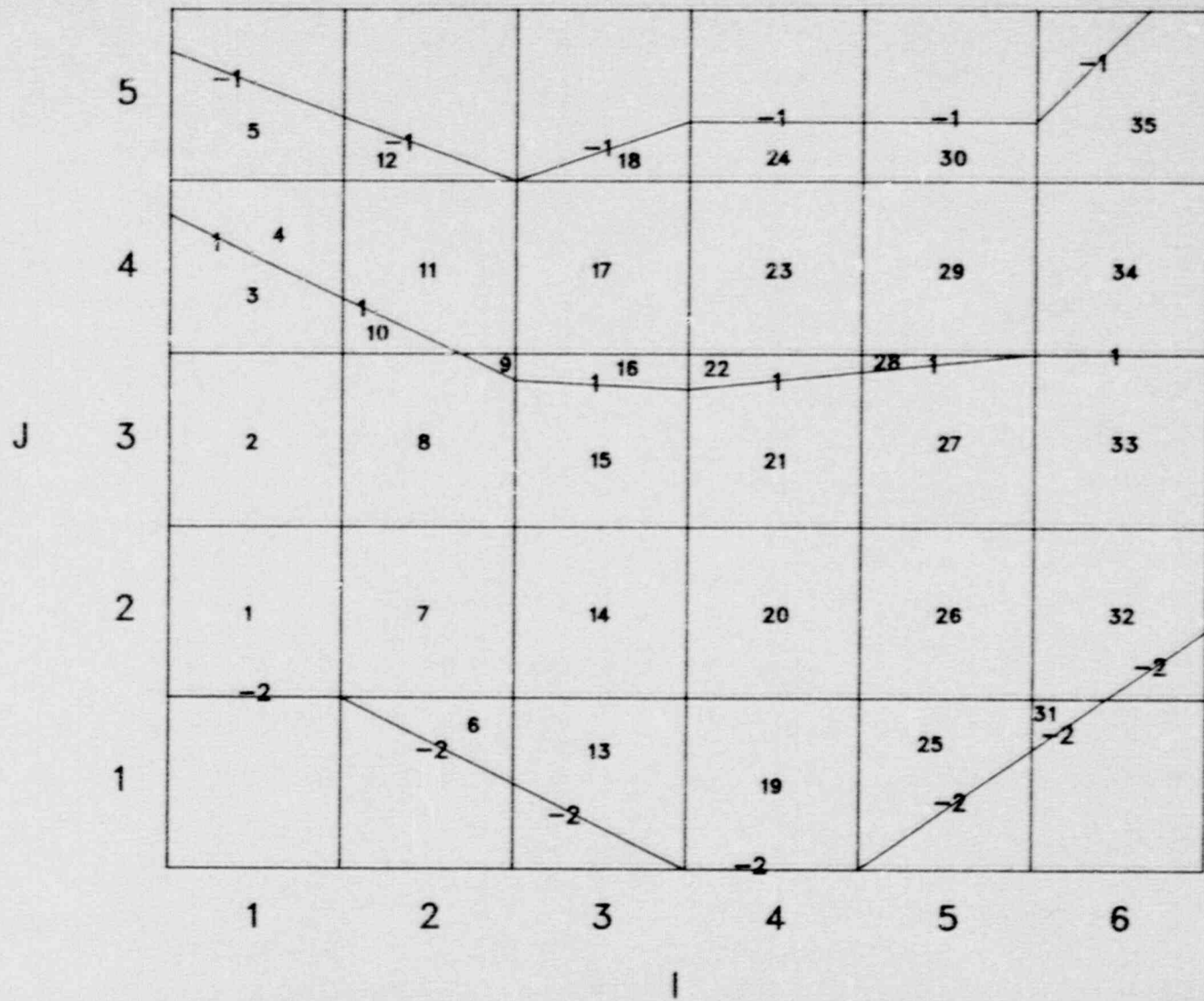
Fig. 2.12. A sample grid with node numbers assigned to computation grid cells according to the numbering convention used in the preprocessor.

the interfacial line splitting the rectangular cell. The split cell node numbering convention is discussed later in this section. Also notice that no numbers are assigned to cells below the -2 or above the -1 interfacial lines, since these cells do not lie within the computational region. Area A(NODE) and centroid coordinates XC(NODE), ZC(NODE) for each computational cell are calculated using the following formulas

$$A = \int_A dx\, dz \ , \tag{1}$$

$$XC = \frac{1}{A} \int_A x\, dx\, dz \ , \tag{2}$$

$$ZC = \frac{1}{A} \int_A z\, dx\, dz \ . \tag{3}$$

The most complex computational cell permitted by the preprocessor is a five-sided one as shown as the shaded area in Fig. 2.13a. For such a cell, the integration over an area can be separated into the integration over three areas, two rectangles, and one right triangle, as

$$\int_A dx\, dz = \int_{X_{min}}^{X_1} dx \int_{Z_{min}}^{Z_{max}} dz + \int_{X_1}^{X_{max}} dx \int_{Z_{min}}^{Z_2} dz + \int_{X_1}^{X_2} dx \int_{Z_2}^{Z_1 + \frac{Z_2 - Z_1}{X_2 - X_1}[x - X_1]} dz \tag{4}$$

Substituting Eq. (4) in Eqs. (1), (2), and (3) yields

$$A = (X_2 - X_{min})(Z_1 - Z_{min}) + \frac{1}{2}(X_2 - X_1)(Z_1 - Z_2) \tag{5}$$

$$XC = C \frac{1}{A}\left[\frac{1}{2}(Z_1 - Z_{min})(X_1^2 - X_{min}^2) + \frac{1}{2}(Z_2 - Z_{min})(X_2^2 - X_1^2) + \right. \tag{6}$$

$$\left. (Z_2 - Z_1)\left(\frac{X_1^2}{3} + \frac{X_2^2}{6} - \frac{X_1 X_2}{6}\right)\right] \ ,$$
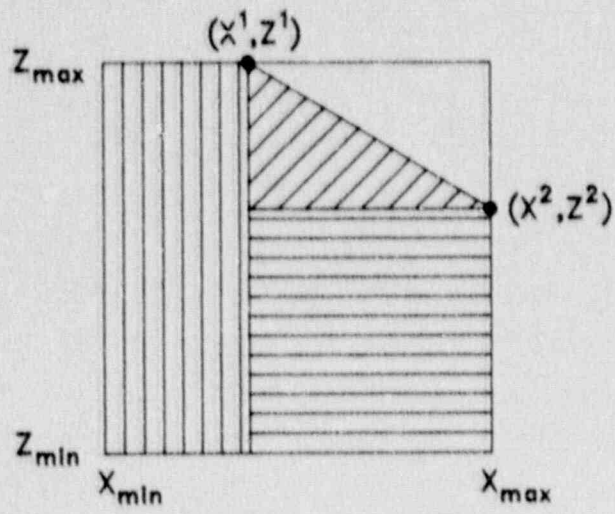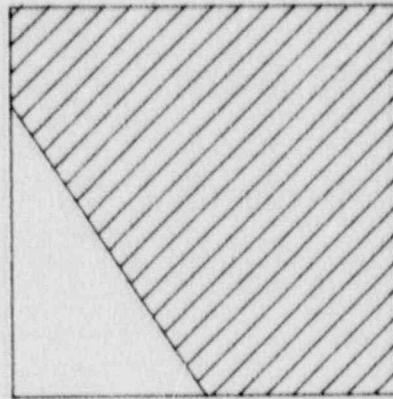
Fig. 2.13. Examples of two five-sided cells. The decomposition used in computing cell areas and centroids is shown in (a).

and

$$ZC = \frac{1}{A} \left[\frac{1}{6} (X_2 - X_1)(Z_2{}^2 + Z_1 Z_2 + Z_1{}^2 - 3Z_{min}{}^2) + \right. \tag{7}$$

$$\left. \frac{1}{2} (Z_1{}^2 - Z_{min}{}^2)(X_1 - X_{min}) \right] .$$

For other five-sided cells such as the one shown in Fig. 2.13b, formulas for areas and centroids are variations of Eqs. (4) through (7). Formulas for three and four-sided cells are degenerate cases of the formulas for five-sided cells. The value of a cell's horizontal centroid coordinate XC is not explicitly required by the MIGRAT code, although it is required by the preprocessor for determination of the cell connection input.

The determination of all the cells which have a side in common with a particular cell is a complex aspect of preprocessor computations. This is accomplished in the preprocessor by using a variation of the convention for connections among rectangular grid cells [i.e., cell (I,J) is connected to cells (I±1,J) and (I,J±1)]. For two adjacent rectangular cells, for example cell (I,J) and cell (I±1,J), two tests are made:

1. Is cell (I,J) split (IS(I,J)≠0)? and
2. Is cell (I±1,J) split (IS(I±1,J)≠0)?

This will yield one of the three possible outcomes:

1. neither cell is split,
2. both cells are split, or
3. only one cell is split.

For the first outcome the connection is simply that the node number assigned to the (I,J) cell is connected to the node number assigned to the (I±1,J) cell. Two node numbers must be associated with a rectangular cell which is split. In order to differentiate these two cells, the split rectangular cell has two assigned node numbers; NODE, which is the number associated with the lower portion of the split cell, and NOD1, which is associated with the upper portion of the split cell. To illustrate this numbering system, observe in

Fig. 2.12 that NODE equals 19 for grid cell (4,1), NODE equals 15 for cell (3,3), and NOD1 equals 16 for cell (3,3).

If only one cell (I,J) is split, then the NODE associated with cell (I±1,J) shares a cell side with either NODE of (I,J) or NOD1 of (I,J). To determine which portion of the split (I,J) cell connects with the rectangular (I±1,J) cell, a test is performed on the slope of the splitting line segment defined by the coordinate pairs $(X_1(I,J), Z_1(I,J))$ and $(X_2(I,J) \; Z_2(I,J))$. If the slope is negative (Fig. 2.14a), NOD1 of (I,J) is connected to NODE of (I±1,J), and, if the slope is positive (Fig. 2.14b), NODE of (I,J) is connected to NODE of (I±1,J). The latter case is seen in Fig. 2.12 for the grid cells (2,4) and (3,4), where NOD1 of (2,4) is 11 and NODE of (3,4) is 17. The preprocessor would determine that cell 11 must be connected to cell 17.

If both the (I,J) and (I±1,J) cells are split, a test is performed to determine if the splitting line passes continuously through both cells as in Figs. 2.15a and b. If this is the case, two connections are made: NODE of (I,J) with NODE of (I±1,J) and NOD1 of (I,J) with NOD1 of (I±1,J). An example of this situation can be seen in cells (2,3) and (3,3) of Fig. 2.12, where NODE of (2,3) (NODE=8) is connected to NODE (3,3) (NODE=15), and NOD1 of (2,3) (NOD1=9) is connected to NOD1 of (3,3) (NOD1=16). Should the splitting line not pass continuously through both cells as in Fig. 2.15c, only one connection is required, and additional slope tests are performed to determine the connection convention.

Connections over the full grid are established by vertically sweeping the rectangular grid system, starting from the lower left. For a cell (I,J), connections are made with the cells (I+1,J) and (I,J+1) in the manner outlined above. If cell (I,J) is split, the additional connection NODE of (I,J) to NOD1 of (I,J) is made. For example at grid cell (3,3) in Fig. 2.12, the following connections would be established:

    15 -> 16

    15 -> 21

    16 -> 22

    16 -> 17.

Cells below the interfacial line -2 and above the interfacial line -1 are not considered.
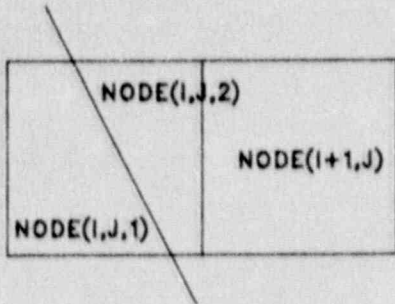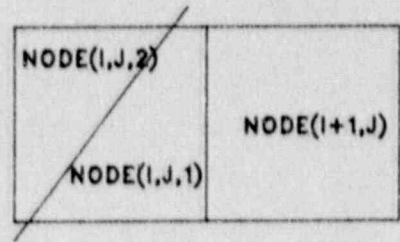
Fig. 2.14. Examples of two possible ways a split cell can connect with a non-split cell.
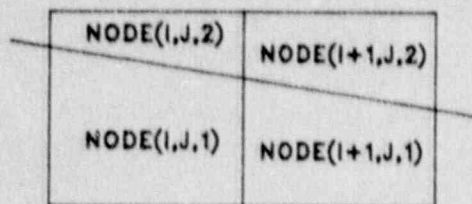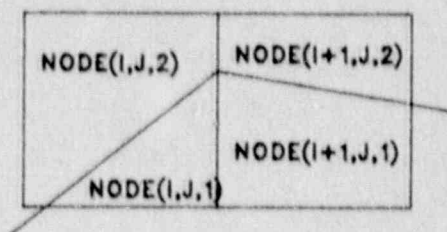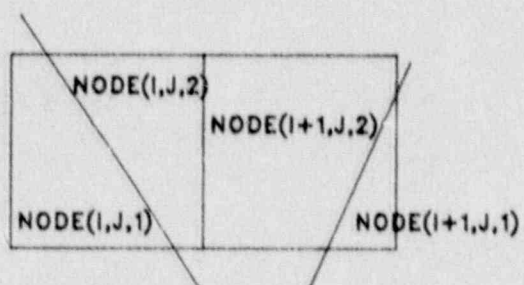
Fig. 2.15. Three samples of adjacent split cells.

The final elements of the connection data that must be generated by the preprocessor are the distances from centroids of adjacent computational cells to their common face, d_{ij} and d_{ji} (Fig. 2.2b), and the length ℓ_{ij} of the common face when projected onto a line normal to d_{ij}. This is performed using existing input data and derived geometric data for each connection determined by the method outlined above. In Fig. 2.16a, points 3 and 4 are the centroids of cells i and j, respectively. These coordinates are calculated using the algorithm described previously, and the slope of line 3-4 is determined. Points labeled 1 and 2 are defined by the rectangular grid and an interfacial line. The point labeled 5 is the intersection of the line segments 3-4 and 1-2. For each connection, the preprocessor calculates the coordinates of this point of intersection and uses this information to calculate the length of the line segment 3-5 (d_{ij}) and the length of the line segment 4-5 (d_{ji}). To determine ℓ_{ij}, the preprocessor calculates the angle θ (Fig. 2.16b) from the slopes of the line segments 1-2 and 3-4. Then, ℓ_{ij} is equal to the product of the length of the line segment 1-2 with the cosine of the angle $90° - \theta$.

The exceptions to this procedure are connections in which the line drawn between centroids of connected computational cells passes through a third cell. In such cases, a third point is introduced which lies on the common interface, and d_{ij} is the length of the line segment connecting node i and this supplemental point. Similarly, d_{ji} is the line segment connecting node j and the supplemental point. Also, in such cases, ℓ_{ij} is taken to be the length of the common side.

2.5 THE ADJUSTED GRID

The MIGRAT preprocessor has an optional feature which, if invoked, will simplify the grid by adjusting the interfacial lines to eliminate small split cells. The purpose of this feature is to allow the user to reduce the total number of computational cells, particularly small cells which can restrict the size of the computational time step. If the smaller portion of a split rectangular cell satisfies one of the following criteria selected by the user, the two points where the interfacial line intersect the rectangular grid cell are moved so as to eliminate the smaller portion of the split cell (Fig 2.17).
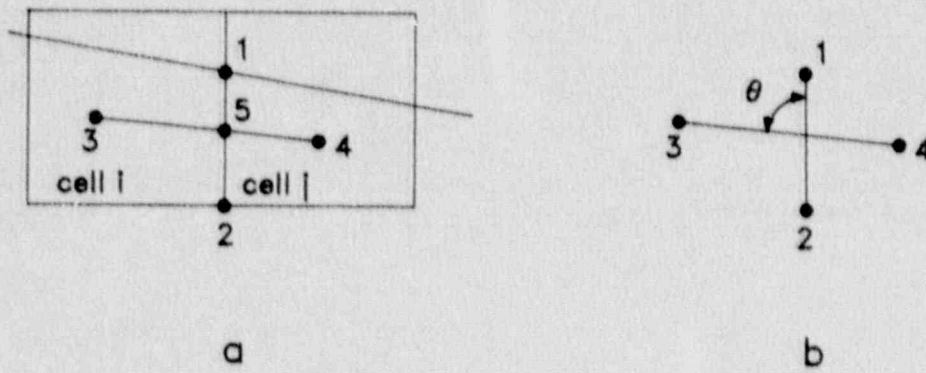
Fig. 2.16. Illustration of the use of five points in determining (a) d_{ij} and d_{ji} and (b) ℓ_{ij}.
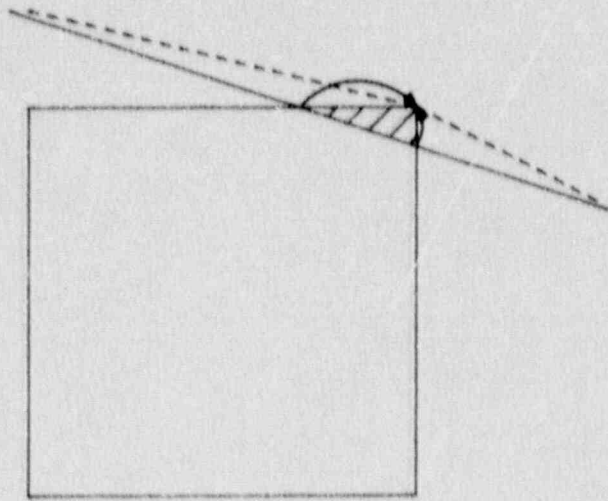
a
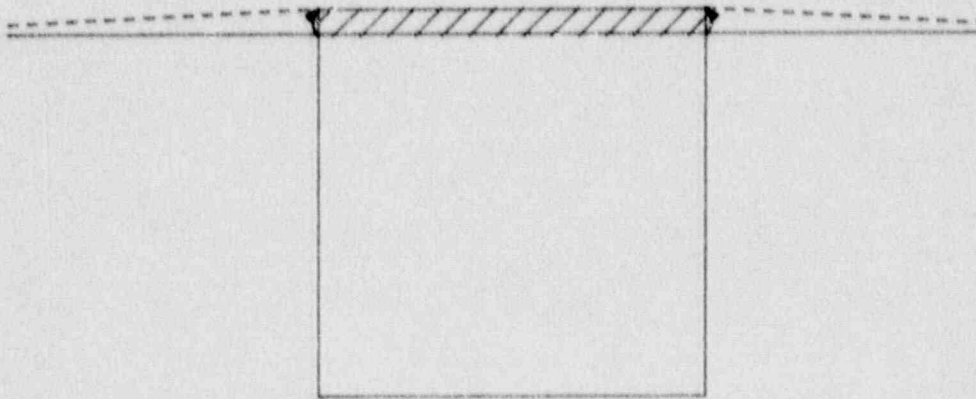
b

Fig. 2.17. Two examples of the man:ar in which the points of intersection of an interfacial line with a rectangular cell are adjusted to eliminate small split cells.

The user may select either of two bases for adjusting:

1. the area of the smaller portion of a split rectangular cell is less than a user-specified fraction of the total area of the rectangular cell in which it is contained, or

2. the area of the smaller portion of a split rectangular cell is less than a user-specified fraction of the total area of the smallest nonsplit rectangular.

Application of the first criterion with a user-specified area fraction of 0.5 will profoundly alter the grid. In this case, the grid will be altered so that all interfacial lines will either coincide with the boundary of a rectangular grid cell or bifurcate a rectangular grid cell along a diagonal. The second criterion will produce a lesser alteration of the grid, eliminating only the small split cells which can impact the time step. In either case, the maximum area fraction the user can specify is 0.5. If a value greater than 0.5 is specified, the preprocessor changes the value to one minus that value. For example, an entered value of 0.7 will result in the preprocessor using a value of 0.3.

Great care must be taken in utilizing the adjustment feature to avoid adjusting two adjacent cells which are split by different interfacial lines. This pitfall is illustrated in Fig. 2.18a and shows rectangular cell (I,J) split by interfacial line 2 and cell (I,J±1) split by interfacial line 3. Adjusting here could result in the superimposition of interfacial lines on each other (Fig. 2.18b). To avoid such situations, an additional horizontal grid line should be added as shown in Fig. 2.18c. It is important to note that the situation shown in Fig. 2.18a represents a poorly conceived grid independent of the above-mentioned adjusting problem. In order to properly represent vertical gradients within a layer, the layer must be a minimum of 3 grid cells thick. Thus, the layer defined by the region bounded by interfacial lines 2 and 3 is only two cells thick as depicted in Fig. 2.18a. This situation is corrected by adding a horizontal grid line as shown in Fig. 2.18c.
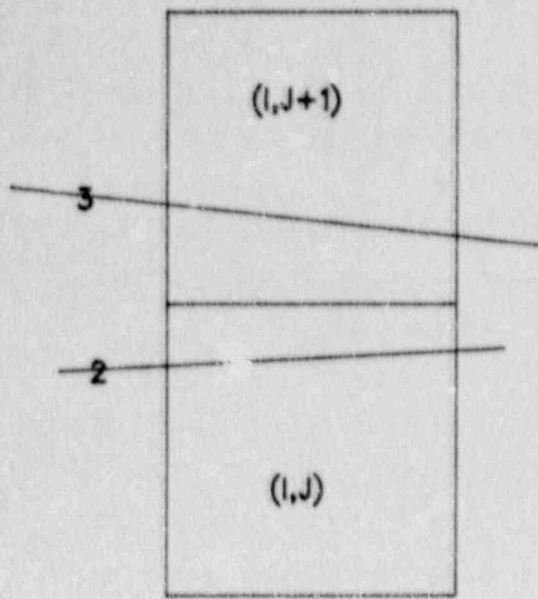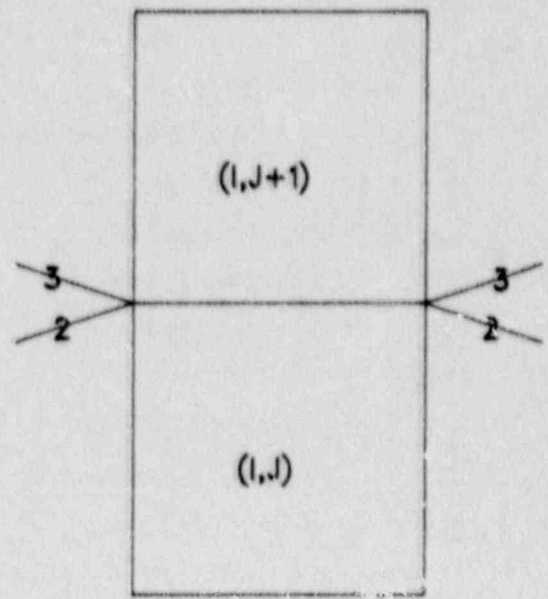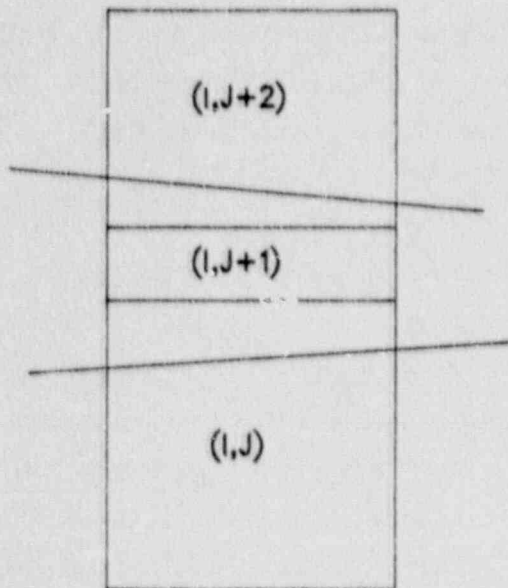
Fig. 2.18. (a) Two split and unadjusted grid cells (b) the non uniqueness which results from adjusting and (c) a three-grid cell system which can be adjusted properly.

2.6 LAYER GENERATION

The input of cell-varying attributes is simplified by defining a system of layers where each layer is selected to be a set of computational grid cells with constant attributes. This greatly reduces the magnitude of the input data that must be provided by the user; however, the preprocessor must convert from layer-based attributes to cell-based attributes to cast these data in the form required by the MIGRAT code. This is done by assigning a layer number to each computational grid cell and then assigning the user-provided attribute for a given layer to every cell having that layer number.

Layer numbers are assigned by the preprocessor by vertically sweeping the grid from bottom to top and from left to right. No layer number is assigned until the -2 (bottom) interfacial line is crossed. The layer number 1 is assigned to cells above the -2 line and below all other interfacial lines. In the vertical sweep whenever an interfacial line other than -2 is crossed, cells above that line are assigned a layer number equal to one plus the interfacial line number. The only exception to this is situations where an interfacial line is crossed for a second time in the vertical sweep. Such situations will occur whenever there are one or more imbedded layers, such as layers 4 and 5 in Fig. 2.1. To properly accommodate these features, the preprocessor will decrement the layer number to the previous layer number whenever an interfacial line is crossed a second time. The user is cautioned that the preprocessor only stores the current layer number and the two preceding layer numbers. This means that three nested, embedded layers cannot be correctly numbered by the preprocessor software.

2.7 LAYER-BASED ATTRIBUTES

The MIGRAT preprocessor allows the user to input the following attributes for each layer:
1. a material name and identifier number,
2. initial level of saturation,
3. initial concentrations of two contaminants,
4. external connections (including hydraulic boundary conditions),
5. contaminant concentration boundary conditions.

The first user-specified attribute is the material name (i.e., sandstone, clay) of which each layer is composed. A unique identifier number for each material is added by the preprocessor for each computational cell in that layer. Each material name (and number) corresponds to material properties such as saturation and conductivity which may be a function of pressure, void fraction, etc.

The MIGRAT code requires that the initial head, Φ, be specified for each computational grid cell. Since this is not, in general, an attribute which will be constant within a layer, the user is asked to specify the initial level of saturation for each layer. The preprocessor calculates the appropriate Φ value for each cell in the layer, based on the selected saturation value. The user is offered three options in selecting initial saturations:

1. Fully saturated - the layer is assumed to be an unconfined aquifer. The value of Φ for every cell in a given column within the layer is set equal to the mean value of the elevation of the upper boundary of the layer for that column. Thus, the upper boundary of the layer is taken as the top of the unconfined aquifer.

2. Equilibrium - the layer is in equilibrium with an underlying unconfined aquifer. In this case the value of Φ for every cell in a given column of the layer is set equal to the mean value of the water table elevation underlying the layer in that column,

3. Arbitrary - the layer is at an arbitrary level of saturation. The user enters any level of saturation for the layer. Using this input value, the preprocessor first converts to a value of pressure, , by interpolation from the user-input saturation vs pressure curve for the appropriate material. A value of Φ is then calculated for each cell in the layer using the relationship

$$\Phi_i = \psi + ZC ,$$

where ZC is the elevation of the cell centroid.

Any layer can have a constant non-zero initial concentration of one or two contaminants. For any layer in which an initial contaminant concentration is specified, the user will be prompted to specify whether or not this layer is a contaminant source. If the response is affirmative, a flag will be set for every cell in this layer, which will result in the

contaminant concentrations in that layer remaining constant in time. Thus, this layer would become a perpetual source of both contaminants at the specified initial conditions.

The MIGRAT code treats permeable boundary cells by connecting each such cell to an imaginary external cell. As input for boundary conditions, MIGRAT requires a specified fixed value for the head at each imaginary external node, a length through which each boundary cell is connected to an external cell, and the conductance between each permeable boundary cell and the associated external cell. Constant head conditions are created by fixing the head of the external cell at the desired head condition and specifying a large value for the conductance. Constant flux conditions are imposed by using a small conductance and adjusting the head so that the product of the conductance, the head, and the connection length is equal to the desired flux.

The MIGRAT preprocessor allows any portion of the left, right, or top boundaries to be permeable. The user specifies the layer which is open, the boundary which is open, and whether constant head or constant flux conditions will be imposed. The preprocessor finds the node numbers of all the cells of the specified layer which are adjacent to the selected boundary. The preprocessor also calculates the length of the side of each boundary cell which lies on the permeable boundary. The boundary conditions make use of the relationship

$$\text{Flux} = \rho \, \text{*HSURE*L*}\Phi_b, \tag{8}$$

where ρ is the density of water, HSURE is the coefficient of conductance, L is the boundary length of the cell, and Φ_b is the boundary head. For constant head conditions, the user specifies the value of Φ_b, and a value for HSURE is set by the preprocessor for each boundary cell as $100/\rho\text{*Lmin}$, where Lmin is the minimum cell boundary length within the particular layer. This yields a conductance ($\rho\text{*HSURE*L}$) which is greater than or equal to 100.

For constant flux conditions, the user provides the total flux into the specified layer. This flux is partitioned into the boundary cells in proportion to the lengths of the boundary sides of the boundary cells. The preprocessor sets HSURE equal to $10^{-5}/(\rho\text{*Lmax})$ where Lmax is the maximum cell boundary side length. This provides a conductance which is less than or equal to 10^{-5}. The boundary potential Φ_b is computed to satisfy Eq. (8)

using the user-specified flux and the established value of HSURE according to

$$Flux = \rho \; *HSURE* \Phi_b \sum L,$$
$$\text{all boundary cells,}$$

where the summation over L represents the total boundary length.

The preprocessor also allows the user to identify any of the layers as drains. Drains are treated in a fashion similar to a constant head boundary. Each cell in a drain layer is connected to an external cell at a potential equal to the elevation of the centroid of the drain cell. The connection occurs through an area equal to the area of the cell. Each external node connected to a drain cell is assigned an external node identification number greater than or equal to 9000. The external node number is checked in the MIGRAT code. If the flux between the drain cell and the external node is positive (into the drain cell), the flux is set to zero. Thus, any movement of moisture and contaminants in the drain region is constrained to be only out of the computational grid.

The remainder of the input to the preprocessor involves constants and coordinate pairs which represent functional forms of material and contaminant properties. No manipulations are performed by the preprocessor for these parameters. They are requested of the user through a sequence of prompts and then formatted in accordance with the MIGRAT input data formats.

3. DESCRIPTION OF MIGRAT INPUT DATA

Input data parameters and formats for the MIGRAT code are presented here. Data entry for this code is a slightly modified version of the TRUST code as required to accommodate the entry of data associated with the additional contaminant transport coding. Input data parameter descriptions and formats are presented here in a manner similar to that provided in the TRUST documentation (Ref. 1). For input parameters which are unchanged from TRUST or unaffected by the MIGRAT preprocessor only an abbreviated parameter description is provided. For more detail the reader is referred to Section 5 of the TRUST documentation. In some cases, either a subset of a block or an entire block is unaltered form TRUST and cannot be generated by the pre-processor. Where encountered, these cases are identified and no description of input data is provided. In such cases, the reader is referred to Sect. 5 of the TRUST documentation for details.

Every input parameter identified below is categorized by one or more superscripts. The superscript indicates that the parameter is one not found in the TRUST code. The * alone indicates that the parameter is unaffected by the preprocessor and that the value of the parameter is requested by the preprocessor and output to the block data set unaltered. The additional + superscript indicates that the input parameter is influenced by the use of the preprocessor. For example, the parameter may be internally generated by the preprocessor, not needed when using the preprocessor, or cannot be input through the preprocessor.

For each card, the column numbers, the variable name, and a brief description are given below.

Block 1 - Problem Controls, Limits, and Constants

Card 1	Format (9I5,5X, 2E10.3)	
1-5	IPRINT*	No. of time steps between printed output.
6-10	NUM*	No. of node to be monitored.
11-15	KDATA*	Output control parameter.
16-20	KSPEC*	Control parameter for computation scheme.
21-25	MCYC*	Maximum number of time steps.
26-30	MSEC*	Maximum machine time.

31 35	NPUNCH*,+	Control parameter for final output. Set to 1 by the preprocessor to create a plotting or restart file for transfer to the PC.
36-40	NDOT*	If non-zero, time derivatives set to 0.
41-45	KSTDAT*	Control parameter for volume strain output.
51-60	TIMEP*	Time interval between data printout.
61-70	SCALE*,+	Scale factor for problem length scales. Set to 1 by preprocessor, user may change by editing completed Block file.

Card 2 Format (I5, 5X, 7E10.3)

1-5	KD*,+	Symmetry Indicator. Set to 1 by preprocessor. Preprocessor cannot be used for axisymmetric or centrisymmetric geometries.
11-20	DELTO*	Maximum time step.
21-30	SMALL*	Minimum allowed time step.
31-40	PSIVARY*	Maximum potential change per time step.
41-50	TAU*	Initial problem time.
51-60	TIMAX*	Maximum allowable problem time.
61-70	PSIMIN*	Minimum allowable pressure head.
71-80	PSIMAX*	Maximum allowable pressure head.

Card 3 Format (8E10.3)

1-10	PHIONE*,+	Initial potential for all nodes not specified in Block 9. The preprocessor generated a Block 9 file with initial conditions for all nodes; consequently, this is not needed when using preprocessor.
11-20	GONE*,+	Constant source or sink rate for all nodes not specified in Block 9. Sources and sinks cannot be entered through the preprocessor. User may enter GONE by editing completed Block 1 file.
21-30	HONE*,+	Fluid mass transfer coefficient for all external connections not specified in Block 6. The preprocessor generates a complete Block 6 file;

		consequently, this is not needed when using preprocessor.
31-40	PCONE*,+	Preconsolidation stresses for nodes not specified in Block 9. Preconsolidation stresses cannot be entered via the preprocessor. User may enter PCONE by editing completed Block 1 file.

Block 2 - System and Material Properties

Card 1

1-4		Word "SYST" written by preprocessor.

Card 2 Format (A4, 6X, 6E10.3)

1-4	APATH*	Select either "WET" for wetting regime or "DRY" for drying regime. Blank for fully saturated conditions.
11-20	THICK*,+	Thickness of flow regime. Generated by preprocessor.
21-30	RD*	Specific gravity of saturated soil.
31-40	XF*,+	Fracture length, set to default value by preprocessor. Flow rate from well. Cannot be entered via preprocessor. If required user may enter by editing completed Block 2 file.
51-60	ALAM(1)	Decay constant time for contaminant 1. Derived from user-entered half-life in preprocessor.
61-70	ALAM(2)	Decay constant time for contaminant 2. Derived from user-entered half-line in preprocessor.

Card 3 Format (A4, 1X, 5I5, 5E10.3)

1-4	AMAT*	Material name.
6-10	MAT*,+	Material identification number. Generated by preprocessor.
11-15	LTABC*,+	Number of tabulated values of saturated; >0 vs pressure, <0 vs time, = 100 uses analytic relationship, = 0 for constant value. Preprocessor generated LTABC assuming it is greater

		than zero. For LTABC < 0 user may edit completed Block 2 file.
16-20	LTTABSC*,+	Number of scanning curves for saturation vs pressure. Set to zero by the preprocessor. User may enter by editing completed Block 2 file.
21-25	LTABK*,+	Number to tabulated values of permeability; >0 vs pressure, <0 vs time, = 100 uses analytical relationship. Preprocessor generates LTABK assuming it is positive. For negative user may edit completed Block 2 file.
26-30	LTABSK*,+	Number of scanning curves for permeability vs pressure. Set to zero by preprocessor. User may enter by editing completed Block 2 file.
31-40	AV*	Coefficient of compressibility.
41-50	EZ*	Reference void ratio.
51-60	PZ*	Reference effective stress.
61-70	CONT*	Constant permeability, only used for LTABK = 0.
71-80	SS *	Specific storage.

Card 4		This card is used for entering parameters associated with compression index and functional void ratios. Cannot be entered via preprocessor. User may enter by editing completed Block 2 file.

Card 5		Format (8E10.3) Assuming LTABC $\geq$ 2 and $\leq$100.
1-10	PSIVRC(1)*	Tabulated values of pressure head in ascending order
11-20	PSIVRC(2)*	vs saturation. Ordering is performed by the
o		preprocessor.
o		
o		

plus additional cards as needed.

Card 6		Format (8E10.3)
1-10	SW(1)*,+	Wetting saturation, SW, and drying saturation, SD,
11-20	SD(1)*,+	corresponding to pressure head values entered in

21-30	SW(2)*,+	previous card. The preprocessor does not allow
31-40	SD(2)*,+	hysteresis, so only a single curve is entered with
o		SW set equal to SD by the preprocessor. To include
o		hysteresis, the user may edit the completed Block 2
o		file.

plus additional cards as needed.

Card 7   This card is used only to enter saturation scanning curves. Since the preprocessor does not accommodate hysteresis, scanning curves, if desired, must be entered by editing a completed Block 2 file.

Card 8   Format (8E10.3)

1-10	PSIVRK(1)*	Tabulated values of pressure head in ascending order
11-20	PSIVRK(2)*	vs permeability. Ordering is performed by the
o		preprocessor.

plus additional cards as needed.

Card 9   Format (8E10.3)

1-10	CONTW(1)*,+	Wetting conductivity, CONTW, and drying conductivity,
11-20	CONTD(1)*,+	CONTD, corresponding to pressure had values
21-30	CONTW(2)*,+	entered in previous card. The preprocessor does
31-40	CONTD(2)*,+	not allow hysteresis, so only a single curve is
o		entered with CONTD set equal to CONTW by the
o		preprocessor. To include hysteresis, the user may
o		edit the completed Block 2 file.

plus additional cards as needed.

Card 10   This card is used only to enter conductivity scanning curves. Since the preprocessor does not allow hysteresis, scanning curves, if desired, must be entered by editing the completed Block 2 file.

Cards 11 and 12   These cards are used only if data related to deformation of the unsaturated zone is to be input. These data cannot be

entered via the preprocessor. If desired, it can be
entered by editing the completed Block 2 file.

Card 13	Format (E10.3)	
1-10	DFUS	Diffusivity of material.

Card 14	Format (I5)	
1-5	LTAB	Number of tabulated values of retardation vs concentration.

Card 15	Format (8E10.3)	
1-10	ABDSI(1)	Values of concentration corresponding to tabulated
11-20	ABDSI(2)	points on the concentration vs retardation curve.
o		
o		
o		
	RD1(1)	Values of retardation of contaminant 1
	RD1(2)	corresponding to concentration values entered
	o	above.
	o	
	o	
	RD2(1)	Values of retardation of contaminant 2
	RD2(2)	corresponding to concentration values entered
	o	
	o	
	o	

plus additional cards as needed.

Block 3 - Properties of the Fluid

Card 1	Format (10A1, 4E10.3)	
1-10	AFLUID*	Name of fluid.
11-20	VISC*	Coefficient of viscosity.
21-30	BETA*	Compressibility of fluid.

31-40	RHOZ*	Density at atmospheric pressure.
41-50	GEE*	Gravitational constant.

Block 4 - Node Descriptions

Card 1 etc. (1 card per node) Format (I1, I4, I2, 2I2, 3E10.3, 4F9.0)

1	NTCONC	=0 if cell is perpetual source of contamination, =1 otherwise.
2-5	NODE*,+	Node identification number. Generated by preprocessor.
6-7	NSEQ*,+	Number of identical sequential nodes. Not used with preprocessor.
8-10	NADD*,+	Incremental value of NODE used with NSEQ. Not used with preprocessor.
11-12	NODMAT*,+	Material identification number. Generated by preprocessor.
13-14	KS*,+	Node type indicator not entered via preprocessor. Only used when KSPEC (Block 1) is negative. User may enter KS by editing the completed Block 4 file.
15-24	DLONG*,+	Volume of cell (assuming two-dimensional cell). Generated by preprocessor.
25-34	DWIDE*,+	Width of cell (assuming three-dimensional cell). Set to 1 by preprocessor.
35-44	DRAD	Used with KD (Block 1 = 2,3. Set to 1 by preprocessor since preprocessor requires KD = 1.
45-53	X	X-coordinate of cell centroid. (Only needed if contouring is performed with MIGRAT code.)
54-62	Y	Y-coordinate of cell centroid (only needed if contouring is performed within MIGRAT code.) Irrelevant in one- or two-dimensional (vertical cross section) problems. Set to 0 by preprocessor.
63-70	DELZ*,+	Increment in node elevations used in conjection NSEQ. Not needed with preprocessor.
71-80	Z*,+	Elevation of node. Generated by preprocessor.

Block 5 - Internal Connections

Card 1 etc. (1 card per connection) Format (2I5, 3I3, I1, 6E101.3)

1-5	NOD1*,+	Identification numbers of the connected nodes.
6-10	NOD2*,+	Generated by the preprocessor.
11-13	NSEQ*,+	Number of identical connections. Not needed with preprocessor.
14-16	NAD1*,+	Incremental values of NOD1 and NOD2 used with NSEQ.
17-19	NAD2*,+	Not needed with preprocessor.
20	NZ*,+	Scale factor which scales NAD1 and NAD2 by 10NZ. Not needed with preprocessor.
21-30	DEL1*,+	Length along line between NOD1, NOD2 from NOD1 (NOD2)
31-40	DEL2*,+	to common cell side. Generated by preprocessor.
41-50	DLONG*,+	Projection of length of cell side common to NOD1, NOD2. Generated by preprocessor.
51-60	DRAD*,+	Used with KD (Block 1) = 2,3. Set to 1 by preprocessor since preprocessor requires KD = 1.
61-70	TSCON1	Used when entering NTCONC(NOD1) = 1 and NTCONC(NOD2) = 0
71-80	TSCON2	or NTCONC(NOD1) = 0 and NTCONC(NOD2) = 1 (Block 4). TSCON1 and TSCON2 are the concentrations of contaminants 1 and 2, respectively, in the cell for which NTCONC = 0. Generated by preprocessor.

Block 6 External Fluid Flow Connections

Card 1	Format	(6I5, 2E10.3, 10A1, 2E10.3)
1-5	NODS*,+	Surface node identification number. Generated by preprocessor.
6-10	NODB*,+	Boundary node identification number. Generated by preprocessor.
11-15	NSEQ*,+	Number of identical connections. Not needed with preprocessor.
16-20	NADS*,+	Increments in NODS and NODB, respectively.
21-25	NADSB*,+	Not needed with preprocessor.

26-30	LTABH*,+	Number of tabulated values of surface fluid transfer coefficient. Cannot be entered via preprocessor. User may enter by editing the completed Block 6 file.
31-40	DLONG*,+	Length over which NODS is connected to NODB. Generated by preprocessor.
41-50	DRAD*,+	Used with KD(Block 1) = 2,3. Set to 1 by preprocessor since preprocessor requires KD = 1.
51-60	HSURE*,+	Constant surface fluid transfer coefficient. Generated by preprocessor.
61-70	TBCON1	Boundary concentrations of contaminants 1 and 2,
71-80	TBCON2	respectively. Generated by preprocessor.

Card 2   This card is used to enter surface fluid transfer coefficients as a function of potential or time. Only used when LTABH = 0. Cannot be entered via preprocessor.

Block 7 - Boundary Nodes and External Potentials

Card 1   Format (2I5, 7E10.3)

1-5	NODB*,+	Boundary node identification number. Generated by preprocessor.
6-10	LTABPHI*,+	Number of tabulated values of external or boundary potential. Cannot be entered via preprocessor.
11-20	ZB*,+	Elevation of boundary node. Set to Z(NODS) (Block 6) by the preprocessor. If a different value is required, the use may edit the completed Block 7 file.
21-30	PHIB*,+	External potentials. Three values may be entered
41-50		for either time-varying or sinusoidal conditions.
61-70		The preprocessor assumes constant boundary conditions or external potentials so that only a single value is used. With preprocessor, PHIB is only user specified for constant head conditions. For constant flux

conditions, the user enters the desired flux and the
preprocessor computes the appropriate PHIB value.

31-40	TIMEB*,+	Times corresponding to PHIB for transient or
51-60		sinusoidal conditions. Not used with the
71-80		preprocessor.

Block 8 - Internal Fluid Generation Variables

This block cannot be entered via the preprocessor. The user may create
a Block 8 file and insert it into the completed input data set generated
by the preprocessor.

Card 1	Format	(4I5, 4E10.3)
1-5	NODG*	Node identification number.
6-10	NSEQ*	Number of identical sequential nodes.
11-15	NADG*	Increment in node numbers used with NSEQ.
16-20	LTABG*	Number of tabulated values of fluid generation.
		LTABG > 0 for function of potential, LTABG < 0 for
		function of time.
21-30	GT(1)*	Volumetric fluid generation rate.
31-40	TVARG(1)*	Potential or time corresponding to GT(1).
41-50	GCONC1	Concentrations of contaminants 1 and 2,
51-60	GCONC2	respectively, for positive fluid generation
		(injection).

Card 2	Format (8E10.3)	
1-10	GT(2)*	Additional values of GT and TVARG, as appropriate.
11-20	GT(3)*	Uses as many cards as necessary.
21-30	GT(4)*	
31-40	GT(5)*	
41-50	TVARG(2)*	
51-60	TVARG(3)*	
61-70	TVARG(4)*	
71-80	TVARG(5)*	

Note: Format of Card 1 has changed to accommodate input of GCONC1, GCONC2.

Block 9 - Initial Conditions

Card 1	Format (3I5, 5X, 5F12.0)	
1-5	NOTE *,+	Node identification number. Generated by preprocessor.
6-10	NSEQ*,+	Number of additional nodes with identical initial conditions. Not needed with preprocessor.
11-15	NADD*,+	Increment in node numbers used with NSEQ. Not needed with preprocessor.
21-32	PPHI*,+	Initial potential. Generated by preprocessor.
33-44	GG*,+	Fluid generation rate. Cannot be entered via preprocessor. If desired, user may enter by editing the completed Block 9 file.
45-56	PC*,+	Initial preconsolidation stress. Cannot be entered via preprocessor. If desired, user may enter by editing the completed Block 9 file.
57-68	CONC1	Initial concentrations of contaminants 1 and 2,
69-80	CONC2	respectively. Generated by preprocessor.

plus additional cards as needed.

Block 10 - Printout of Dimensionless Well Variables

This block cannot be entered via the preprocessor. The user may create a Block 10 file and add it to the input data set generated by the preprocessor.

4. EXECUTION OF THE MIGRAT PREPROCESSOR

This section describes and illustrates the step sequence on the IBM-XT
needed to create the input data for the MIGRAT computer code. The steps must
be executed sequentially because each step uses input data from the previous
step and creates input for the next step. A visual check after most steps
can be made to ensure the validity of the step. The source language for all
steps is FORTRAN 77.[1] The graphics are accomplished by using DISSPLA/PC[2] on
an IBM color graphics or compatible monitor. The graphics monitor must have
an Enhanced Graphics Adapter, Professional Graphics Adapter, or Color
Graphics Adapter. Because there are many steps that are necessary to
generate the data for MIGRAT, three menus (DOS batch files) have been created
to ease the user progression through the steps. These are called grid1.bat,
grid2.bat, and grid3.bat. To demonstrate the use of the preprocessor, this
section details the entry of data via the preprocessor for the sample problem
shown in Fig. 4.1. A description of each step and the associated entry of
data for the sample problem are given below.

4.1 GRID1

The grid1 batch file drives the first nine steps of the preprocessor.
Table 4.1 contains the listing of the grid1 menu. Option 0 returns the user
to DOS and is not part of the preprocessor programs. Table 4.2 lists the
grid1 batch file, grid1.bat. Typing grid1 and a carriage return calls up the
menu (see Table 4.1). The user selects an option by entering any one-digit
number from zero to nine. (Note: Menu selections do not need to be followed
by a carriage return. Also, a "Return to DOS" option is necessary because
the user would have to reboot the PC to escape from the menu programs.) The
following is a description of the nine options in the grid1 menu.

---

[1]Microsoft FORTRAN version 4.0 or higher, Microsoft Corp., Box 97017,
Redmond, WA 98073-9717.

[2]DISSPLA/PC, Integrated Software Systems Corp., 10505 Sorrento Valley
Road, San Diego, CA 92121-1698.
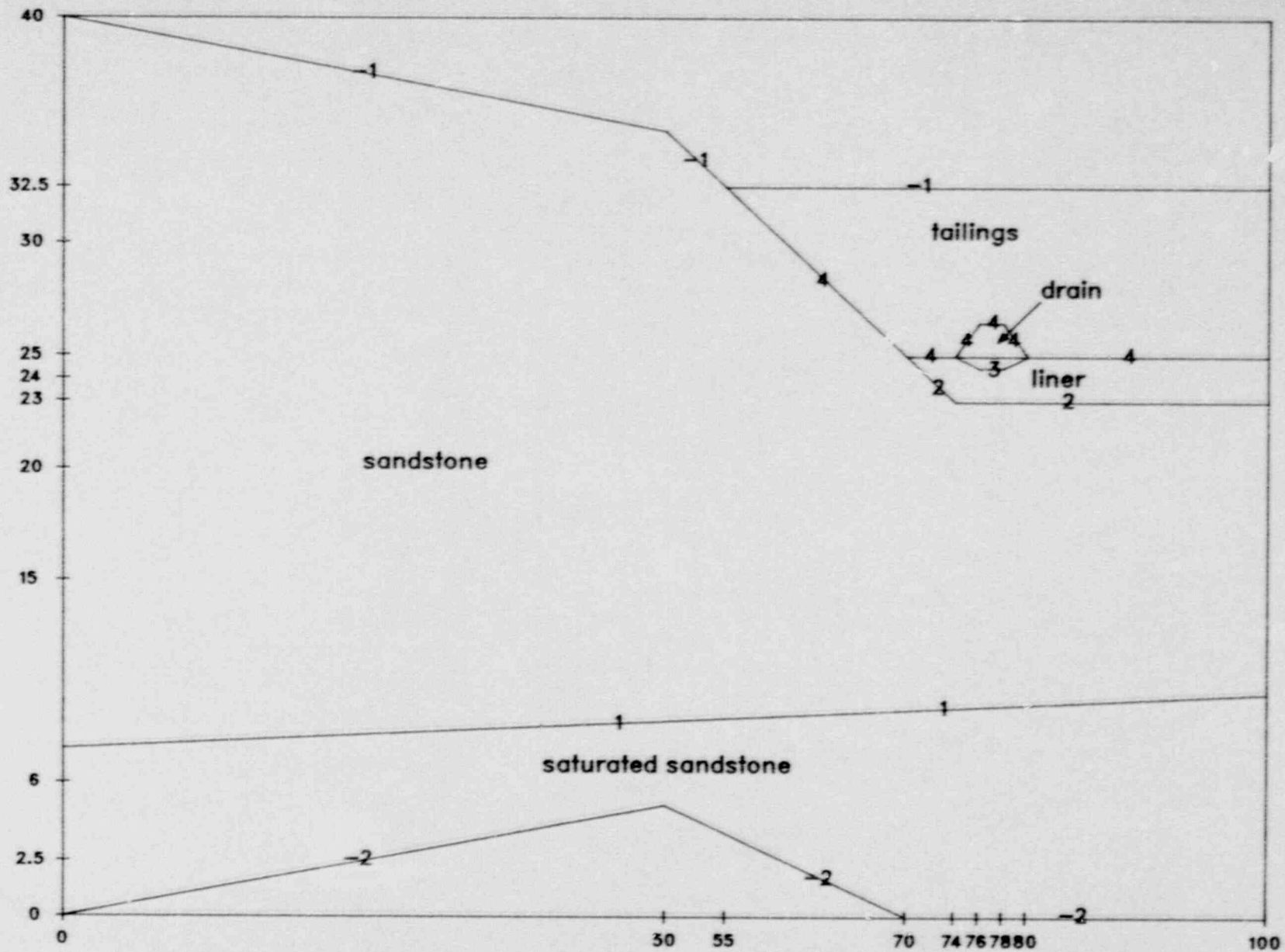
Fig. 4.1. Schematic of the sample problem. The locations of the horizontal and vertical grid lines are indicated by the tick marks on the left and bottom, respectively.

Table 4.1.   MIGRAT Preprocessor (grid1) Menu

```
          ====>     MIGRAT Preprocessor    <====

Note:  Do not strike carriage return for menu selection!

    0 - Exit to DOS .....................................

    1 - Create Site Name File for the MIGRAT Case .......

    2 - Create the Initial Grid Lines (STEP1) ...........

    3 - Plot the Initial Grid ...........................

    4 - Adjust the Initial Grid (STEP2 - necessary) .....

    5 - Determine Layers (STEP3) ........................

    6 - Plot the Layer Map ..............................

    7 - Assign Material Indices to Layers (STEP4) .......

    8 - Plot Material Map ...............................

    9 - Determine Centroid Locations - NODES (STEP5) ....
```

Table 4.2.   Listing of the file gridl.bat

```
:menu
echo off
assign
cls
type gridl.txt
getdigit                          Press key for desired option:
cls
echo working....
if errorlevel 9 goto step5
if errorlevel 8 goto plom
if errorlevel 7 goto step4
if errorlevel 6 goto ploll
if errorlevel 5 goto step3
if errorlevel 4 goto adjust
if errorlevel 3 goto plogri
if errorlevel 2 goto stepl
if errorlevel 1 goto maknam
if errorlevel 0 goto exit
:badopt
echo Invalid option
pause
goto exit
:step1
step1
goto menu
:plogri
plogri /r 2000
goto menu
:adjust
step2
goto menu
:step3
step3
goto menu
:ploll
ploll /r 2000
goto menu
:step4
step4
goto menu
:plom
plom /r 2000
goto menu
:step5
step5
goto menu
:plocen
plocen /r 2000
goto menu
:maknam
maknam
goto menu
:exit
cls
ver
cd
```

Option 1 assigns a case identifier that appears on all later plots. Table 4.3 shows a sample interactive session using this option. Ten characters or two consecutive blank spaces, whichever comes first, mark the end of the case-identifying string. The result of Option 1 (MAKNAM.EXE) is a one-record file, sitnam.dat.

Option 2 uses the executable program STEP1.EXE to enter data which define the computational grid. Two data sets are created in this step which are required for subsequent steps. STEP1 must be executed prior to STEP2, a later step in the sequence. The user responds to a set of inquiries concerning the grid layout and interface curves. Table 4.4 is a listing of a sample interactive session with Option 1.

There are several constraints in STEP1. First, the maximum number of grid lines in each direction is 26. The source code can easily be modified to change this constraint, however. A second and third constraint are strictly unchangeable. The second constraint is that all interface lines must end on an X(vertical)-grid line. The third rule is that no grid cell can be cut by more than one interface line. If an interface line lies on a horizontal (Z)-grid line, that line belongs to the grid cell above it, and no other line can cut that cell. If more than one line cuts a grid cell, it is imperative that the interface line is changed or another grid line is added so that no grid cell is cut more than once. The two data sets created during STEP1 are named MIGSAV.GRD and INTERF.CON. MIGSAV.GRD contains the coordinates for all grid lines and the endpoints for all interface lines. The data set INTERF.CON contains the interface line endpoints grid cell by grid cell. Because there is always the possibility that problems may exist in the grid data entered during STEP1, a safeguard has been added to preserve an interactive session and to later make corrections or changes in the grid. When running STEP1, the user can enter the interactive mode in which he enters his data at the keyboard, or he can enter the batch mode, which uses MIGRAT.BAT (created during the interactive mode of STEP1) as data. The sample grid in Fig. 4.1 shows a problem that may occur when a grid is created; the numerous lines in the 24 to 25 vertical range might cause Step 1 processes to operate as if some of the cells were split more than once. By editing MIGRAT.BAT with the two changes noted (see Table 4.5), rerunning STEP1 through the batch mode, and selecting Option 3—and for all later

Table 4.3. Listing of the interactive session for the input of
the case name - Option 1 (grid1)

maknam (0)
Enter the site identifier (10 char. or less) for the MIGRAT pre-processor.
        Note: 2 consecutive blanks end the identifier.

Site1
Site Identifier = Site1   Is this correct?
        N means reenter.

N
Enter the site identifier (10 char. or less) for the MIGRAT pre-processor.
        Note: 2 consecutive blanks end the identifier.

Site Identifier = Site 1   Is this correct?
        N means reenter.

Stop - Program terminated.

. Creates file sitnam.dat

Table 4.4. Listing of the interactive session for the input of
grid data - Option 2 (gridl)

Enter IN; 0 means interactive, 8 means batch
0
Enter the number of grid cells in the X-dir.
8
The number of cells in the X-dir. (NX)=008
Is the entry correct? N means reenter the data

Enter the number of grid cells in the Y-dir.
10
The number of cells in the Y-dir. (NY) =010
Is the entry correct? N means reenter the data

Enter the X coordinate for grid line #001
0
Grid Line #001 has X =   .000
Is the entry correct? N means reenter the data

Enter the X coordinate for grid line #002
50
Grid Line #002 has X =   50.000
Is the entry correct? N means reenter the data

Enter the X coordinate for grid line #003
55
Grid Line #003 has X =   55.000
Is the entry correct? N means reenter the data

Enter the X coordinate for grid line #004
70
Grid Line #004 has X =   70.000
Is the entry correct? N means reenter the data

Enter the X coordinate for grid line #005
74
Grid Line #005 has X =   74.000
Is the entry correct? N means reenter the data

Enter the X coordinate for grid line #006
76
Grid Line #006 has X =   76.000
Is the entry correct? N means reenter the data

Enter the X coordinate for grid line #007
78

Table 4.4 (continued)

```
Grid Line #007 has X =    78.000
Is the entry correct?  N means reenter the data

Enter the X coordinate for grid line #008
80
Grid Line #008 has X =    80.000
Is the entry correct?  N means reenter the data

Enter the X coordinate for grid line #009
100
Grid Line #009 has X =   100.000
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #001
0
Grid Line #001 has Y =      .000
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #002
2,5
Grid Line #002 has Y =     2.000
Is the entry correct?  N means reenter the data
n
Enter the Y Coord. for grid line #002
2.5
Grid Line #002 has Y =     2.500
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #003
6
Grid Line #003 has Y =     6.000
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #004
15
Grid Line #004 has Y =    15.000
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #005
20
Grid Line #005 has Y =    20.000
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #006
23
```

Table 4.4 (continued)

```
Grid Line #006 has Y =    23.000
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #007
24
Grid Line #007 has Y =    24.000
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #008
25
Grid Line #008 has Y =    25.000
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #009
30
Grid Line #009 has Y =    30.000
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #010
32.5
Grid Line #010 has Y =    32.500
Is the entry correct?  N means reenter the data

Enter the Y Coord. for grid line #011
40
Grid Line #011 has Y =    40.000
Is the entry correct?  N means reenter the data

Enter the number of top boundary points
4
The number of top boundary points =004
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
1 40
X and Y boundary coord.= 0.000E+00 4.000E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
2 35
X and Y boundary coord.= 5.000E+01 3.500E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
3 32.5
```

Table 4.4 (continued)

```
X and Y boundary coord.= 5.500E+01 3.250E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
9 32.5
X and Y boundary coord.= 1.000E+02 3.250E+01
Is the entry correct?  N means reenter the data

Enter the number of bottom boundary points
4
The number of bottom boundary points = 004
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
1 0
The X and Y coord.= 0.000E+00 0.000E+00
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
2 5
The X and Y coord.= 5.000E+01 5.000E+00
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
4 0
The X and Y coord.= 7.000E+01 0.000E+00
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
9 0
The X and Y coord.= 1.000E+02 0.000E+00
Is the entry correct?  N means reenter the data

Enter the number of interface curves
4 0
The number of interface curves=04
Is the entry correct?  N means reenter the data

Enter the number of points for interface curve # 01
2
The number of points in interface curve # 01 = 02
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
1 7.5
```

Table 4.4 (continued)

```
X and Y boundary coord.= 0.000E+00 7.500E+00
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
9 10
X and Y boundary coord.= 1.000E+02 1.000E+01
Is the entry correct?  N means reenter the data

Enter the number of points for interface curve # 02
3
The number of points in interface curve # 02 = 03
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
4 25
X and Y boundary coord.= 7.000E+01 2.500E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
5 23
X and Y boundary coord.= 7.400E+01 2.300E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
9 23
X and Y boundary coord.= 1.000E+02 2.300E+01
Is the entry correct?  N means reenter the data

Enter the number of points for interface curve # 03
4
The number of points in interface curve # 03 = 04
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
5 25
X and Y boundary coord.= 7.400E+01 2.500E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
6 24.5
X and Y boundary coord.= 7.600E+01 2.450E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
7 24.5
```

Table 4.4 (continued)

```
X and Y boundary coord.= 7.800E+01 2.450E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
8 25
X and Y boundary coord.= 8.000E+01 2.500E+01
Is the entry correct?  N means reenter the data

Enter the number of points for interface curve # 04
7
The number of points in interface curve # 04 = 07
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
3 32.5
X and Y boundary coord.= 5.500E+01 3.250E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
4 25
X and Y boundary coord.= 7.000E+01 2.500E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
5 25
X and Y boundary coord.= 7.400E+01 2.500E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
6 26.5
X and Y boundary coord.= 7.600E+01 2.650E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
7 26.5
X and Y boundary coord.= 7.800E+01 2.650E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
8 25
X and Y boundary coord.= 8.000E+01 2.500E+01
Is the entry correct?  N means reenter the data

Enter the X-grid index and the Y coord.
9 25
```

Table 4.5. Listing of the MIGRAT.BAT file

```
 8 NX
11 NY (changed - was 10)
 1        .000   IC,XC(IC)
 2      50.000   IC,XC(IC)
 3      55.000   IC,XC(IC)
 4      70.000   IC,XC(IC)
 5      74.000   IC,XC(IC)
 6      76.000   IC,XC(IC)
 7      78.000   IC,XC(IC)
 8      80.000   IC,XC(IC)
 9     100.000   IC,XC(IC)
 1        .000   IC,YC(IC)
 2       2.500   IC,YC(IC)
 3       6.000   IC,YC(IC)
 4      15.000   IC,YC(IC)
 5      20.000   IC,YC(IC)
 6      23.000   IC,YC(IC)
 7      24.000   IC,YC(IC)
 0      24.5     (added)
 8      25.000   IC,YC(IC)
 9      30.000   IC,YC(IC
10      32.500   IC,YC(I'
11      40.000   IC,YC(IC
 .1000000E-04   .2000          TOL,VMIN
 4  NBT
 1        .000   40          ,XBT(IP),YBT(IP)
 2      50.000   35          ,XBT(IP),YBT(IP)
 3      55.000   32.         IP,XBT(IP),YBT(IP)
 4     100.000   32.500   IP,XBT(IP),YBT(IP)
 4  NBB
 1        .000       .000 IP,XC(IP),YBB(IP)
 2      50.000      5.000 IP,XC(IP),YBB(IP)
 3      70.000       .000 IP,XC(IP),YBB(IP)
 4     100.000       .000 IP,XC(IP),YBB(IP)
 4  NIC
 1  2  ICU,NCI(ICU)
 1        .000      7.500
 2     100.000     10.000
 2  3  ICU,NCI(ICU)
 1      70.000     25.000
 2      74.000     23.000
 3     100.000     23.000
 3  4  ICU,NCI(ICU)
 1      74.000     25.000
 2      76.000     24.500
 3      78.000     24.500
 4      80.000     25.000
 4  7  ICU,NCI(ICU)
 1      55.000     32.500
 2      70.000     25.000
 3      74.000     25.000
 4      76.000     26.500
 5      78.000     26.500
 6      80.000     25.000
 7     100.000     25.000
```

plotting programs (options)—the user can see the plot at the graphics monitor, send it to an HP 7475 (HP 7550) plotter, or create a POP file which includes all plotting instructions. The POP file can be saved and then sent to a graphics monitor or an HP plotter at a later time. To generate a map of the grid system as entered in STEP1, the user may select option 3 (plogri.exe). STEP1 will always assign line numbers -2 and -1 to lower and upper boundaries, respectively. To verify that no cell is cut more than once by interface lines, the user can execute CHKLIN. This routine will return the indices of all rectangular cells split more than once. For example, if the interfacial line labeled 3 in Fig. 4.2 was selected to lie along the horizontal grid line Z = 25, cells (5,8) (6,8) and (7,8) would be split by both lines 3 and 4. The message returned by CHKLIN for this case would be

Cell with I = 5 and J = 8 has more than one interface line
Cell with I = 6 and J = 8 has more than one interface line
Cell with I = 7 and J = 9 has more than one interface line
Cell with I = 5 and J = 8 has more than one interface line
Cell with I = 7 and J = 8 has more than one interface line
Cell with I = 7 and J = 8 has more than one interface line

Option 4 (STEP2.EXE) can adjust the original grid to enhance computational efficiency. Computational cells with very small volumes may require small time steps. The user, therefore, has the option to adjust the interface lines to improve time of computation. The user can select one of two options for adjusting interface lines. Adjustment option one means that eligible interface lines will be adjusted until the lesser volume of a split cell is not less than the entered fraction. The user responds to the prompt:

Enter the minimum allowable fraction for the lesser volume of a split cell

with a non zero fraction. For example, a response of 0.2 would mean that the interface line of any eligible split cell with a lesser volume of 20% of the total cell volume would be adjusted so as to eliminate the small portion of the split cell.

ORIGINAL GRID FOR SITE 1
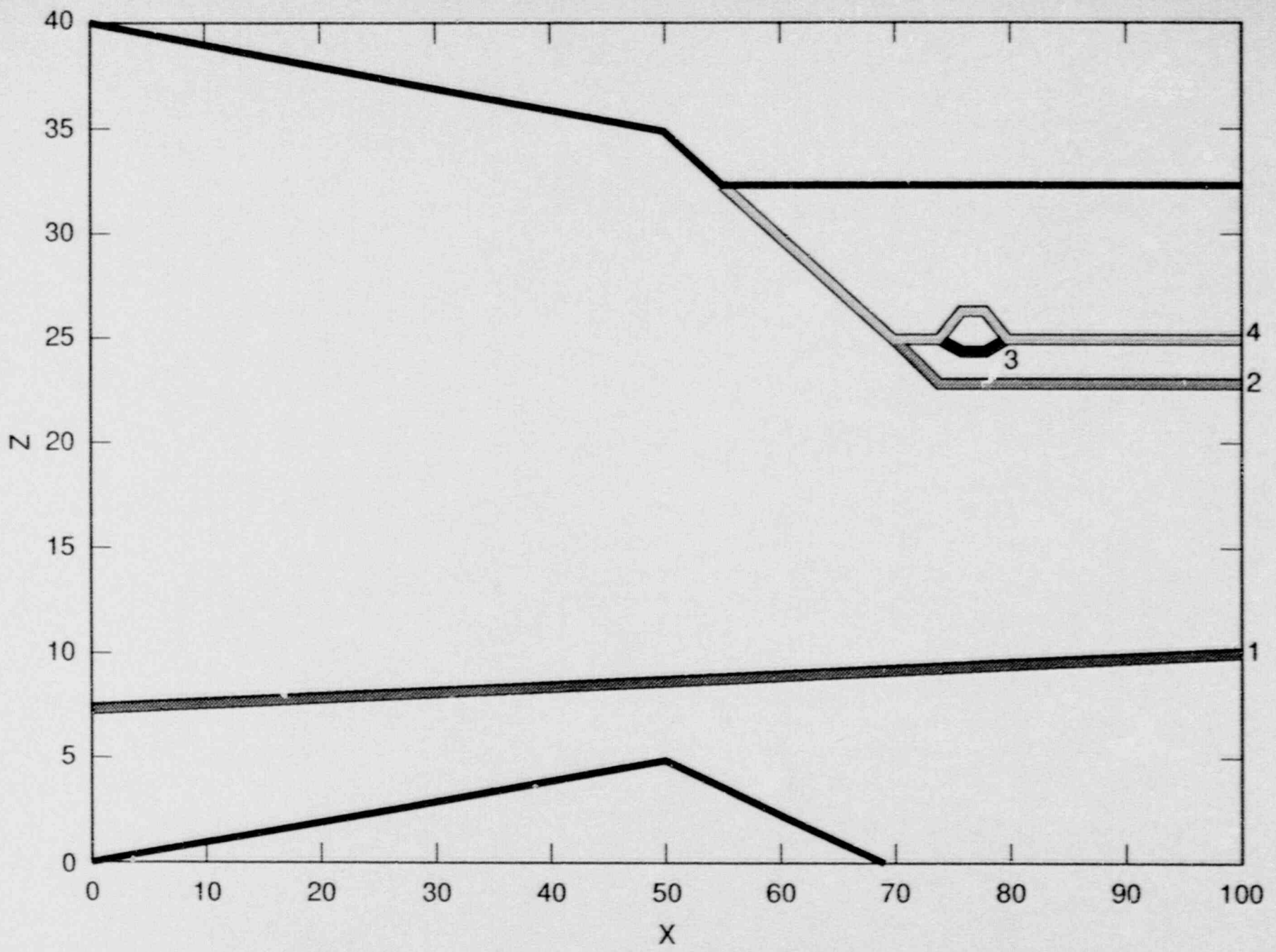
Fig. 4.2. Plot of the user-input grid system with numbered interfacial
lines as generated by Option 3 of GRID1.

The second adjustment option requires entering a negative fraction to the above prompt. This option uses the absolute value of the entered negative fraction multiplied by the smallest rectangular grid cell volume to obtain the lower tolerance for a split cell.

In portions of the grid where accurate representation is important, selected interface lines can be protected from adjustment. The following two prompts will appear on the screen:

Enter the number of lines not to be adjusted

and

Enter the line number not to be adjusted.

For example, to ensure that the drain representation does not change from that illustrated in Fig. 4.1, interfacial line numbers 3 and 4 must be protected from adjustment. Table 4.6 shows an interactive session with an adjustment factor of 0.4 but maintaining the drain configuration. To verify the integrity of the adjusted grid, CHKLIN may again be executed.

STEP2 creates the data set MIGRD.REV required for STEP3. Consequently, STEP2 must be executed even if no grid adjustment is desired. In such cases, an adjustment factor of zero is specified.

For the remainder of this section, the unadjusted grid is used.

Option 5 (STEP3.EXE) assigns a layer number to each computational grid cell. The input data to this step is a data set from STEP2, MIGRD.REV and a data set from STEP1, MIGSAV.GRD. The resultant file from STEP3 is the data set MMMM.RES. Upon completion of STEP3, the total number of layers in the grid is displayed on the screen. The option for viewing the layer map is Option 6.

STEP3 requires no user-supplied input. This step must be executed to generate the MMMM.RES file needed in subsequent steps and to provide the user with the layer map (Fig. 4.3) necessary for specifying layer-based attributes.

Option 7 (STEP4.EXE) assigns a material index to each layer. The user must respond to several prompts during this step. The first prompt is

LAYER MAP FOR SITE 1
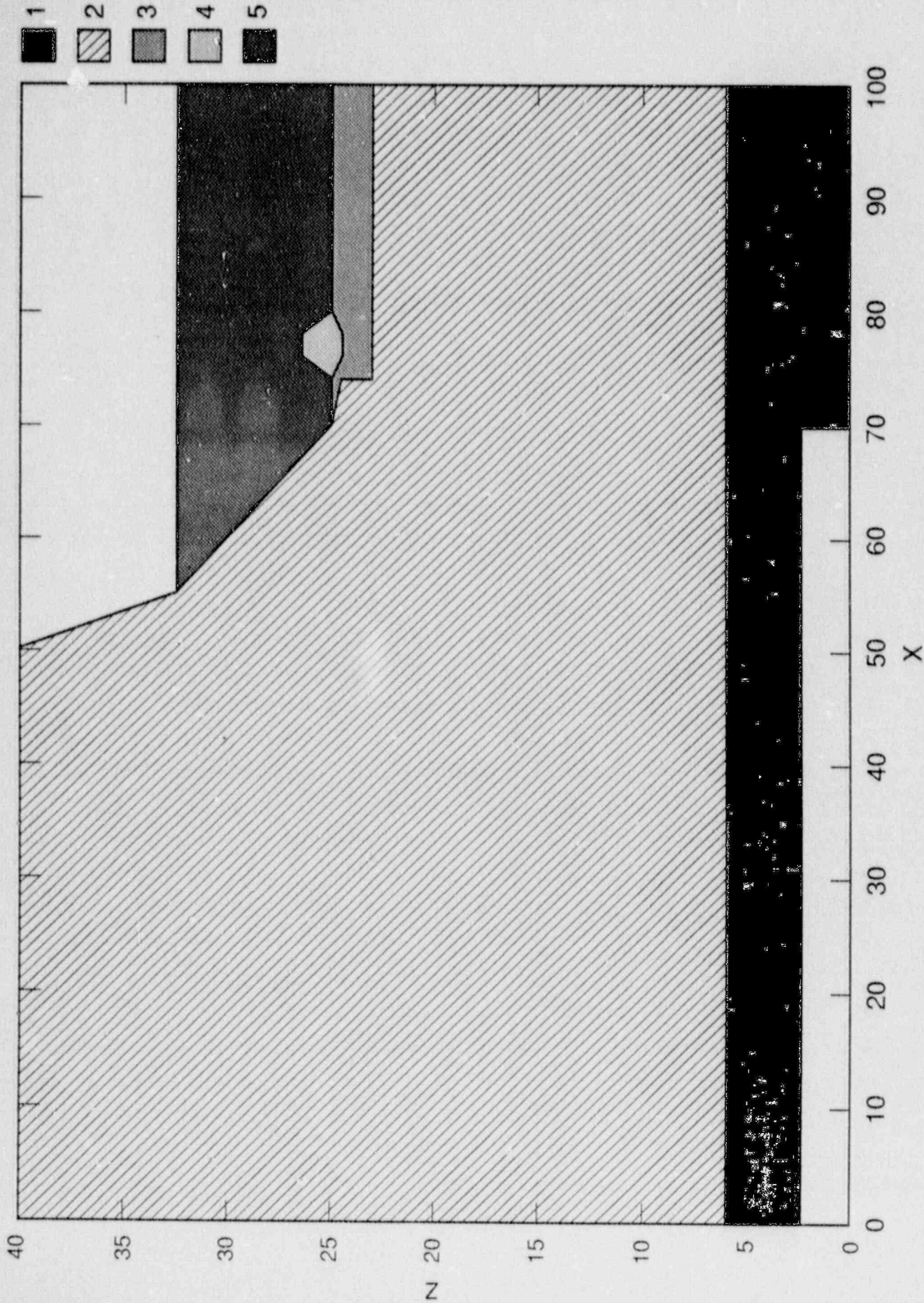
Fig. 4.3. The layer map showing the system created by STEP3 and returned by Option 5 of GRID1.

Table 4.6. Listing of the interactive session for grid
adjustment - Option 4 (grid1)

Enter the minimum allowable fraction for the lesser area of a split cell
If fraction < 0, minimum allowable volume is |fraction| times least rectangular
.4
The minimum allowable fraction =   .400 Is this correct? N means reenter.

Enter the number of lines not to be adjusted
2
Enter the line number not be adjusted
3
Enter the line number not be adjusted
4
start adjusting
I,J cell to be adj=   1   1
I,J cell to be adj=   1   2
I,J cell to be adj=   1   3
I,J cell to be adj=   1   11
I,J cell to be adj=   2   2
I,J cell to be adj=   2   3
I,J cell to be adj=   3   1
I,J cell to be adj=   3   3
I,J cell to be adj=   4   3
I,J cell to be adj=   4   6
I,J cell to be adj=   4   7
I,J cell to be adj=   5   3
I,J cell to be adj=   6   3
I,J cell to be adj=   7   3
I,J cell to be adj=   8   3
Stop - Program terminated.

Enter the number of different materials.

Presently there is a maximum of ten different materials. The second prompt is:

Enter the name (A10) of material #__.

To this prompt enter the layer indices from the layer map (Fig. 4.4) that correspond to the given material. The resultant files from this step are MMMM.REV and MATERL.NAM. The file MMMM.REV contains grid coordinates, layer identifiers, and an added material number from this step for each grid cell. MATERL.NAM is a key to the material map. (See Table 4.7 for the sample interactive session in STEP4 and Fig. 4.4 for the material map generated by Option 8.)

Option 9 (STEP5.EXE) calculates the centroid location of each grid cell. The area (or areas within a split cell) is also calculated for each cell. By the time this total grid generation program has progressed through STEP5, a large data file, CENTRO.DAT, has been created. This data set contains the following variables:

NY - index denoting the type of cell,

    0 means non-split

    1 means lower part (cell) of a split cell pair

    2 means upper part (cell) of a split cell pair,

IX - grid index number in the horizontal direction (increasing from left to right),

JY - grid index number in the vertical direction (increasing from bottom to top),

N - node number assigned to the centroid of the cell,

ILAY - layer number assigned to the cell,

IMAT - material number assigned to the cell,

XNI - horizontal coordinate of the centroid of the cell,

YNI - vertical coordinate of the centroid of the cell,

AI - area of the cell,

NPTS - number of points to define the cell boundary,

Table 4.7.   Listing of the interactive session for the assignment of
material names and material indices - Option 7 (grid1)

```
Enter the number of different materials
4
The number of different materials =   4
Is the entry correct? N means reenter the datum

Enter the name (A10) of material #  1
SANDSTONE
The name of material #  1 = SANDSTONE
Is the entry correct? N means reenter the datum

Enter the number of layers of material SANDSTONE
2
The number of layers of material SANDSTONE  = 02
Is the entry correct? N means reenter the datum

Enter the layer #_s of material SANDSTONE
1 2
Material SANDSTONE  exists in layer(s)   1  2
Is the entry correct? N means reenter the datum

Enter the name (A10) of material #  2
LINER
The name of material #  2 = LINER
Is the entry correct? N means reenter the datum
```

Table 4.7 (continued)

```
Enter the number of layers of material LINER
1
The number of layers of material LINER      = 01
Is the entry correct? N means reenter the datum

Enter the layer #_s of material LINER
3
Material LINER        exists in layer(s)    3
Is the entry correct? N means reenter the datum

Enter the name (A10) of material #  3
DRAIN
The name of material #  3 = DRAIN
Is the entry correct? N means reenter the datum

Enter the number of layers of material DRAIN
1
The number of layers of material DRAIN      = 01
Is the entry correct? N means reenter the datum

Enter the layer #_s of material DRAIN
4
Material DRAIN        exists in layer(s)    4
Is the entry correct? N means reenter the datum

Enter the name (A10) of material #  4
TAILINGS
The name of material #  4 = TAILINGS
Is the entry correct? N means reenter the datum

Enter the number of layers of material TAILINGS
1
The number of layers of material TAILINGS   = 01
Is the entry correct? N means reenter the datum

Enter the layer #_s of material TAILINGS
5
Material TAILINGS    exists in layer(s)    5
Is the entry correct? N means reenter the datum

Stop - Program terminated.
```

MATERIAL MAP FOR SITE 1
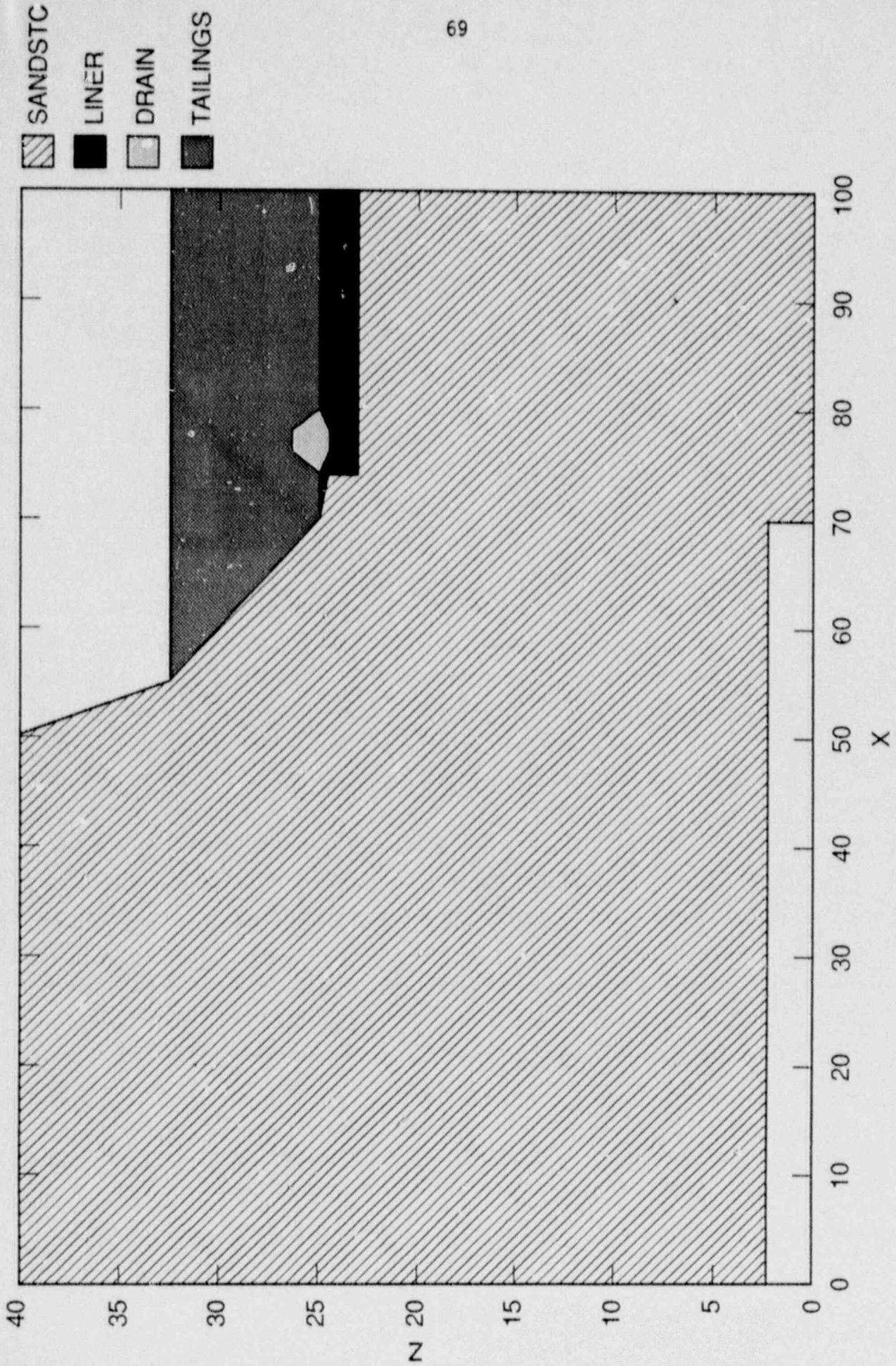
Fig. 4.4. The material map as generated by Option 8 of GRID1.

XP(K) - horizontal coordinates of the cell boundary points, K=1, NPTS

YP(K) - vertical coordinates of the cell boundary points, K=1, NPTS.

STEP5 requires no user supplied input but creates the CENTRO.DAT file which contains both the data to be input to the MIGRAT code and the data required by subsequent steps.

4.2 GRID2

The GRID2 options (Table 4.8) are the last of the MIGRAT preprocessor steps. This menu and associated programs are driven by the grid2.bat file (see Table 4.9). Option 1 generates the centroid map shown in Fig. 4.5.

The user must tell the plotting program if he wants the node identifier written next to each node. These numbers have been omitted in Fig. 4.5. Option 2, STEP6.EXE, determines the connectivity of nodes for the MIGRAT grid. Three data sets are created during this step. The first is file NODCON.DAT. This file contains the node identifier with X and Y coordinates, an "END OF NODE DATA" record followed by the pairs of node indices of the connected nodes. The second data set, ZEROV.CON, has three sets of X and Z coordinate pairs per line. The middle pair is the location of an imposed zero volume node (Sect. 2.4). This data set is used only for plotting by Option 3. See Fig. 4.6 for the connectivity map from Option 3. The third data set is BLOCK45.DAT which contains the Block 4 and 5 data from the MIGRAT code.

Option 4, INMAT1.EXE, allows the user to enter material properties. These may be either functional relations including saturation vs pressure, conductivity vs pressure, retardation vs concentration, or constants such as diffusivity, reference void ratio, etc., as described in the previous section. This step creates the BLOCK2.DAT file which contains the input data for Block 2 of the MIGRAT code. This step also creates files which are used in Option 5 to plot saturation vs Φ and conductivity vs Φ. Table 4.10 shows an interaction session of INMAT1. Selecting Option 5 produces plots of the material property curves as shown in Fig. 4.7. With this step, the user also has the option for an interactive or a batch mode of operation. If during an interactive session the user determines that he has made a mistake, he can finish the interactive session. The interactive session creates a data file

Table 4.8.   MIGRAT Preprocessor (grid2) menu

```
------> MIGRAT Preprocessor cont.  <------

Note:  Do not strike carriage return for menu selection!

0 - Exit to DOS ........................................

1 - Plot Centroid Locations - NODES (STEP5) ..........

2 - Determine Node Connectivity (STEP6) ..............

3 - Plot Connection Map ...............................

4 - Define Material Properties (BLOCK2.DAT) ..........

5 - Plot Material Property Curves ....................

6 - Create Initial BLOCKS 1 and 3 Data (BLK13.DAT) ..

7 - Define Initial PHI's and Conc.s (STEP7) ..........

8 - Define Boundary Conditions (STEP8) ...............

9 - EDIT - Edit Layer Map or Create Restart Data ....
```

Table 4.9. Listing of the grid2.bat file

```
:menu
echo off
assign
cls
type grid2.txt
getdigit                        Press key for desired option:
cls
echo working....
if errorlevel 9 goto edit
if errorlevel 8 goto step8
if errorlevel 7 goto step7
if errorlevel 6 goto inib13
if errorlevel 5 goto plomat
if errorlevel 4 goto inmatl
if errorlevel 3 goto plocon
if errorlevel 2 goto step6
if errorlevel 1 goto plocen
if errorlevel 0 goto exit
:badopt
echo Invalid option
pause
goto menu
:plocen
plocen /r 2000
goto menu
:step6
step6
goto menu
:plocon
plocon /r 2000
goto menu
:inmatl
inmatl
goto menu
:plomat
plomat /r 2000
goto menu
:inib13
inib13
goto menu
:step7
step7
goto menu
:step8
step8
goto menu
:edit
edit
goto menu
:exit
cls
ver
cd
```

Centroid Map for Site 1
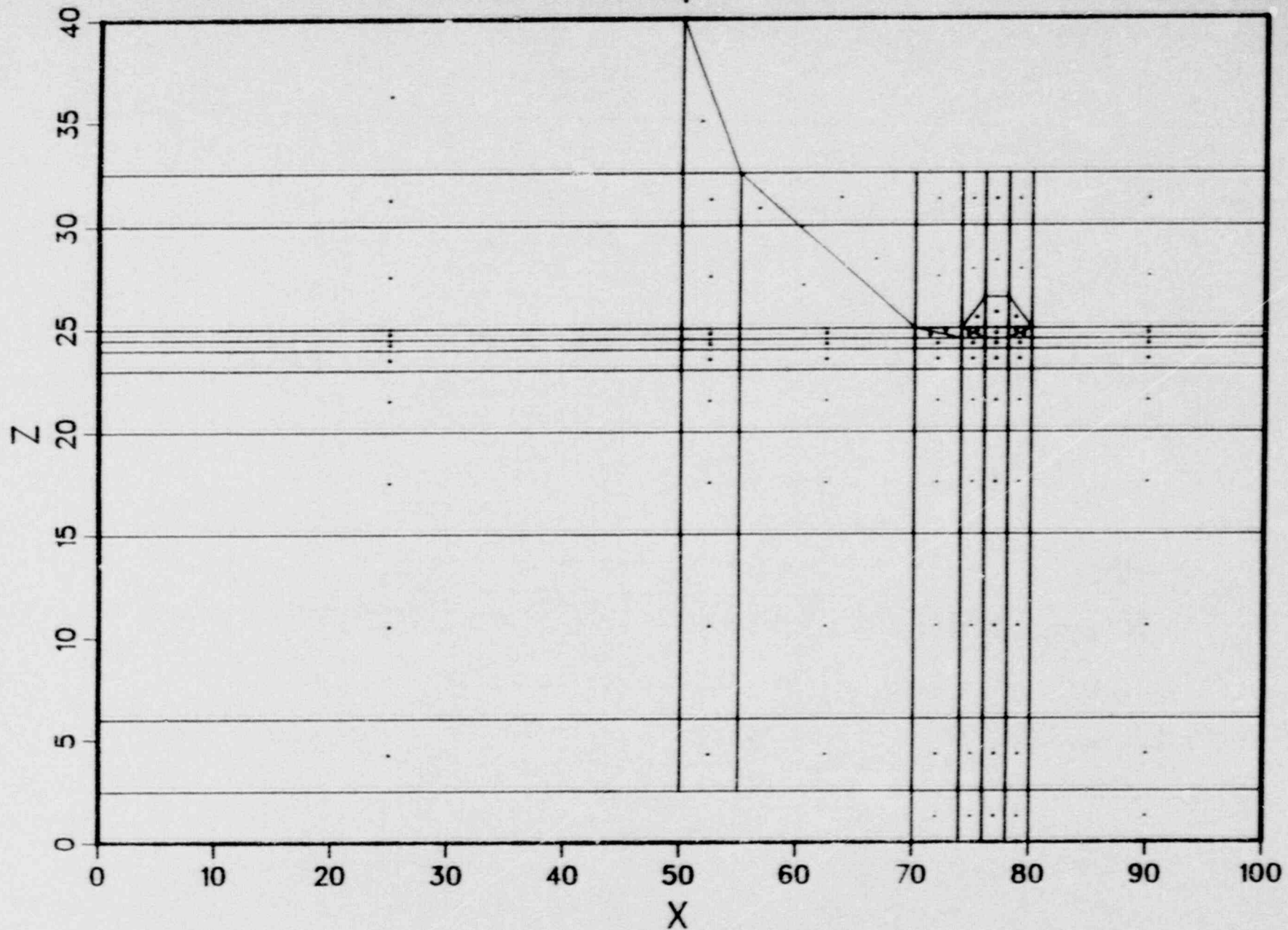
Fig. 4.5. A plot showing the locations of the centroids of each cell as
computed by Option 9 of GRID1 and generated by Option 1 of GRID2.
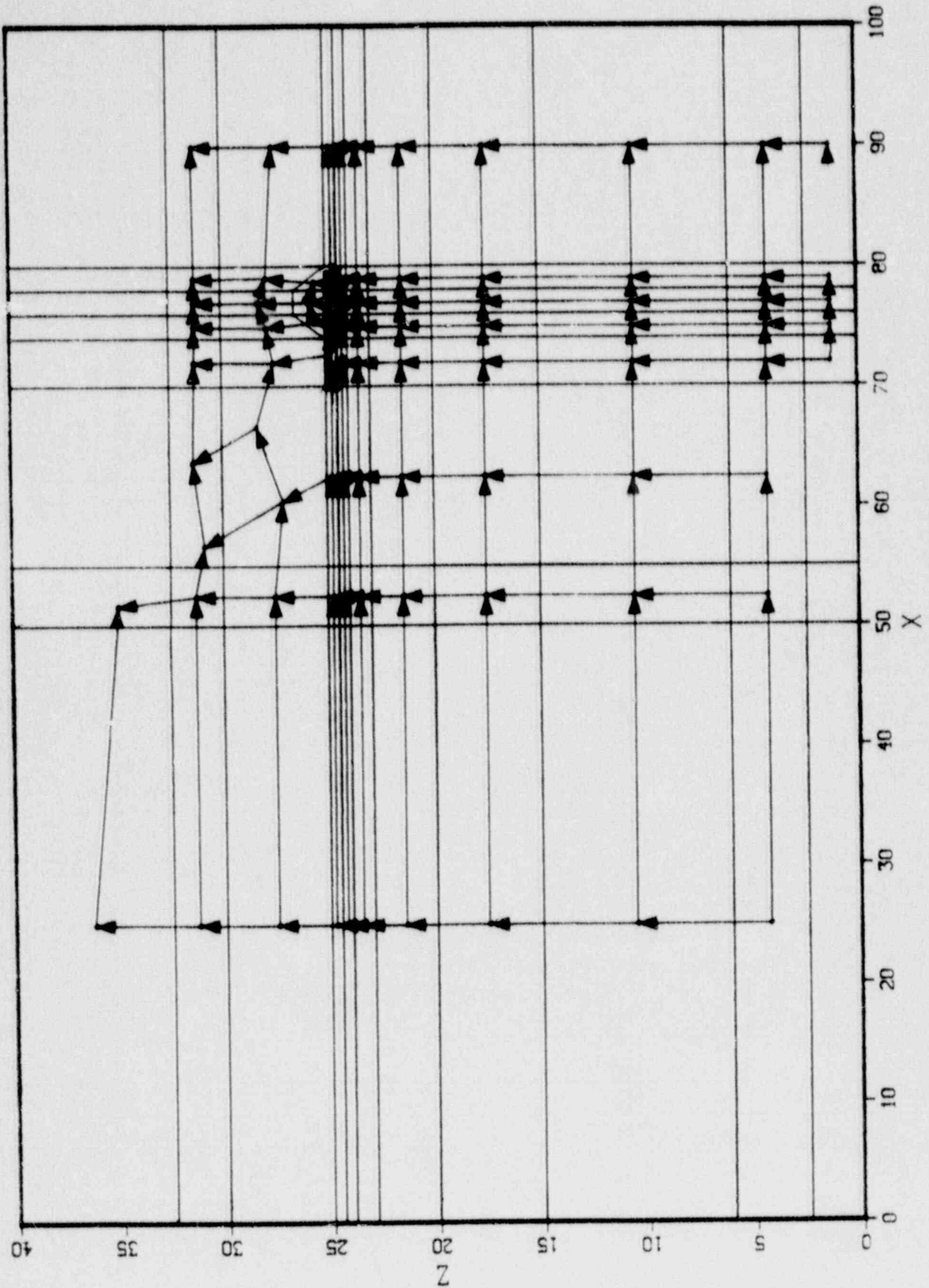
Fig. 4.6. A plot indicating the cell connections as computed in STEP6 of Option 2 and generated by Option 3 of GRID2.

Table 4.10. Listing of the interactive session for entering
             material properties - Option 4 (grid2)

Enter type of execution: 0 means interactive
                         1 means batch (from MATCRV.BAT).
0
This is an interactive run.
Is the entry correct? N means reenter.

Enter RD - the specific gravity of saturated soil.
2
RD = 2.000E+00
Is the entry correct? N means reenter.

Enter the number of contaminants (0,1, or 2)
2
The number of contaminants = 2
Is the entry correct? N means reenter.

Does contaminant # 1 decay? Y means yes.
Y
Contaminant # 1 decays.
Is the entry correct? N means reenter.

Enter the half life for contaminant # 1
1.5E2
The half life for contaminant # 1 = 1.5000E+02.
Is the entry correct? N means reenter.

Does contaminant # 2 decay? Y means yes.

Contaminant # 2 DOES NOT DECAY.
Is the entry correct? N means reenter.

You will now enter material-specific constants and parameters.

Enter AV - coefficient of compressibility (1/pressure)
for material SAND
6.E-16
AV for Material SAND   = 6.000E-16
Is the entry correct? N means reenter.

Enter EZ - reference void ratio for material SAND
.5
EZ = 5.0000E-01
Is the entry correct? N means reenter.

Enter PZ - relative effective stress corresponding to EZ (M/LT**2).
1.E13
PZ = 1.0000E+13
Is the entry correct? N means reenter.

Enter DFUS - the diffusivity for material SAND
1
DFUS = 1.000E+00 for material SAND
Is the entry correct? N means reenter.

Is permeability constant for material SAND   ? Y means yes.
N
Constant Permeability = N
Is the entry correct? N means reenter.

Table 4.10 (continued)

Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 1
3.E-2 5.e-25 -2.5e4
The SATURATION,COND. and PSI for data point # 1 =   3.000E-02   5.000E-25   -2.500E+04
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 2
6.e-2 2.e-23 -2.5e3
The SATURATION,COND. and PSI for data point # 2 =   6.000E-02   2.000E-23   -2.500E+03
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 3
9.5e-2 2.e-23 -2.5e2
The SATURATION,COND. and PSI for data point # 3 =   9.500E-02   2.000E-23   -2.500E+02
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 4
1.e-1 1.e-18 -2.5e1
The SATURATION,COND. and PSI for data point # 4 =   1.000E-01   1.000E-18   -2.500E+01
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 5

1.7e-1 8.e-17 -5
The SATURATION,COND. and PSI for data point # 5 =   1.700E-01   8.000E-17   -5.000E+00
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 6
2.e-1 1.e-15 -2.5
The SATURATION,COND. and PSI for data point # 6 =   2.000E-01   1.000E-15   -2.500E+00
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 7
4.4e-1 1.e-13 -1
The SATURATION,COND. and PSI for data point # 7 =   4.400E-01   1.000E-13   -1.000E+00
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 8
8.e-1 rel -.5

The SATURATION,COND. and PSI for data point # 8 =   8.000E-01   0.000E+00   0.000E+00
Is the entry correct? N means reenter.
N
Enter the SATURATION fraction, COND. and PSI for data point # 8
8.e-1 4.e-12 -.5
The SATURATION,COND. and PSI for data point # 8 =   8.000E-01   4.000E-12   -5.000E-01
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 9
9.9e-1 5.e-11 -.3
The SATURATION,COND. and PSI for data point # 9 =   9.900E-01   5.000E-11   -3.000E-01
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 10
1 8.e-11 1.e3
The SATURATION,COND. and PSI for data point # 10 =   1.000E+00   8.000E-11   1.000E+03
Is the entry correct? N means reenter.

Enter the number of data points in the retardation
 curve for the contaminants in material SAND   .
5

Table 4.10 (continued)

for each contaminant in material SAND   .
1.e-4 0 4
Point # 1 has conc. = 1.000E-04 and retard. =   0.000E+00   4.000E+00
Is the entry correct? N means reenter.

Enter the concentration and retardation data point # 2
for each contaminant in material SAND   .
1.e-3 0 3
Point # 2 has conc. = 1.000E-03 and retard. =   0.000E+00   3.000E+00
Is the entry correct? N means reenter.

Enter the concentration and retardation data point # 3
for each contaminant in material SAND   .
1.e-2 0 2
Point # 3 has conc. = 1.000E-02 and retard. =   0.000E+00   2.000E+00
Is the entry correct? N means reenter.

Enter the concentration and retardation data point # 4
for each contaminant in material SAND   .
1.e-1 0 1
Point # 4 has conc. = 1.000E-01 and retard. =   0.000E+00   1.000E+00
Is the entry correct? N means reenter.

Enter the concentration and retardation data point # 5
for each contaminant in material SAND   .
1 0 0
Point # 5 has conc. = 1.000E+00 and retard. =   0.000E+00   0.000E+00
Is the entry correct? N means reenter.

Enter AV - coefficient of compressibility (1/pressure)
for material LINER   .
5.9e-15
AV for Material LINER   = 5.900E-15
Is the entry correct? N means reenter.

Enter EZ - reference void ratio for material LINER
.63
EZ = 6.3000E-01
Is the entry correct? N means reenter.

Enter PZ - relative effective stress corresponding to EZ (M/LT**2).
1.e13
PZ = 1.0000E+13
Is the entry correct? N means reenter.

Enter DFUS - the diffusivity for material LINER
.5
DFUS = 5.000E-01 for material LINER   .
Is the entry correct? N means reenter.

Is permeability constant for material LINER   ? Y means yes.
N
Constant Permeability = N
Is the entry correct? N means reenter.

YOU ARE NOW ENTERING SATURATION & CONDUCTIVITY VS PSI DATA.
Enter the # of data points for material LINER
7
The # of data points = 7
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 1

Table 4.10 (continued)

Enter the SATURATION fraction, COND. and PSI for data point # 2
.7 1.5e-19 1e-2
The SATURATION,COND. and PSI for data point # 2 =   7.000E-01   1.500E-19   1.000E-02
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 3
.76 7e-19 -5e1
The SATURATION,COND. and PSI for data point # 3 =   7.600E-01   7.000E-19   -5.000E+01
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 4
.88 2e-17 -1e1
The SATURATION,COND. and PSI for data point # 4 =   8.800E-01   2.000E-17   -1.000E+01
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 5
.97 1.5e16 -5
The SATURATION,COND. and PSI for data point # 5 =   9.700E-01   1.500E+16   -5.000E+00
Is the entry correct? N means reenter.
N
Enter the SATURATION fraction, COND. and PSI for data point # 5
.97 1.5e-17 -5
The SATURATION,COND. and PSI for data point # 5 =   9.700E-01   1.500E-17   -5.000E+00
Is the entry correct? N means reenter.
N
Enter the SATURATION fraction, COND. and PSI for data point # 5
.97 1.5e-16 -5
The SATURATION,COND. and PSI for data point # 5 =   9.700E-01   1.500E-16   -5.000E+00
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 6
1 2.7e-16 -3e-2
The SATURATION,COND. and PSI for data point # 6 =   1.000E+00   2.700E-16   -3.000E-02
Is the entry correct? N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point # 7
1 2.7e-16 1e4
The SATURATION,COND. and PSI for data point # 7 =   1.000E+00   2.700E-16   1.000E+04
Is the entry correct? N means reenter.

Enter the number of data points in the retardation
 curve for the contaminants in material LINER   .
5
The number of points = 5
Is the entry correct? N means reenter.

Enter the concentration and retardation data point # 1
for each contaminant in material LINER   .
1.e-4 0 8
Point # 1 has conc. = 1.000E-04 and retard. =   0.000E+00   8.000E+00
Is the entry correct? N means reenter.

Enter the concentration and retardation data point # 2
for each contaminant in material LINER   .
1.e-3 0 6
Point # 2 has conc. = 1.000E-03 and retard. =   0.000E+00   6.000E+00
Is the entry correct? N means reenter.

Enter the concentration and retardation data point # 3
for each contaminant in material LINER   .
1.e-2 0 4
Point # 3 has conc. = 1.000E-02 and retard. =   0.000E+00   4.000E+00

Table 4.10 (continued)

```
1.e-1 0 2
Point # 4 has conc. = 1.000E-01 and retard. =        0.000E+00     2.000E+00
Is the entry correct?  N means reenter.

Enter the concentration and retardation data point # 5
for each contaminant in material LINER      .
1 0 0
Point # 5 has conc. = 1.000E+00 and retard. =        C.000E+00     0.000E+00
Is the entry correct?  N means reenter.

Enter AV - coefficient of compressibility (1/pressure)
for material DRAIN      .
6.e-16
AV for Material DRAIN      = 6.000E-16
Is the entry correct?  N means reenter.

Enter EZ - reference void ratio for material DRAIN
.6
EZ = 6.0000E-01
Is the entry correct?  N means reenter.

Enter PZ - relative effective stress corresponding to EZ (M/LT**2).
1.e13
PZ = 1.0000E+13
Is the entry correct?  N means reenter.

Enter DFUS - the diffusivity for material DRAIN
2
DFUS = 2.000E+00 for material DRAIN
Is the entry correct?  N means reenter.

Is permeability constant for material DRAIN      ?  Y means yes.
Y
Constant Permeability = Y
Is the entry correct?  N means reenter.

Enter CONT - constant permeability.
1.e-10
CONT = 1.000E-10 for material DRAIN
Is the entry correct?  N means reenter.

YOU ARE NOW ENTERING SATURATION VS PSI DATA.
Enter the # of data points for material DRAIN
9
The # of data points = 9
Is the entry correct?  N means reenter.

Enter the SATURATION fraction and PSI for data point # 1
1.e-3 -1e4
The SATURATION and PSI for data point # 1 =        1.000E-03     -1.000E+04
Is the entry correct?  N means reenter.

Enter the SATURATION fraction and PSI for data point # 2
1.5e-3 -1e3
The SATURATION and PSI for data point # 2 =        1.500E-03     -1.000E+03
Is the entry correct?  N means reenter.

Enter the SATURATION fraction and PSI for data point # 3
2.e-3 -1e2
The SATURATION and PSI for data point # 3 =        2.000E-03     -1.000E+02
Is the entry correct?  N means reenter.
```

Table 4.10 (continued)

Enter the SATURATION fraction and PSI for data point # 5
1.e-2 -4e-2
The SATURATION and PSI for data point # 5 =   1.000E-02   -4.000E-02
Is the entry correct? N means reenter.

Enter the SATURATION fraction and PSI for data point # 6
1.e-1 -3e-2
The SATURATION and PSI for data point # 6 =   1.000E-01   -3.000E-02
Is the entry correct? N means reenter.

Enter the SATURATION fraction and PSI for data point # 7
6.3e-1 -2e-2
The SATURATION and PSI for data point # 7 =   6.300E-01   -2.000E-02
Is the entry correct? N means reenter.

Enter the SATURATION fraction and PSI for data point # 8
1 -1e-2
The SATURATION and PSI for data point # 8 =   1.000E+00   -1.000E-02
Is the entry correct? N means reenter.

Enter the SATURATION fraction and PSI for data point # 9
1 1e3
The SATURATION and PSI for data point # 9 =   1.000E+00   1.000E+03
Is the entry correct? N means reenter.

Enter the number of data points in the retardation
 curve for the contaminants in material DRAIN
0
The number of points = 0
Is the entry correct? N means reenter.

Enter AV - coefficient of compressibility (1/pressure)
for material TAILINGS .
5.9e-16
AV for Material TAILINGS   = 5.900E-16
Is the entry correct? N means reenter.

Enter EZ - reference void ratio for material TAILINGS
7.9e-1
EZ = 7.9000E-01
Is the entry correct? N means reenter.

Enter PZ - relative effective stress corresponding to EZ (M/LT**2).
1e13
PZ = 1.0000E+13
Is the entry correct? N means reenter.

Enter DFUS - the diffusivity for material TAILINGS .
0
DFUS = 0.0000E+00 for material TAILINGS .
Is the entry correct? N means reenter.

Is permeability constant for material TAILINGS ? Y means yes.

Constant Permeability =
Is the entry correct? N means reenter.
N
Is permeability constant for material TAILINGS ? Y means yes.
N
Constant Permeability = N
Is the entry correct? N means reenter.

Table 4.10 (continued)

```
The # of data points =  9
Is the entry correct?  N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point #  1
2.3e-1 3.2e-20 -1e3
The SATURATION,COND. and PSI for data point #  1 =      2.300E-01      3.200E-20      -1.000E+03
Is the entry correct?  N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point #  2
3.e-1 5.e-19 -1e2
The SATURATION,COND. and PSI for data point #  2 =      3.000E-01      5.000E-19      -1.000E+02
Is the entry correct?  N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point #  3
4.e-1 1.e-16 -1e1
The SATURATION,COND. and PSI for data point #  3 =      4.000E-01      1.000E-16      -1.000E+01
Is the entry correct?  N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point #  4
8.e-1 1.e-13 -1
The SATURATION,COND. and PSI for data point #  4 =      8.000E-01      1.000E-13      -1.000E+00
Is the entry correct?  N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point #  5
9.e-1 4.e-13 -1e-1
The SATURATION,COND. and PSI for data point #  5 =      9.000E-01      4.000E-13      -1.000E-01
Is the entry correct?  N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point #  6
9.3e-1 6.e-13 -1e-2
The SATURATION,COND. and PSI for data point #  6 =      9.300E-01      6.000E-13      -1.000E-02
Is the entry correct?  N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point #  7
9.6e-1 1.e-12 -1e-3
The SATURATION,COND. and PSI for data point #  7 =      9.600E-01      1.000E-12      -1.000E-03
Is the entry correct?  N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point #  8
9.8e-1 2.e-12 -1e-4
The SATURATION,COND. and PSI for data point #  8 =      9.800E-01      2.000E-12      -1.000E-04
Is the entry correct?  N means reenter.

Enter the SATURATION fraction, COND. and PSI for data point #  9
1 2.e-12 1e3
The SATURATION,COND. and PSI for data point #  9 =      1.000E+00      2.000E-12       1.000E+03
Is the entry correct?  N means reenter.

Enter the number of data points in the retardation
 curve for the contaminants in material TAILINGS  .
0
The number of points =  0
Is the entry correct?  N means reenter.

Stop - Program terminated.

C:\>
```
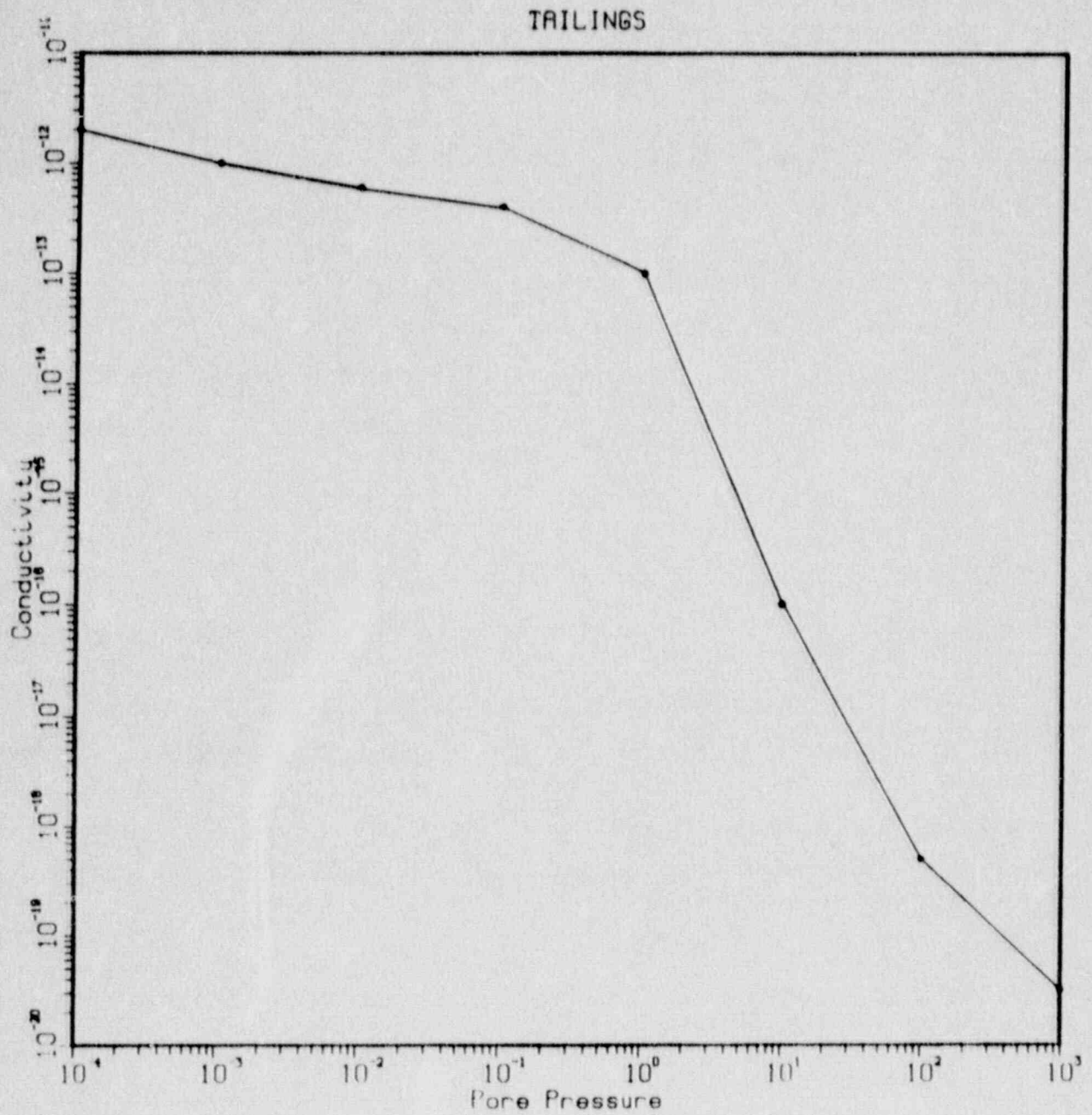
Fig. 4.7. Seven examples (a-g) of material property curves from data entered in INMAT1 and generated by Option 5 of GRID2.
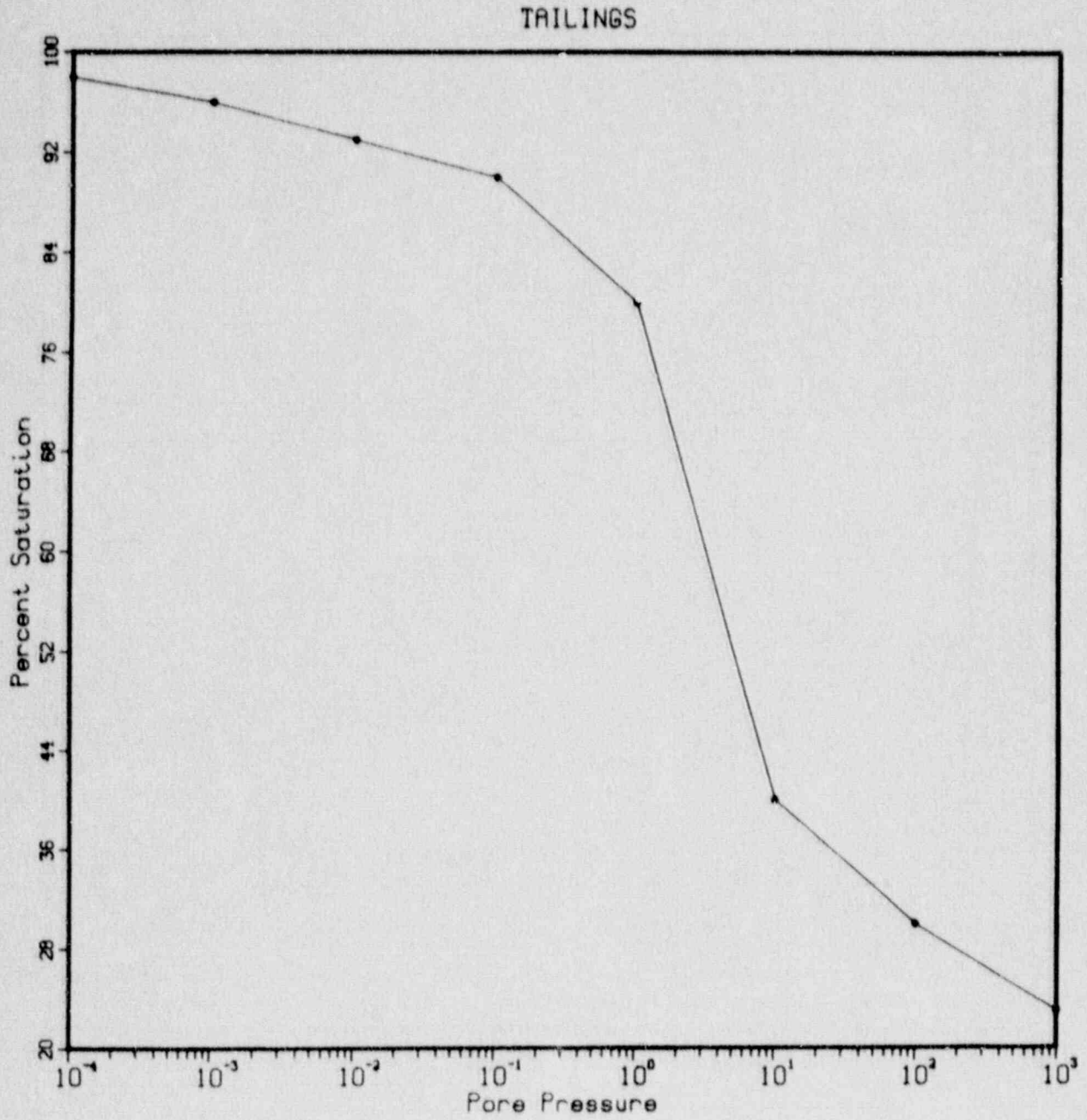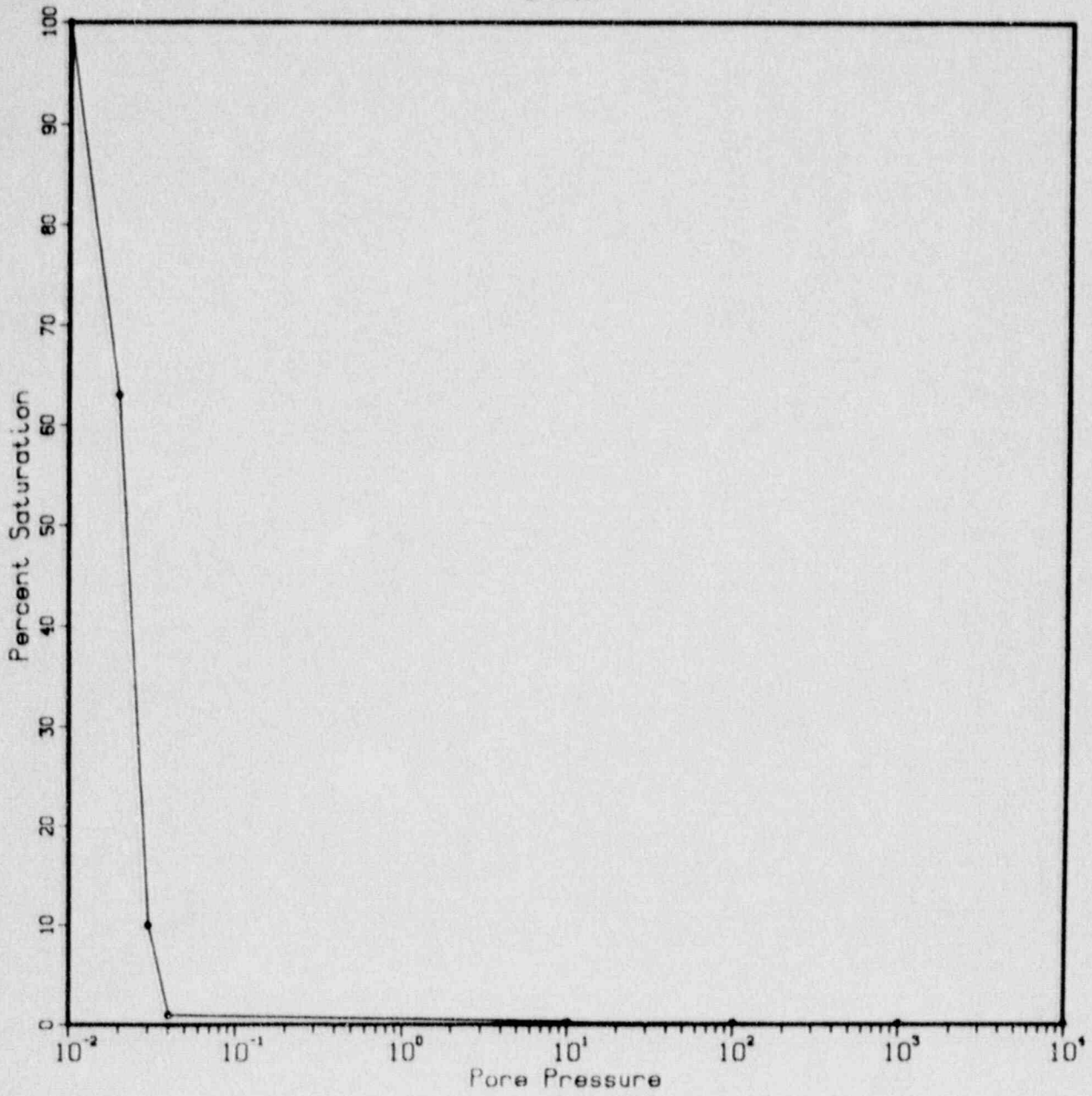
Fig. 4.7. Example 2.

Fig. 4.7. Example 3.

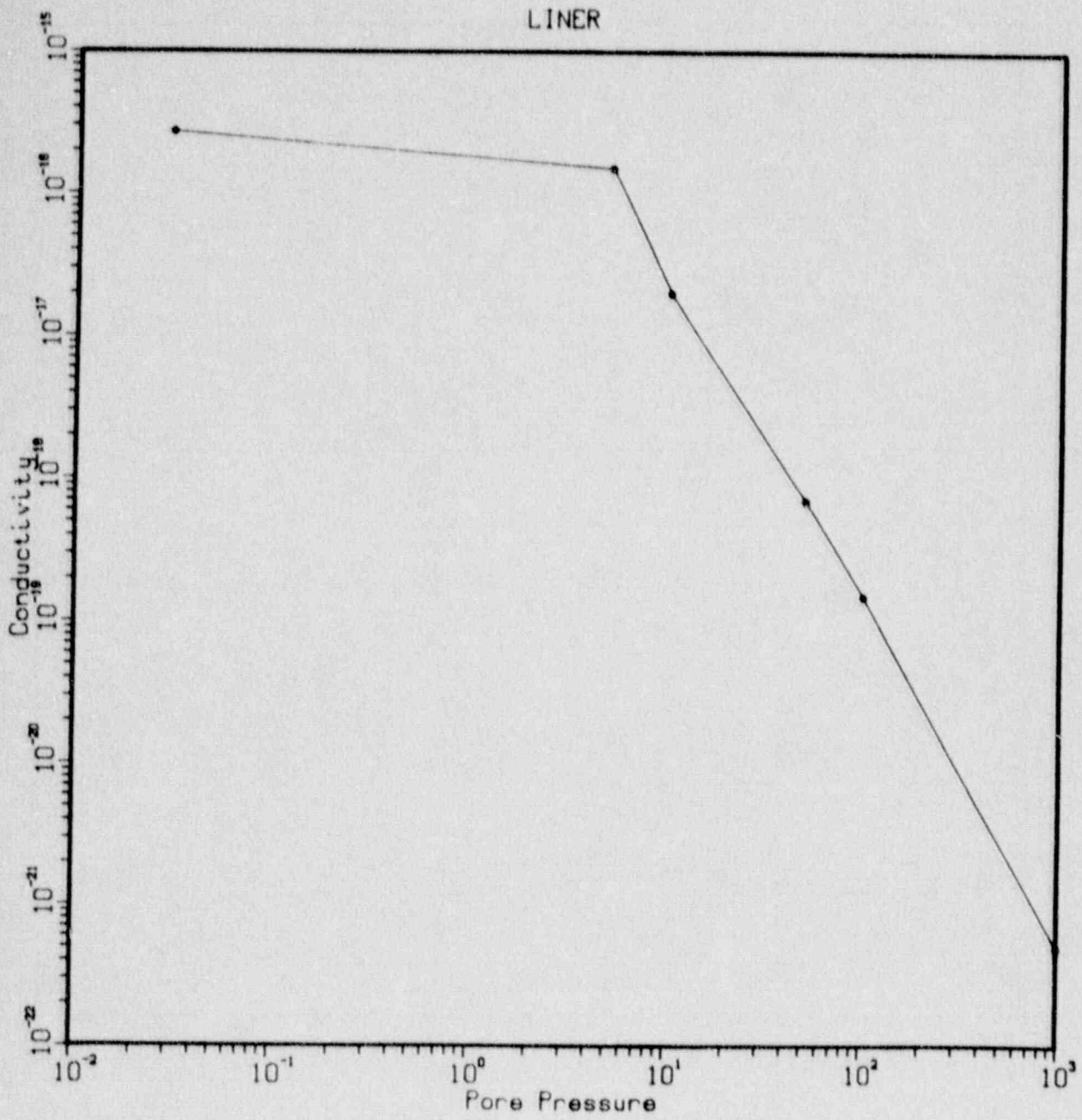Fig. 4.7. Example 4.

LINER

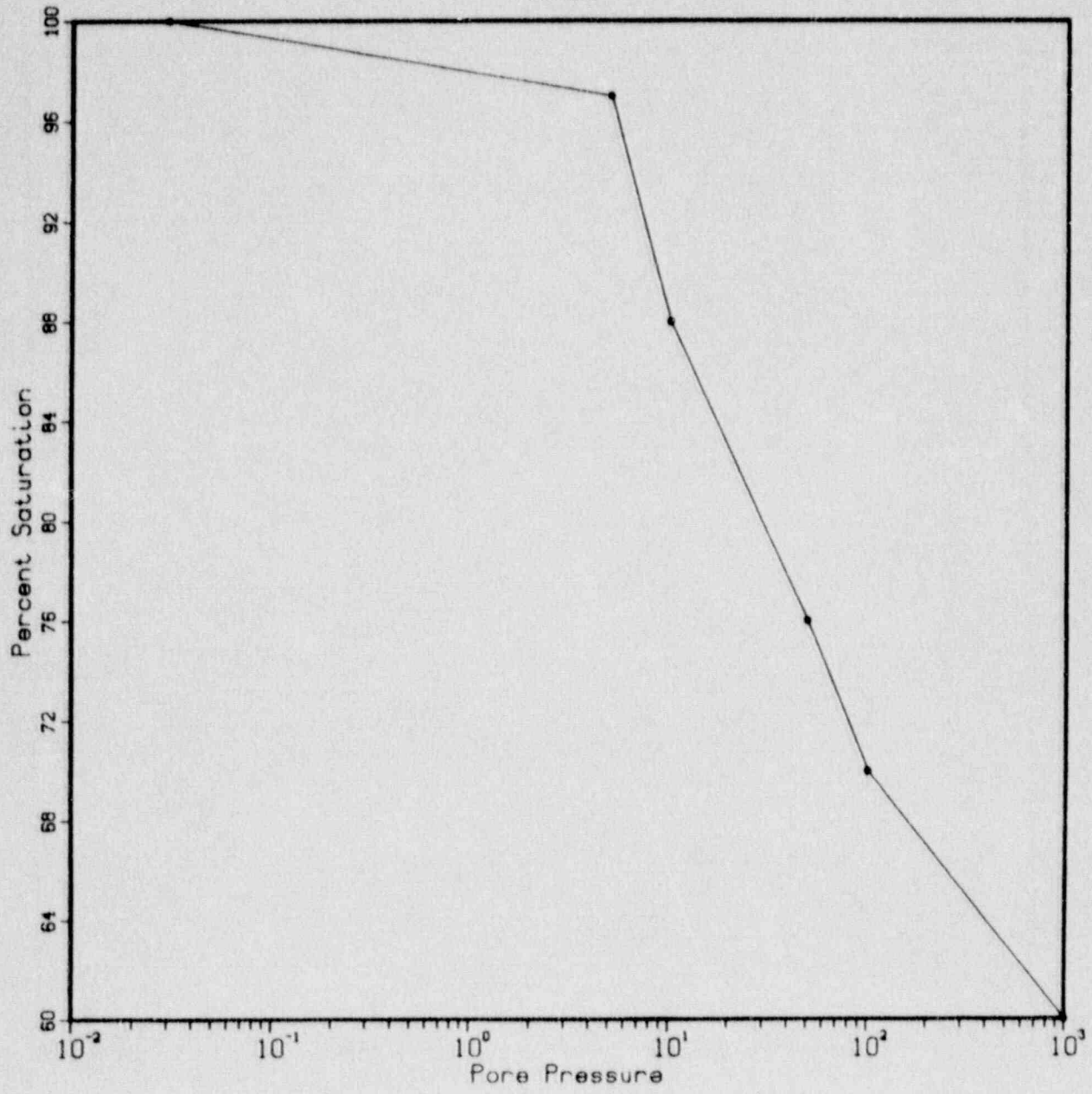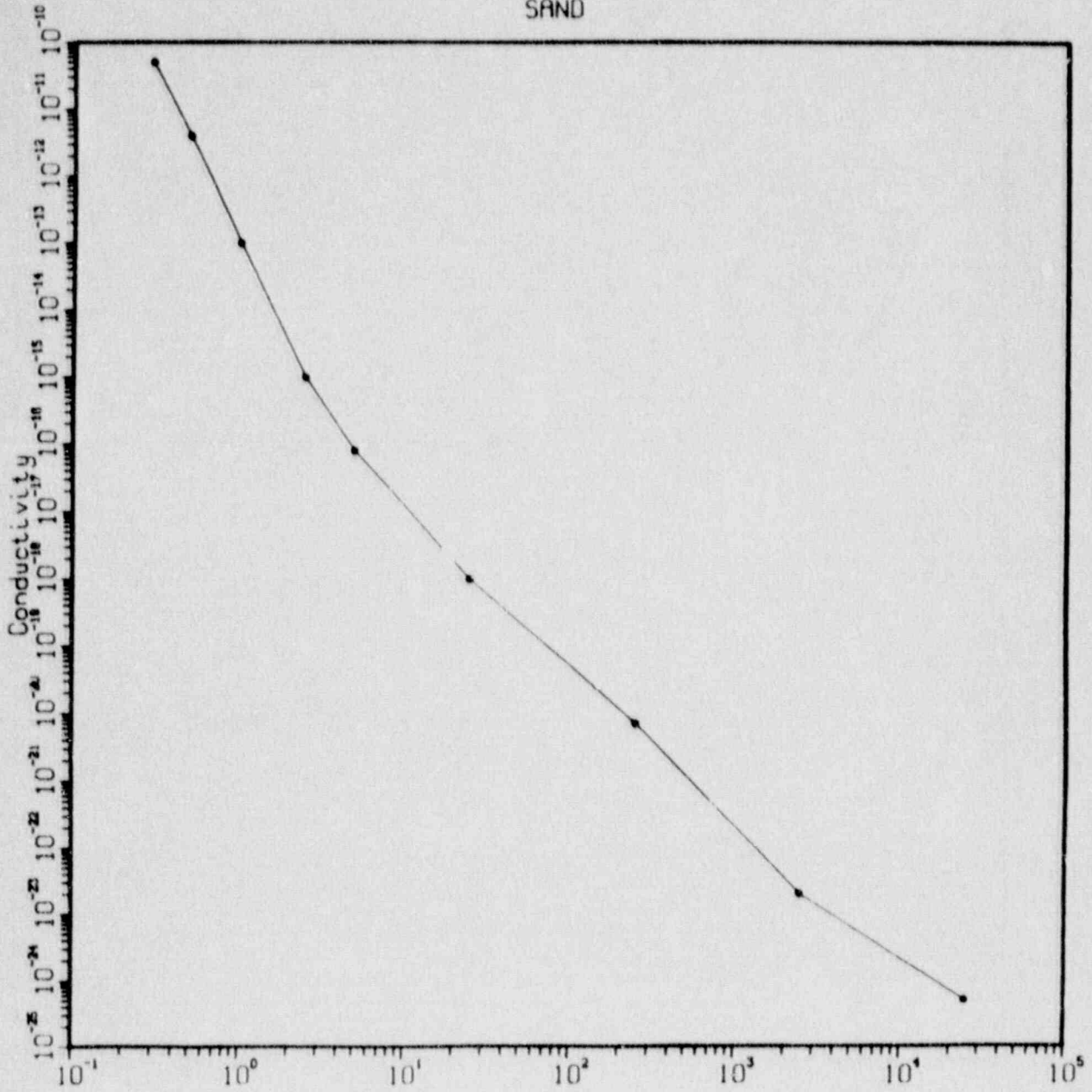Fig. 4.7. Example 5.
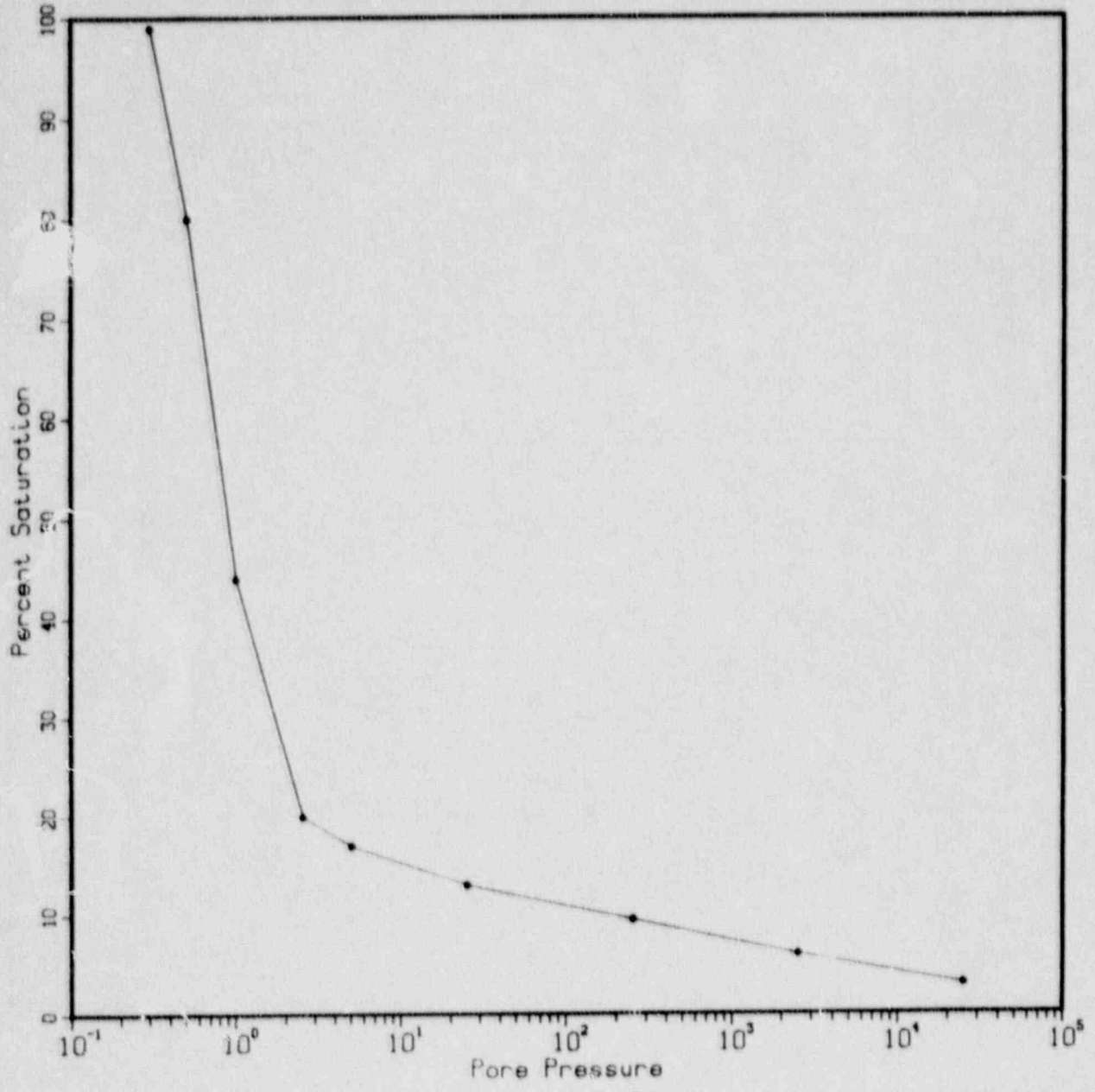
Fig. 4.7.   Example 6.

Fig. 4.7. Example 7.

of the responses, MATCRV.BAT. This file can be edited with the appropriate changes, and the user can then select the batch mode.

Option 6, INIB13.EXE, allows the user to enter the required constants for Blocks 1 and 3 described in the previous section. This step must be executed prior to entry of initial conditions, Option 7. This step creates the data file BLK13.DAT. Table 4.11 illustrates an interactive session using 4 INIB13. This session creates a data file of control parameters for an initial MIGRAT run for a simulation time beginning at zero and continuing through day 40, generating output data sets for plotting at 10-day intervals. The value of MCYC is selected to be 20,000 cycles, which is sufficiently large to allow the simulations to run for the full 40 days. A value of PSIVRY of 10^{-3} was selected to allow a reasonably large time step.

Option 7, STEP7.EXE, is used to enter initial conditions which must be specified in Block 9 of the MIGRAT input data set. In this step, the user is asked for initial levels of saturation and initial concentrations of two contaminants for each layer and shown in Fig. 4.3.

The user has three options in specifying initial saturation conditions: (1) fully saturated, (2) equilibrium, and (3) an arbitrary level of saturation. For options (1) or (2), no additional information is requested of the user. The STEP7 software assumes that equilibrium conditions are with respect to an unconfined aquifer in layer 1. Consequently, this option is only appropriate for situations in which layer 1 is specified as fully saturated. For option (3), the user is requested to enter the desired level of saturation. The level of saturation is converted to potential for every cell within the layer by the STEP7 software. In any layer in which a non-zero initial contaminant concentration is specified, the user is asked if this layer is a perpetual source of concentration. If it is, the concentrations in this layer are held constant at the initial values. STEP7 creates the BLOCK9.DAT file which contains the MIGRAT Block 9 input data.

Table 4.12 documents a STEP7 interactive session. In this session, initial saturation values are full saturation for layers 1, 4, and 5, equilibrium for layer 2, and 80% saturation for layer 3. Layer 4 has initial concentrations of 0.001 and 0.1 for contaminants 1 and 2, respectively. Layer 5 is a perpetual source of contaminant 1 at a concentration of 0.001 and contaminant 2 at a concentration of 0.1.

Table 4.11. Listing of the interactive session for creating
Blocks 1 and 3

This program creates the BLOCK 1 and BLOCK 3 data as input to MIGRAT.
We begin with BLOCK 1.
Enter IPRINT - # of time steps between data output.
0
IPRINT =   0
Is the response correct? N means reenter.

Enter NUM - node # for which potential, rate of change of potential,
            source rate and time will be written for each time step.
0
NUM =   0
Is the response correct? N means reenter.

Enter KDATA - flag for controlling output: 0 normal,
            -1 minimal, 1 maximum.
-1
KDATA =   -1
Is the response correct? N means reenter.

Enter KSPEC - controls node classification and
            implicit difference calculations.
0
KSPEC =   0
Is the response correct? N means reenter.

Enter MCYC - maximum # of time steps:
            0 not used, negative #, problem ends after one time step.
20000
MCYC = 20000
Is the response correct? N means reenter.

Enter MSEC - maximum allowed machine time in seconds:
            0 not used, negative #, problem ends after one time step.
0
MSEC =   0
Is the response correct? N means reenter.

NPUNCH - flag for saving a restart data set upon normal termination of a job.
Always enabled (set to 1).
NPUNCH =   1
Enter NDOT -
0
NDOT =   0
Is the response correct? N means reenter.

Enter KSTDATA - nonzero, data or volume strain will be printed out.
0
KSTDATA =   0
Is the response correct? N means reenter.

Enter TIMEP - problem time interval between data output.
10
TIMEP = 1.000E+01
Is the response correct? N means reenter.

KD - symmetry-type indicator: 1 nonsymmetric,
            2 axisymmetric, 3 centrisymmetric.
   is always set to 1.
Enter DELT0 - maximum allowed time step; must be in range 10**-12 to 10**12

Table 4.11 (continued)

```
                    (10**12 is default or used if entered value is not within range.
                    Must be specified if KSPEC > 0!
2
DELTO =  2.000E+00
Is the response correct?  N means reenter.

Enter SMALL - minimum allowed time step (default is 2/3 of 1% of the
                    smallest time constant of any explicit node.  If at least
                    1/4 of the nodes are explicit, SMALL=10**-12).
1.e-12
SMALL =  1.000E-12
Is the response correct?  N means reenter.

Enter PSIVARY - desired maximum change in potential in each time step
                    (default=5.0).
1.e-3
PSIVARY =  1.000E-03
Is the response correct?  N means reenter.

Enter TAU - initial problem time.
0
TAU =  0.000E+00
Is the response correct?  N means reenter.

Enter TIMAX - maximum allowable problem time.  If negative
                    problem will end after first time step.
40
Is the response correct?  N means reenter.

Enter PSIMIN - minimum allowable pressure head in the flow domains.
                    Set to 10**-12 if ge PSIMAX or if unspecified.
-1e-12
PSIMIN =  -1.000E-12
Is the response correct?  N means reenter.

Enter PSIMAX - maximum allowable pressure head in the flow domains.
Set to 10**12 if le PSIMIN or if unspecified.
1.e12
PSIMAX =  1.000E+12
Is the response correct?  N means reenter.

PHIONE - initial potential (PHI=z+PSI) for all nodes for which PPHI is not specified
 is always set to zero (0.).
GONE - constant source or sink rate for all nodes for which GG is not specified
 is always set to zero (0.).
HONE - fluid mass transfer coefficient for all eternanal connections
for which no HSURE or a HSURT table is specified in BLOCK 6
 is always set to zero (0.)
PCONE - preconsolidation stress for all nodes
for which no PC(N) is specified in BLOCK 9
 is always set to zero (0.).
BLOCK 1 in now complete.  Begin BLOCK 3 data.
Enter AFLUID - name of the fluid (10 char. or less).
WATER
AFLUID = WATER
Is the response correct?  N means reenter.

Enter VISC - coefficient of viscosity (M/LT).
58
VISC =  5.800E+01
```

Table 4.11 (continued)

Is the response correct? N means reenter.

Enter BETA - compressibility of the fluid (LT**2/M).
1.17e-21
BETA = 1.170E-21
Is the response correct? N means reenter.

Enter RHOZ - density at PSI=0 (M/L**3).
62.5
RHOZ = 6.250E+01
Is the response correct? N means reenter.

Enter GEE - gravitational constant (L/T**2).
2.4e11
GEE = 2.400E+11
Is the response correct? N means reenter.

You have now completed the BLOCK 1, BLOCK 3 data set.
Stop - Program terminated.

Table 4.12. Listing of the interactive session for defining
initial conditions - Option 7 (grid2)

Is layer # 1 saturated (1), in equilibrium (2), or other (3)?
1
Layer # 1 is saturated   . Is that correct? N means reenter.

Is layer # 2 saturated (1), in equilibrium (2), or other (3)?
2
Layer # 2 is in equilibrium. Is that correct? N means reenter.

Is layer # 3 saturated (1), in equilibrium (2), or other (3)?
3
Layer # 3 is other   . Is that correct? N means reenter.

Is layer # 4 saturated (1), in equilibrium (2), or other (3)?
1
Layer # 4 is saturated   . Is that correct? N means reenter.

Is layer # 5 saturated (1), in equilibrium (2), or other (3)?
1
Layer # 5 is saturated   . Is that correct? N means reenter.

Enter the % saturation for layer # 3
80
The % saturation for layer # 3 = 80.0. Is the entry correct? N means reenter

Enter the total number pollutants
2
The total # of pollutants =   2
Is the response correct? N means reenter

Enter initial concentration of pollutant # 1 in layer # 1
0
The init .1 conc. of pollutant # 1 in layer # 1 =   .0000000E+00
Is the response correct? N means reenter

Is layer # 1 a perpetual source of contamination? Y means yes.

Layer # 1 is not a perpetual source of contamination.
i.e. concentrations are calculated in this layer.
Is the response correct? N means reenter

Enter initial concentration of pollutant # 1 in layer # 2
0
The initial conc. of pollutant # 1 in layer # 2 =   .0000000E+00
Is the response correct? N means reenter

Is layer # 2 a perpetual source of contamination? Y means yes.

Layer # 2 is not a perpetual source of contamination.
i.e. concentrations are calculated in this layer.
Is the response correct? N means reenter

Enter initial concentration of pollutant # 1 in layer # 3
1.e-3
The initial conc. of pollutant # 1 in layer # 3 =   .1000000E-02
Is the response correct? N means reenter

Is layer # 3 a perpetual source of contamination? Y means yes.

Layer # 3 is not a perpetual source of contamination.

Table 4.12 (continued)

i.e. concentrations are calculated in this layer.
Is the response correct? N means reenter

Enter initial concentration of pollutant # 1 in layer # 4
0
The initial conc. of pollutant # 1 in layer # 4 =   .0000000E+00
Is the response correct? N means reenter

Is layer # 4 a perpetual source of contamination? Y means yes.

Layer # 4 is not a perpetual source of contamination.
i.e. concentrations are calculated in this layer.
Is the response correct? N means reenter

Enter initial concentration of pollutant # 1 in layer # 5
1.e-3
The initial conc. of pollutant # 1 in layer # 5 =   .1000000E-02
Is the response correct? N means reenter

Is layer # 5 a perpetual source of contamination? Y means yes.
y
Layer # 5 is a perpetual source of contamination.
Is the response correct? N means reenter

Enter initial concentration of pollutant # 2 in layer # 1
0
The initial conc. of pollutant # 2 in layer # 1 =   .0000000E+00
Is the response correct? N means reenter

Is layer # 1 a perpetual source of contamination? Y means yes.

Layer # 1 is not a perpetual source of contamination.
i.e. concentrations are calculated in this layer.
Is the response correct? N means reenter

Enter initial concentration of pollutant # 2 in layer # 2
0
The initial conc. of pollutant # 2 in layer # 2 =   .0000000E+00
Is the response correct? N means reenter

Is layer # 2 a perpetual source of contamination? Y means yes.

Layer # 2 is not a perpetual source of contamination.
i.e. concentrations are calculated in this layer.
Is the response correct? N means reenter

Enter initial concentration of pollutant # 2 in layer # 3
0
The initial conc. of pollutant # 2 in layer # 3 =   .0000000E+00
Is the response correct? N means reenter

Is layer # 3 a perpetual source of contamination? Y means yes.

Layer # 3 is not a perpetual source of contamination.
i.e. concentrations are calculated in this layer.
Is the response correct? N means reenter

Enter initial concentration of pollutant # 2 in layer # 4
0
The initial conc. of pollutant # 2 in layer # 4 =   .0000000E+00

Table 4.12 (continued)

Is the response correct? N means reenter

Is layer # 4 a perpetual source of contamination? Y means yes.

Layer # 4 is not a perpetual source of contamination.
i.e. concentrations are calculated in this layer.
Is the response correct? N means reenter

Enter initial concentration of pollutant # 2 in layer # 5
1.e-1
The initial conc. of pollutant # 2 in layer # 5 =   .1000000E+00
Is the response correct? N means reenter

Is layer # 5 a perpetual source of contamination? Y means yes.
y
Layer # 5 is a perpetual source of contamination.
Is the response correct? N means reenter

Stop - Program terminated.

Option 8, STEP8.EXE, allows the entry of boundary conditions and external potentials. The user will be asked in sequence if the left, right, or top boundary is open (i.e., will have a boundary condition other than impermeable). For any boundary for which a positive response is provided, the user is prompted to enter the number of a layer (see Fig. 4.3) for which a boundary condition will be specified. The STEP8 software checks to verify that the selected layer intersects the selected boundary. If it does not, the user may reenter the data. Otherwise, a prompt appears to specify if a contaminant is entering the system through this boundary. If it is, the user will be asked to provide the appropriate contaminant concentration boundary conditions. The user is then asked if this is a constant head or constant flux boundary and subsequently requested to specify the desired head or flux. For the constant flux condition, the total length over which this flux is distributed is calculated and appears on the screen.

After all boundary conditions are entered, the user is asked if any drain (external potentials) layers (such as layer 4, Fig. 4.3) are included. If yes, the user will be prompted to enter the layer numbers of all layers that are drains.

STEP8 creates the BLOCK67.DAT file which contains input data for Blocks 6 and 7 of the MIGRAT code. Table 4.13 documents a STEP8 interactive session. The boundary conditions entered in this session are as follows: layer 1 is fixed at a constant head of 7.5 on the left and a constant flux of 10 on the right. A boundary concentration of 10^{-5} for contaminant 1 is specified for the right side of layer 1 to simulate the flux of contamination into the aquifer. A constant head of 32.5 is specified at the top of layer 5 to represent the perpetual presence of ponded water above the tailings.

Option 9, EDIT.EXE, has two main functions: The first is to allow the user to delete a layer for subsequent addition in conjunction with a program restart. For example, EDIT would be used if layers of mill tailings will be added at later times in the simulation. To accomplish this the user executes all previous steps and includes all layers. EDIT is used to remove all tailings layers not desired at the initial time. To use EDIT in this mode, the user is requested to specify data files to be edited and the layers to be

Table 4.13. Listing of the interactive session for defining
initial conditions - Option 8 (grid2)

You need to know the grid layer numbers for this program.
Look at the layer map.
rhoz=   .6250000E+02
You will be given a chance to enter drain data
 later. Do not consider a drain as an open boundary as
 response to the next inquiry.
Is the LEFT boundary open? Y means yes.
Y
Enter the layer # for an open boundary on the LEFT
1
The entered layer # = 1
Is the response correct? N means reenter.

Is contamination inflowing through this boundary? Y means yes.

left boundary at node =   1
left boundary at node =   2
left boundary at node =   3
amn= .1500000E+01
Is the boundary a constant head? Y means yes.
Y
Enter PHIB - the constant head at the boundary.
7.5
PHIB for LAYER #   1 = 7.500E+00
Is the response correct? N means reenter.

Is the LEFT boundary open? Y means yes.

Is the RIGHT boundary open? Y means yes.
Y
Enter the layer # for an open boundary on the RIGHT
1
The entered layer # = 1
Is the response correct? N means reenter.

Is contamination inflowing through this boundary? Y means yes.
Y
Contamination is inflowing through this open boundary.
Is the response correct? N means reenter.

Enter the boundary concentration for contaminant # 1
in layer # 1.
1.e-5
The boundary conc. for contaminant # 1 = 1.000E-05
in layer # 1
Is the response correct? N means reenter.

Enter the boundary concentration for contaminant # 2
in layer # 1.
0
The boundary conc. for contaminant # 2 = 0.000E+00
in layer # 1
Is the response correct? N means reenter.

right boundary at node =   89
right boundary at node =   90
right boundary at node =   91
amn= .2500000E+01
Is the boundary a constant head? Y means yes.

Table 4.13 (continued)

```
Total boundary area of layer #   1 =  9.500E+00
Enter the total flux (mass/time) through this layer.
10
Total flux =  1.000E+01
Is the response correct?  N means reenter.

Is the RIGHT boundary open?  Y means yes.

Is the TOP  boundary open?  Y means yes.
y
Enter the layer # for an open boundary on the TOP
5
The entered layer # =  5
Is the response correct?  N means reenter.

top boundary at node =   36
top boundary at node =   50
top boundary at node =   63
top boundary at node =   75
top boundary at node =   88
top boundary at node =   99
Is contamination inflowing through this boundary?  Y means yes.

amn=  .2000000E+01
Is the boundary a constant head?  Y means yes.
y
Enter PHIB - the constant head at the boundary.
32.5
PHIB for LAYER #   5 =  3.250E+01
Is the response correct?  N means reenter.

Is the TOP  boundary open?  Y means yes.

You are now ready to enter DRAIN data.
Enter the layer # for the drain.  0 means there
 are none or no more drains.
4
The entered layer # for a drain =  4
Is the response correct?  N means reenter.

drain at node =   60
drain at node =   61
drain at node =   72
drain at node =   73
drain at node =   85
drain at node =   86
Enter the layer # for the drain.  0 means there
 are none or no more drains.
0
The entered layer # for a drain =  0
Is the response correct?  N means reenter.

Stop - Program terminated.
```

deleted. The EDIT software creates a new MIGRAT input data set in which all
the computational cells within the delayed layers have been removed.
Table 4.14 illustrates an interactive session in which EDIT is used to remove
layer 5 (Fig. 4.3).

EDIT is also used to restart the MIGRAT code. In this mode, EDIT will
replace the original initial condition with the output of the previous MIGRAT
run. The user may also add previously deleted layers at this time. The user
is asked to enter layers to be added and the EDIT software extracts the
appropriate data from a specified master file and inserts these, where
appropriate, into the MIGRAT restart input data set.

An additional routine has been included with preprocessor software.
LAYOUT.FOR is not a step in the generation of input data by the preprocessor.
When executed, LAYOUT.EXE will create a file which contains a tabulation of
node numbers as assigned in STEP3. The output of LAYOUT.FOR is a file called
LAYOUT.PRT. Table 4.15 shows a listing of this file for the example problem.
The table contains node number as a function of the I,J indices of the
rectangular grid. Each I,J pair has two node number entries. For split
cells both entries are non-zero and correspond to node numbers associated
with the upper and lower portion of this split cell. For non-split cells,
only one entry is non-zero and corresponds to the assigned node number of
this single cell. To aid in understanding the reading of this table,
Fig. 4.8 shows the grid map with node numbers identified.

LAYOUT.FOR was developed to allow the user to enter certain parameters
which cannot be entered through the preprocessor. It is anticipated that
this routine will be used to assist in the entry of Block 8 data pertaining
to internal fluid generation and/or contaminant sources and sinks. This
Block requires the user to identify the node numbers corresponding to all
cells which are either source or sinks.

Table 4.14. Listing of the interactive session for editing
grid data - Option 9 (grid2)

Is this the first run of EDIT for this case?
EDIT needs to rewrite the BLOCK5 data set once to add contaminant concentrations
Y
          1 File(s) copied
          1 File(s) copied
          1 File(s) copied
Enter the desired action: 0 means exit from the program
                            1 means edit the master BLOCK 4, 5 and BLOCK 67 files
                            2 means edit the BLOCK 9 data set
                            3 means edit the BLK13.DAT data set by changing the time
                            4 means add layers to the BLOCK 4, BLOCK 5, BLOCK 6&7
1
The desired action indicator = 1
Is the response correct? N means reenter.

How many layers do you want removed from the master BLOCK 4, 5, and 67 data sets
1
The number of layers to remove = 1
Is the response correct? N means reenter.

Enter the index for layer # 1 to be removed.
5
Layer # 1 to be removed has index = 5
Is the response correct? N means reenter.

          34
          36
          49
          50
          62
          63   (nodes removed)
          74
          75
          87
          88
          98
          99
Enter the desired action: 0 means exit from the program
                            1 means edit the master BLOCK 4, 5 and BLOCK 67 files
                            2 means edit the BLOCK 9 data set
                            3 means edit the BLK13.DAT data set by changing the time
                            4 means add layers to the BLOCK 4, BLOCK 5, BLOCK 6&7
0
The desired action indicator = 0
Is the response correct? N means reenter.

Stop - Program terminated.

Table 4.15. Listing of the results from LAYOUT.FOR
(LAYOUT.PRT - file of node numbers)

NODE NUMBER MAP

J

| 11	0	0	0	0	0	0	0	0
	12	23	0	0	0	0	0	0
10	0	0	36	0	0	0	0	0
	11	22	35	50	63	75	88	99
9	0	0	34	0	62	74	87	0
	10	21	33	49	61	73	86	98
8	0	0	0	48	60	0	85	0
	9	20	32	47	59	72	84	97
7	0	0	0	46	0	0	0	0
	8	19	31	45	58	71	83	96
6	0	0	0	44	0	0	0	0
	7	18	30	43	57	70	82	95
5	0	0	0	0	0	0	0	0
	6	17	29	42	56	69	81	94
4	0	0	0	0	0	0	0	0
	5	16	28	41	55	68	80	93
3	4	15	27	40	54	67	79	92
	3	14	26	39	53	66	78	91
2	2	13	25	0	0	0	0	0
	0	0	0	38	52	65	77	90
1	1	0	24	0	0	0	0	0
	0	0	0	37	51	64	76	89
I	1	2	3	4	5	6	7	8

Centroid Map for Site 1
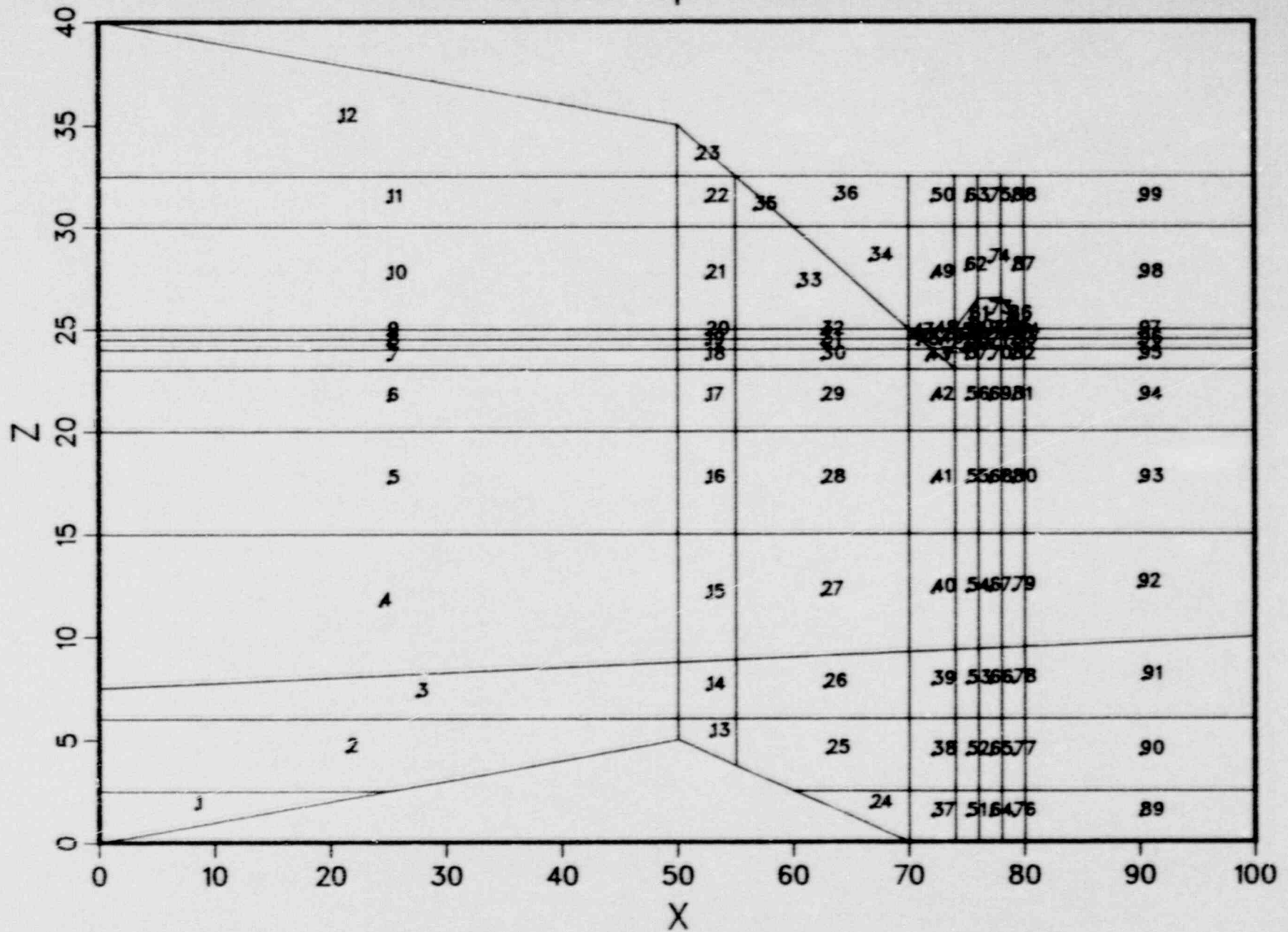
Fig. 4.8. The sample problem grid system showing the assigned node numbers.

5. MIGRAT EXECUTION

5.1 CONTROL PARAMETERS

The execution of the MIGRAT code requires the input of job control parameters in addition to the Block data sets described in Sect. 3. These parameters are input on logical unit 1005. These parameters and their format are given below.

Card 1   Format (1613)

1-3	I006	Logical unit number for standard MIGRAT output. If = 0 standard output is suppressed. A non-zero value specified for I006 will yield more detailed output than the user typically requires. It is recommended that this output only be generated when diagnostic information is required.
4-6	I007	Logical unit number for punched output. Not needed if output is returned to PC. If = 0, punched output is omitted.
10-12	IB13	Logical unit number for the input of Blocks 1 and 3 data.
13-15	IB02	Logical unit number for the input of Block 2 data.
16-18	IB04	Logical unit number for the input of Block 4 data.
19-21	IB05	Logical unit number for the input of Block 5 data.
22-24	IB67	Logical unit number for the input of Blocks 6 and 7 data.
25-27	IB08	Logical unit number for the input of Block 8 data.
28-30	IB19	Logical unit number for the input of Block 9 data.
31-33	IB09	Logical unit number for saving restart data.
34-36	IBT9	Logical unit number for saving restart data in case of abnormal program termination.
37-39	IB10	Logical unit number for the input of Block 10 data.
40-42	I031	Logical unit number for saving saturation output data.

| 43-45 | I032 | Logical unit number for saving moisture content output data. If = 0, moisture content output is suppressed. |
| 46-48 | I033 | Logical unit number for saving contaminant concentration output data. If = 0, contaminant concentration output is suppressed. |

The MIGRAT source code has a program statement that lists 30 tape units (TAPE11-TAPE40). All the logical unit numbers assigned in this card must be between 11 and 40.

<u>Card 2</u> Format (A1, 17A4, A2, A1, 4A2)

This is the problem name card. An asterisk (*) must appear in column 1 followed by a descriptive problem name.

<u>Card 3</u> Format (2I4)

| 1-4 | NTAPE | Output interval for writing to I007. |
| 5-8 | KKTRAN | Control parameter for the calculation of contaminant migration is =0 to suppress contaminant migration calculations and =1 to calculate contaminant migration. |

<u>Card 4</u> Format (A3, A2, I2, A1, 15A4)

1-5	ADATA	The work "BLOCK."
6-7	IBLOCK	Number of Block used.
8-78	ABLOCK	Optional user comment describing Block data set.

Note: One card is required for each Block data set to be input. The first card must either be blank or "BLOCK" in the above format.

The final two cards are:

ENDED - 2
*SPLIT

Table 5.1 lists the control cards for the problem developed in Sect. 4 and executed in Sect. 6.

Table 5.1.   Listing of CONTRL.DAT file (control cards for sample problem).

File: CONTRL.DAT

```
         10        20        30        40        50        60        70
.........|.........|.........|.........|.........|.........|.........|...|.

rec#
  1     6   0 30   1   2   4 11 12   0 13 17 19   0 31 32 33
  2   *     SAMPLE NRC CASE
  3   2000   1
  4
  5   BLOCK 1
  6   BLOCK 2
  7   BLOCK 3
  8   BLOCK 4
  9   BLOCK 5
 10   BLOCK 6
 11   BLOCK 7
 12   BLOCK 9
 13   ENDED-2
 14   *SPLIT

      .........|.........|.........|.........|.........|.........|.........|...|.
               10        20        30        40        50        60        70
```

5.2 PC-MAINFRAME COMMUNICATIONS

Communications between the PC and mainframe, either for transferring input data developed on the PC via the preprocessor for MIGRAT execution or for capturing MIGRAT output for graphical display on the PC, can be accomplished using appropriate communications software packages which are commercially available (e.g., ST100, XTALK, SCOM). This section provides communications information for the user which is specific to MIGRAT and its preprocessor. It is assumed that execution of the communications software can be accomplished by user.

All necessary input data for MIGRAT (with exceptions as noted in Sect. 3) are generated on the PC as data sets named BLK13.DAT. BLOCK2.DAT, BLOCK4.DAT, BLOCK5.DAT, BLK67.DAT, and BLOCK9.DAT. These files are transferred to the mainframe via the communications software. In the jobstream, the user must equate each of these file names with the tape number which corresponds to the logical unit specified in the first card of the control parameters (Sect 5.1). For example, if logical unit number 13 is assigned to the blocks 1 and 3 (columns 10-12 of control parameter card 1), the file BLK13.DAT must be equated to TAPE13. On computers such as the CYBER-176, these input data sets can be treated as "indirect files."

MIGRAT output to be transferred via the communications software to the PC for plotting or restart are output to logical units I031 (percent saturation), I032 (moisture content), and I033 (contaminant concentration) on the mainframe. When capturing these files on the PC, the user can assign arbitrary file names. It is recommended that the following file names be assigned for consistency with the graphics software: SATRES.DAT for logical unit I031, MOIST.RES for logical unit I032, and CONTAM.RES for logical unit I033.

5.3 OUTPUT DISPLAY AND RESTART

The steps necessary to see the results from MIGRAT are enabled with the GRID3 menu. See Table 5.2 for a listing of the GRID3 menu. Table 5.3 shows the grid3.bat file that drives the menu program.

The sequence of steps for using the PC to analyze the MIGRAT output and preparing for a restart are as follows:

Table 5.2.   MIGRAT Postprocessor (grid3) Menu

```
            ------>    MIGRAT Postprocessor    <------

Note:  Do not strike carriage return for menu selection!

    0 - Exit to DOS ......................................

    1 - Plot Saturation Results from MIGRAT (FOR31.RES) .

    2 - Plot Conc. Results from MIGRAT (FOR33.RES) ......

    3 - Expand Saved Plots (Pop Files) ..................
```

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Table 5.3.   Listing of the grid3.bat file

```
:menu
echo off
assign
cls
type grid3.txt
getdigit                        Press key for desired option:
cls
echo working....
if errorlevel 3 goto exppop
if errorlevel 2 goto plotcc
if errorlevel 1 goto plosat
if errorlevel 0 goto exit
:badopt
echo Invalid option
pause
goto exit
:plosat
plosat /r 2000
goto menu
:plotcc
plotcc /r 2000
goto menu
:exppop
coppop
expnrc /r 2000
goto menu
:exit
cls
ver
cd
```

(1) Use the grid3 menu to plot saturation or contaminant concentrations at time intervals TIMEP specified in Block 1. See Table 5.2 for the listing of the grid3 menu. Table 5.3 is the grid3.bat file that drives the postprocessor menu.

(2) Use EDIT, which is the grid2 menu, to create restart Block data sets by (a) changing initial and final simulation times, output time interval, total number of time steps, PSIVRY if smaller or larger time steps are desired, etc.; (b) modifying Blocks 4, 5, 6, 7, and 9 as a result of inclusion or deletion of layers.

(3) Transfer the revised input data sets to the mainframe for restart.

Figure 5.1 is a sample plot of concentration for pollutant #1 results from executing MIGRAT on the mainframe and capturing and plotting the FOR33.RES file on the PC. This plot was received from Option 2. In addition, the user can expand the saved plots (pop files) from the grid1 and grid2 menus by using Option 3 of the grid3 menu. That option requires a response to the following query (Note that the appropriate plot must have previously been saved in a pop file.):

Enter the indicator for the type of plot:

  1 means ORIGINAL GRID

  2 means LAYER MAP

  3 means MATERIAL MAP

  4 means CENTROID MAP

  5 means CONNECTION MAP

  6 means MATERIAL PROPERTIES

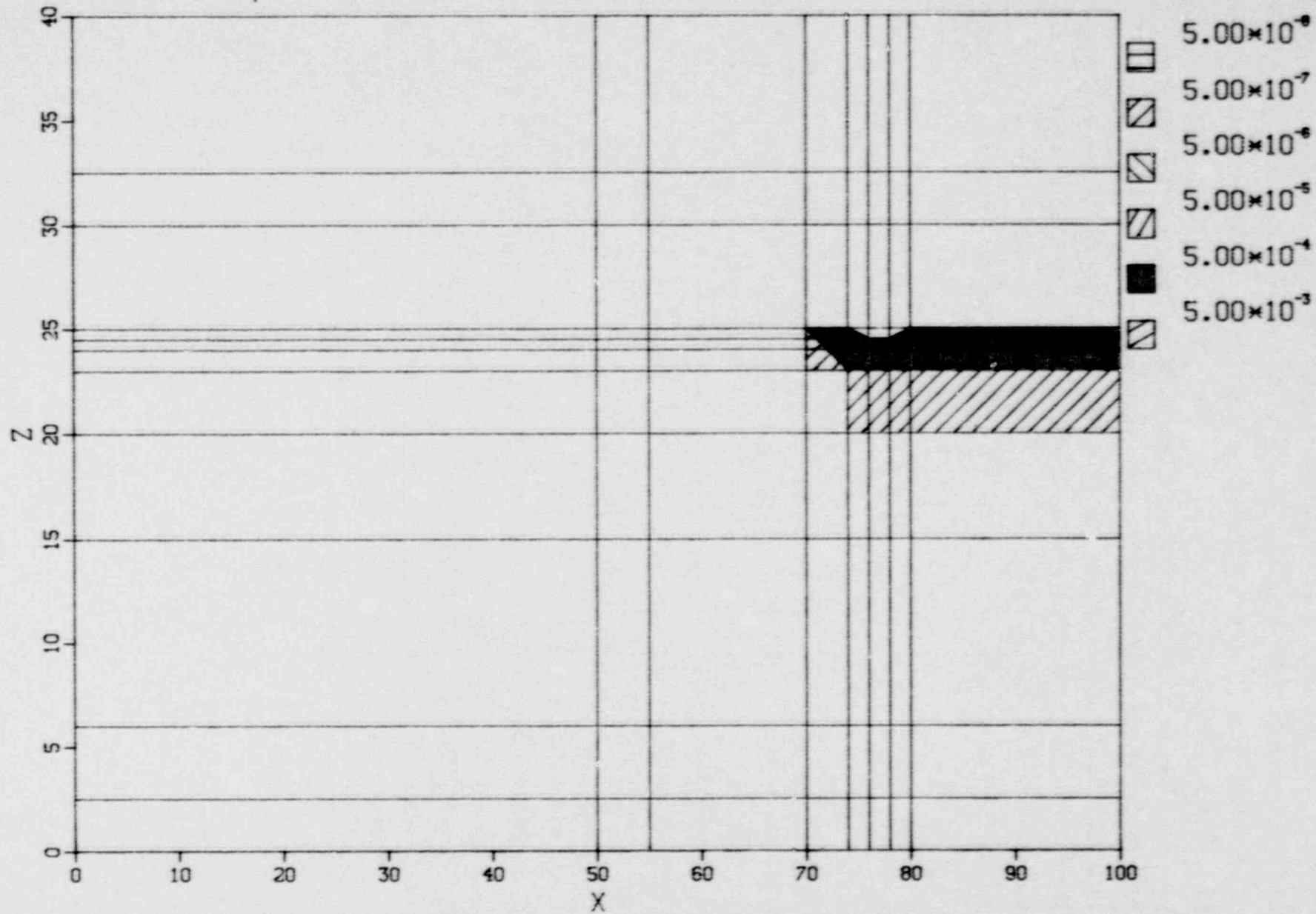 7 means SATURATION RESULTS

  8 means CONCENTRATION RESULTS.

Fig. 5.1. Concentrations of contaminant 1 at 10 days.

6. TEST CASE SIMULATIONS

Results of the MIGRAT code applied to the sample problem introduced in Sect. 4 are provided here. The code was first run for a simulation period of 40 days without the tailings layer (layer 5). Figures 6.1 through 6.3 show contaminant concentration levels at 10-day intervals from day 20 through day 40. The results for day 10 are shown in Fig. 5.1. Table 6.1 is a listing of the interactive session used to generate these plots. Features of interest in these plots include the advection of contaminant 1 from right to left across the aquifer and the migration of both contaminants into the drain and adjacent sandstone.

Following the initial 40-day simulation period, the code was restarted with the inclusion of the tailings layer. The simulation was continued until day 200. Table 6.2 is a listing of the EDIT interactive session used to generate the modified input data set for the restart. Figure 6.4 shows the distribution of both contaminants at day 200. At this time, contaminant 1 has been advected across the entire unconfined aquifer, and both contaminants have migrated out of the tailings pit.

The sample problem executed here was developed to illustrate the use of the preprocessor. To reach this end, the minimum grid system for this case was used. Therefore, the results of the simulation should be viewed in this context and with the knowledge that the grid system must be finer particularly in the neighborhood of the tailings pit sidewall in order to realistically represent migration from the tailings pit.

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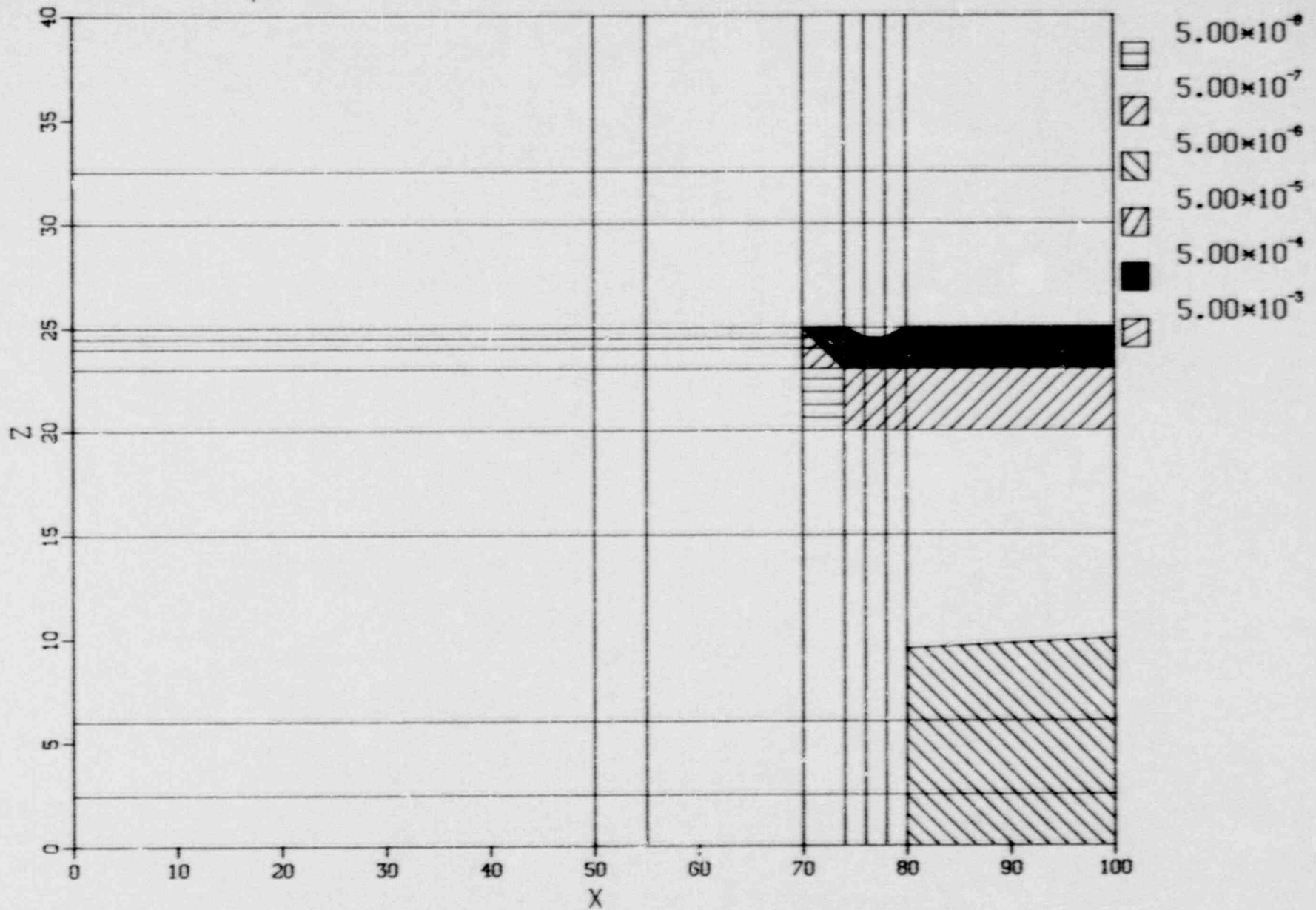
Fig. 6.1. Concentrations of contaminant 1 at 20 days.
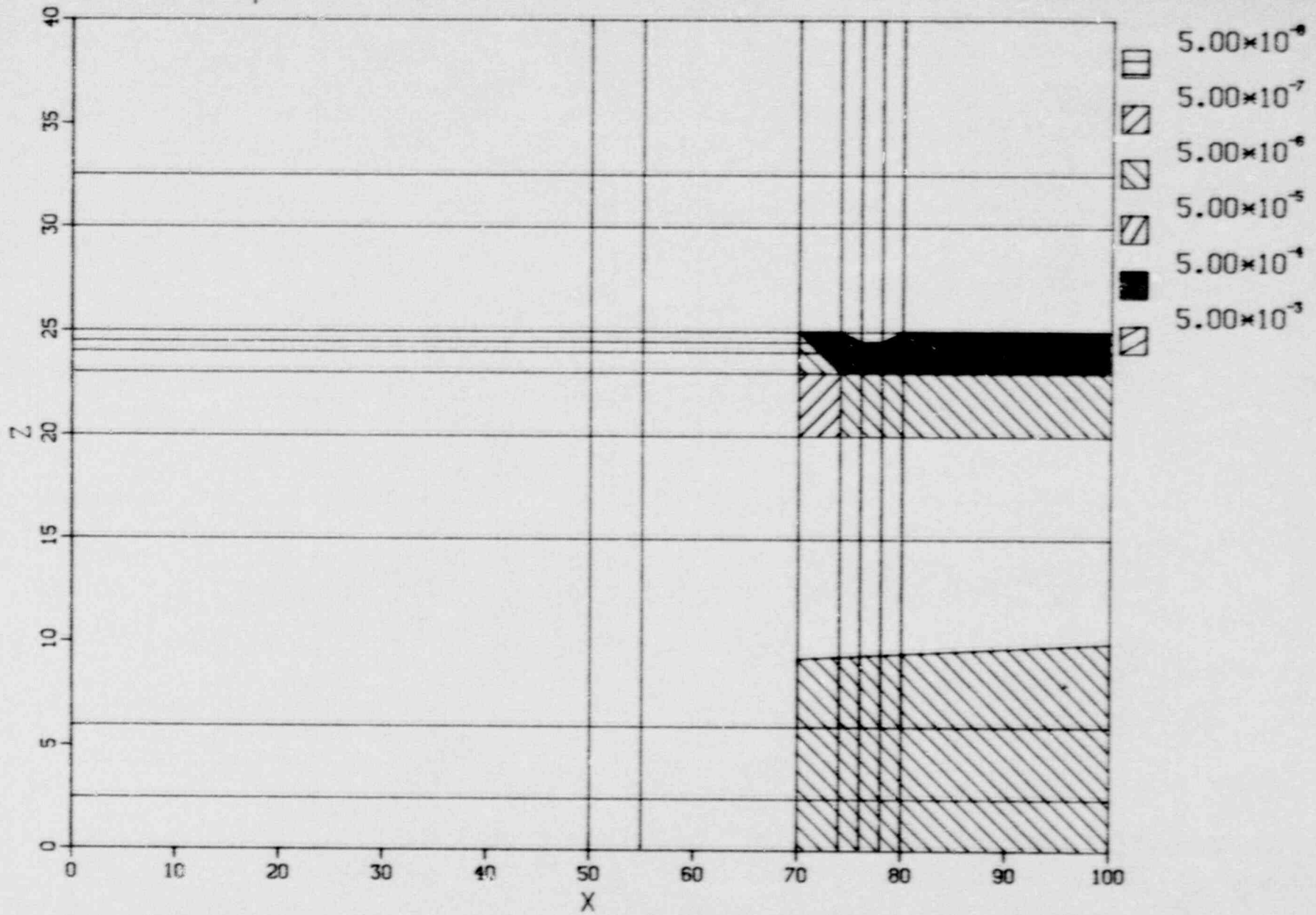
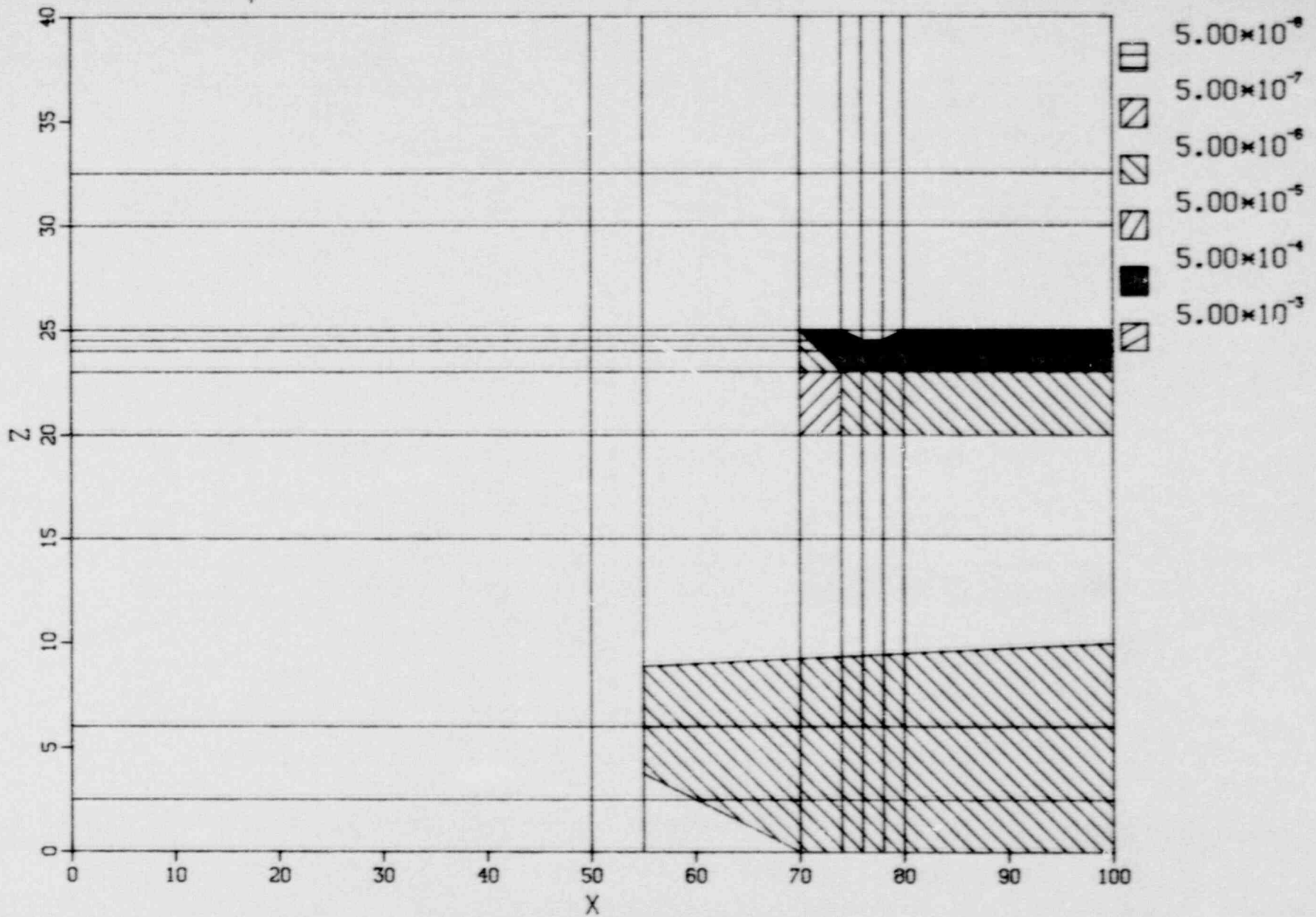Fig. 6.2. Concentrations of contaminant 1 at 30 days.

Fig. 6.3. Concentrations of contaminant 1 at 40 days.

Table 6.1. Listing of the interactive session used to plot contaminant
concentration results - Option 2 (grid3)

=====>   MIGRAT Postprocessor   <=====

Note: Do not strike carriage return for menu selection!

   0 - Exit to DOS ....

   1 - Plot Saturation Results from MIGRAT (FOR31.RES) .

   2 - Plot Conc. Results from MIGRAT (FOR33.RES) ......

   3 - Expand Saved Plots (Pop Files) ....

           Press key for desired option:2working....
Enter type of plot: 1 means to the IBMEGA,
                    2 means to the IBMCGA,
                    3 means to the IBMPGA,
                    4 means to the HP7475 Plotter,
                    5 means save the plot (pop file).
4
How many contaminants do you want plotted?
     1 means contaminant # 1, -1 means contaminant # 2
1
Do you want to assign the contour levels? Y means yes.
y
How many levels are there (must be < 7)?
for contaminant # 1
6
The # of contour levels for contaminant # 1 = 6
Is the response correct? N means reenter.

Enter the contour levels in ascending order!
Enter contour level # 1
5.e-8
Contour level # 1 = 5.000E-08
Is the entry correct? N means reenter.

Enter contour level # 2
5.e-7
Contour level # 2 = 5.000E-07
Is the entry correct? N means reenter.

Enter contour level # 3
5.e-6
Contour level # 3 = 5.000E-06
Is the entry correct? N means reenter.

Enter contour level # 4
5.e-5
Contour level # 4 = 5.000E-05
Is the entry correct? N means reenter.

Enter contour level # 5
5.e-4

Table 6.1 (continued)

Contour level # 5 = 5.000E-04
Is the entry correct? N means reenter.

Enter contour level # 6
5.e-3
Contour level # 6 = 5.000E-03
Is the entry correct? N means reenter.

Stop - Program terminated.

Table 6.2. Listing of the EDIT interactive session - Option 9 (grid2)

Is this the first run of EDIT for this case?
EDIT needs to rewrite the BLOCK5 data set once to add contaminant concentrations
n
Enter the desired action: 0 means exit from the program
                            1 means edit the master BLOCK 4, 5 and BLOCK 67 files
                            2 means edit the BLOCK 9 data set
                            3 means edit the BLK13.DAT data set by changing the time
3   4 means add layers to the BLOCK 4, BLOCK 5, BLOCK 6&7
The desired action indicator = 3
Is the response correct? N means reenter.

        1 File(s) copied
You are changing the time of simulation in the BLK13.DAT data set.
Enter the starting time for this simulation.
40
The starting for the simulation = 4.0000E+01
Is the response correct? N means reenter.

Enter the ending time for this simulation.
2000
The ending time for the simulation = 2.0000E+02
Is the response correct? N means reenter.

Do you want to change PSIVARY? Y means yes.
n
Enter the desired action: 0 means exit from the program
                            1 means edit the master BLOCK 4, 5 and BLOCK 67 files
                            2 means edit the BLOCK 9 data set
                            3 means edit the BLK13.DAT data set by changing the time
4   4 means add layers to the BLOCK 4, BLOCK 5, BLOCK 6&7
The desired action indicator = 4
Is the response correct? N means reenter.

You will add layers to BLOCKS 4,5,6,7 & 9.
Enter the # of layers to add and their indices.
1 7
The layer(s) to be added =   7
Is the response correct? N means reenter.

        1 File(s) copied
        1 File(s) copied
        1 File(s) copied
Enter the desired action: 0 means exit from the program
                            1 means edit the master BLOCK 4, 5 and BLOCK 67 files
                            2 means edit the BLOCK 9 data set
                            3 means edit the BLK13.DAT data set by changing the time
0   4 means add layers to the BLOCK 4, BLOCK 5, BLOCK 6&7
The desired action indicator = 0
Is the response correct? N means reenter.

Stop - Program terminated.

Conc. Map for Pollutant #1 at Site 1 at time 200.0

Legend:
- 5.00×10^{-8}
- 5.00×10^{-7}
- 5.00×10^{-6}
- 5.00×10^{-5}
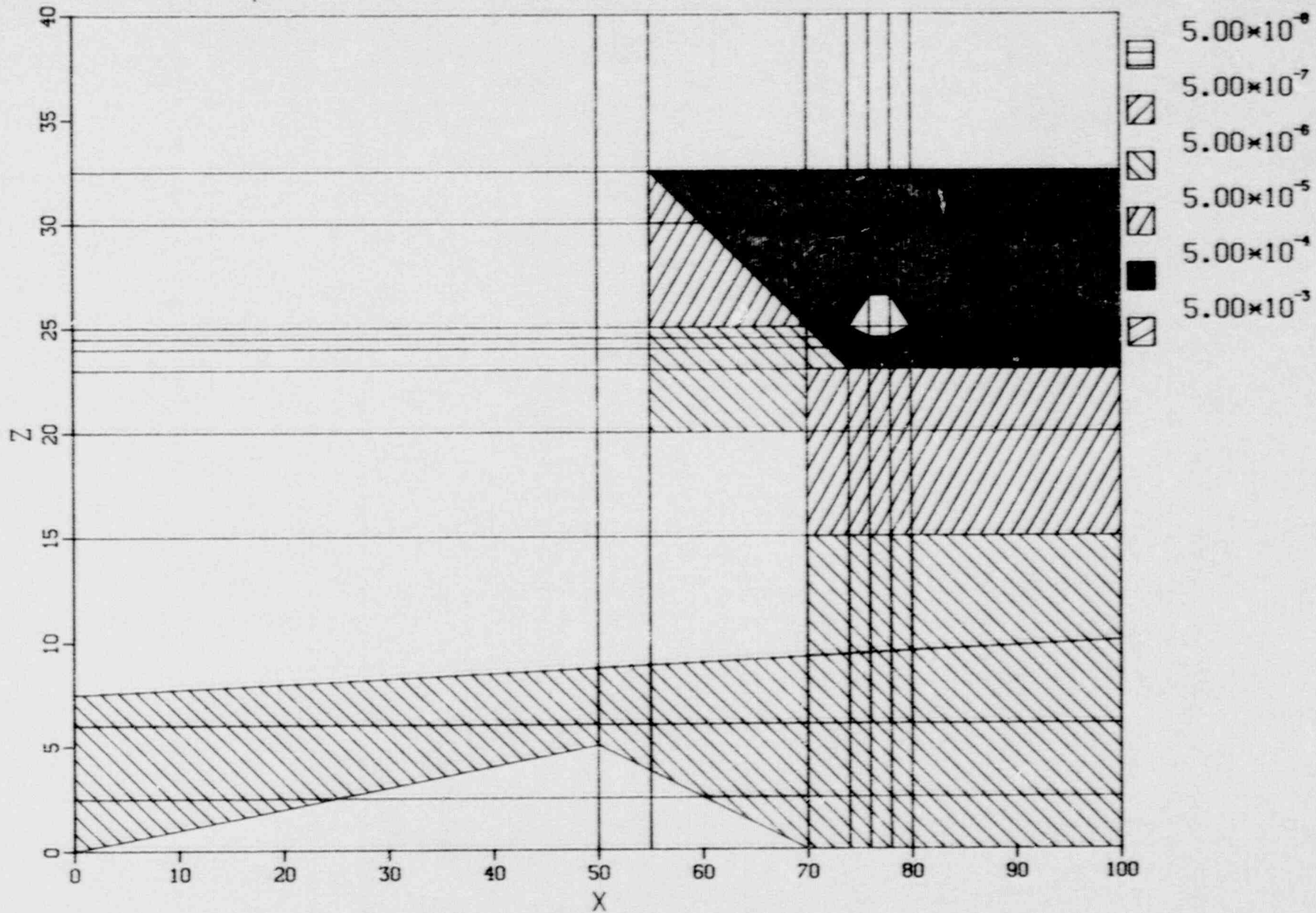- 5.00×10^{-4}
- 5.00×10^{-3}

Fig. 6.4(a). Concentration of contaminant 1 at 200 days.
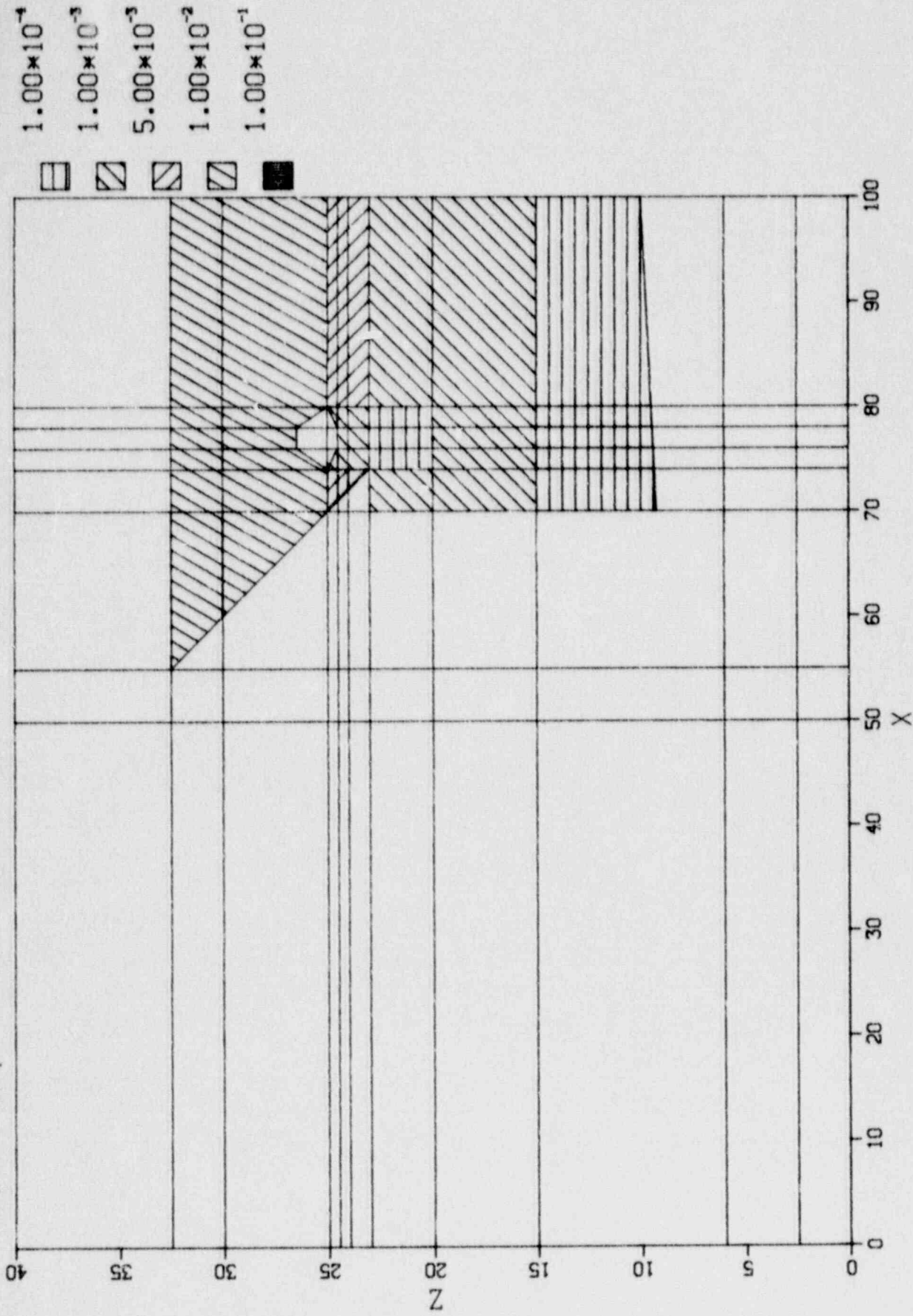
Conc. Map for Pollutant #2 at Site 1 at time 200.0

Fig. 6.4(b). Concentration of contaminant 2 at 200 days.

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10. SUPPLEMENTARY NOTES

11. ABSTRACT *(200 words or less)*

MIGRAT is a state-of-the-art computer code that numerically solves Richard's equation for the migration of moisture in the unsaturated zone and the advective diffusion equation for the associated movement of contaminants. This code utilizes the integral form of these governing equations. This formulation allows the use of polygonal computational cells which can provide an accurate representation of the modeled region. The penalty for this realism is the extensive input data necessary for model applications. In order to render the MIGRAT code more suitable for routine applications, an interactive preprocessor has been developed which allows a user to enter input data rapidly and in a more convenient format. The preprocessor is designed for use on a personal computer to allow the user to develop, modify, and display input data prior to its transmission to a mainframe for MIGRAT execution. Model output can be captured by the personal computer for display utilizing the preprocessor's graphics software.

12. KEY WORDS/DESCRIPTORS *(List words or phrases that will assist researchers in locating the report.)*

MIGRAT code
contaminant transport