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MEMORANDUM FOR: Malcolm R. Knapp
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FROM: Michael F. Weber
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SUBJECT: SUPPLEMENTAL INFORMATION ABOUT SWIFT

During the Hydrogeology Modeling Meeting of March 7 and 8, 1983, Mark Reeves, of GeoTrans, Inc., answered several questions about the implementaion of SWIFT (version 4.81). These questions evolved during the application of SWIFT in the NRC 2-D modeling of BWIP. The following memorandum provides the specific questions and their answers discussed by NRC, GAI, and Dr. Reeves.

1. Where are the Aquifer Influence Functions (AIF's) enforced and how is this information interpreted by the code?

(AIF's are described on pages 76-79 in User's Manual.)

For the side boundary conditions (VAB=[1.0, 2.0, 3.0 or 4.0]), constant pressures are specified at the top center of the external side face of the grid block. Constant temperatures and concentrations are specified in the center of the external side face. Figure 1 illustrates the enforcement location of all AIF's.

Constant Pressures along the top of the grid (VAB=5.0) are enforced at the top center of the grid block. Constant temperatures and concentrations are also enforced at the top center of the grid block. If ΔZ is the vertical grid block spacing for the top layer, then the desired boundary pressure is chosen $\Delta Z/2$ above the top of the grid block. This pressure is then hydrostatically corrected back to the top face-center of the grid block. The user enters the pressure at this location by using the following formula:

$$P_o = P_o' + \rho g \, (\Delta z/2)$$

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where P_o' = desired boundary pressure at $\Delta z/2$ above top block center
$\Delta Z/2$ = the displacement above the top grid block where the boundary pressure is chosen but not enforced
ΔZ = the vertical thickness of the top layer grid blocks
ρ = average density of fluid within top layer grid blocks
P_o = constant boundary pressure actually enforced
g = gravitational constant

Along the base of a model, VAB=6.0, the user must manipulate head (or pressure) data to prepare the boundary pressures for input into SWIFT. Pressure AIF's are enforced $\Delta Z/2$ above the grid block center of the bottom layer, i.e., at the top center of the block. AIF's for temperature and concentration are enforced at the bottom block center.

To specify a constant pressure along the base, the user should first determine the pressure to be maintained at the grid block center in the lowest layer. These pressures must then be corrected to compensate for hydrostatic translation of the grid block center pressure to a grid-block top center location. The constant pressure specified as an AIF influences, but does not control absolutely, the pressure at this location (i.e., top face center of the lowest layer blocks). Mathematically,

if P_o' = the desired boundary pressure at the grid block-center,

then $P_o = P_o' - \rho g\ (\Delta Z/2)$

where P_o = enforced pressure at top center of grid block
ρ = average density of water within lowest layer grid block (at input T)
$\Delta Z/2$ = half the thickness of the lowest layer grid block

The following approach is taken to calculate the flow rate to the lowest layer blocks from the external system underlying the grid, or

$$U \alpha T\ (p_o' - \rho g(\Delta Z/2) - P)$$
$$\text{or } U \alpha T(P_o - P)$$

where U = flow rate across the lower grid block face in the Z direction; the positive direction is into "the grid"
T = transmissivity of bottom grid block
P_o' = pressure at grid block center (lower layer)

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DATE	83/03/21					

ρ = average density within the grid block
ΔZ = thickness of grid block in lowest layer
P = pressure as determined at grid block face center
P_o = P_o' corrected for hydrostatic decrease in pressure

Thus, if there is flow in the vertical direction, the enforced pressure boundary condition, P_o, will not equal the calculated pressure, P, even though they are both referenced to the same point.

For purposes of the external hydrostatic correction to the boundary pressures, one would probably use a reference density. The calculation density is, however, permitted to vary within the bottom layer.

2. What is the ITHRU=2 option and how does this alter the output?

When ITRHU=2 is specified on the R2-1 card, the pressure maps will reflect the variations in density due to thermal perturbations within the flow system. Two pressure maps for a 2-D transient simulation of BWIP are included as Figures 5 and 6 to illustrate the effect of changing ITHRU from 0 to 2. The initialization parameters are shown in Figure 2. These changes result from differences in the datum pressure equation. When ITHRU=0,

$$P_{datum} = P_{node} - \rho g\ (h-h_{datum})$$

where P_{datum} = pressure at datum as printed in the pressure maps
P_{node} = pressure at grid block node (block center)
ρ = reference density
h = elevation at node (elevation increases downward)
h_{datum} = elevation at datum

When ITHRU=2, however, $P_{datum} = P_{node} - (\rho g)dz$, since ρ is no longer constant through the system. This is particularly important in transient simulations of HLW repositories as the decaying radioactive wastes emit heat to the surrounding geohydrologic system. So for any node within the reservoir, when ITHRU=2, the pressure at datum calculation may be shown schematically as in Figure 3.

Once the pressures have been plotted with ITHRU=2, they may be converted into hydraulic heads using the reference ρg term in SWIFT.

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DATE	83/03/21					

3. Can AIF's and overburden/underburden (OB/UB) boundaries be used along the same boundary blocks?

If boundary blocks are specified as OB/UB blocks, then they should not also be specified as AIF blocks. Otherwise the specified thermal boundaries will be physically inconsistent. The constant temperature of the AIF simulates an external system that is at constant temperature, whereas the OB/UB blocks simulate a thermal gradient within this same external system. The AIF temperature, a constant boundary temperature, will generally result in the sharpest temperature gradient and, therefore yield the largest heat transport out of the system. The temperature AIF will probably dominate the OB/UB heat transport.

This effect can be illustrated in the temperature profiles for the various temperature boundary options available in SWIFT as shown in attached Figure 4.

If a modeler wishes to use OB/UB with in transient non-isothermal models with flow boundaries at top and bottom, then wells must be utilized as water sources or sinks. The use of wells as boundary conditions may be difficult if the direction of flow changes as the system heats up. In this situation, the wells will "shut-in."

4. Can the solution technique L2SOR be used in vertical 2-D models (i.e., J=1)?

L2SOR can often be used to solve the flow and transport equations when J=1, but there is a bug in the 4.81 version of SWIFT arising from the inadvertant use of the same memory location of a mapping variable and a L2SOR variable. Code users will recognize this failure easily, as the model will crash prior to completion.

L2SOR is an overrelaxation method which calculates spectral radii and optimal relaxation parameters of the solution matrix for the first and second time solutions. Radii(ρ_s) and relaxation parameters (ω_i) are also determined for every fifth solution thereafter. The iterative procedure of radius and relaxation parameter determination is detailed below.

For Solutions 1, 2, and 5n+2, where n = integer > 0

(1) calculate ρ_s for x, y, and z directions through iteration (maximum number of iterations is 10).

(2) compute $\omega_i = \omega_i(\rho)$, i=x, y and z
$f_{it} = \omega f_{it+1} + (\omega-1)f_{it}$, where $1 < \omega < 2$ for overrelaxation

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NAME						
DATE	83/03/21					

(3) choose direction i for which ω_i = maximum ω

(4) print ω_i as X-DIR, y-DIR, and/or Z-DIR parameters

(5) print $it_{\rho(max)}$ as the number of iterations (ITNS)

Other comments:

- The finite difference solution for a block-centered mesh with unequal node spacing, in general, will not be consistent locally with decreasing Δx, Δy, and/or Δz spacings for unequal spacings. "Consistent" means reduction to the analytical solution in the limit. The effect of inconsistencies is generally smoothed out throughout the grid, and the deviations from the analytical solution are small (see Aziz and Settari, pp. 78ff).

- Where i and j are adjacent grid blocks, and k is a coordinate direction, the ratio of $\Delta k_i/\Delta k_j$ should either be maintained as 1, or they should be adjusted so that $\Delta k_{i+1} - 2\Delta K_i + \Delta K_{i-1} = 0$. Thus, a set of dimensions such as 2, 3/2, 4/3, 5/4 would yield a consistent solution, ~0.

- The aspect ratio (the ratios of block dimensions) can be extreme (>20 to 1) in models with flow predominantly in the direction of a principal axis (x, y, or z). If flow is diagonal compared to the principal axes, the grid orientation effects will be severe, so that the aspect ratio should be minimized to reduce these numerical problems.

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cc: Eileen Poeter
Mark Reeves
Nestor Ortiz
Ellen Quinn
Ben Ross
Roy Williams

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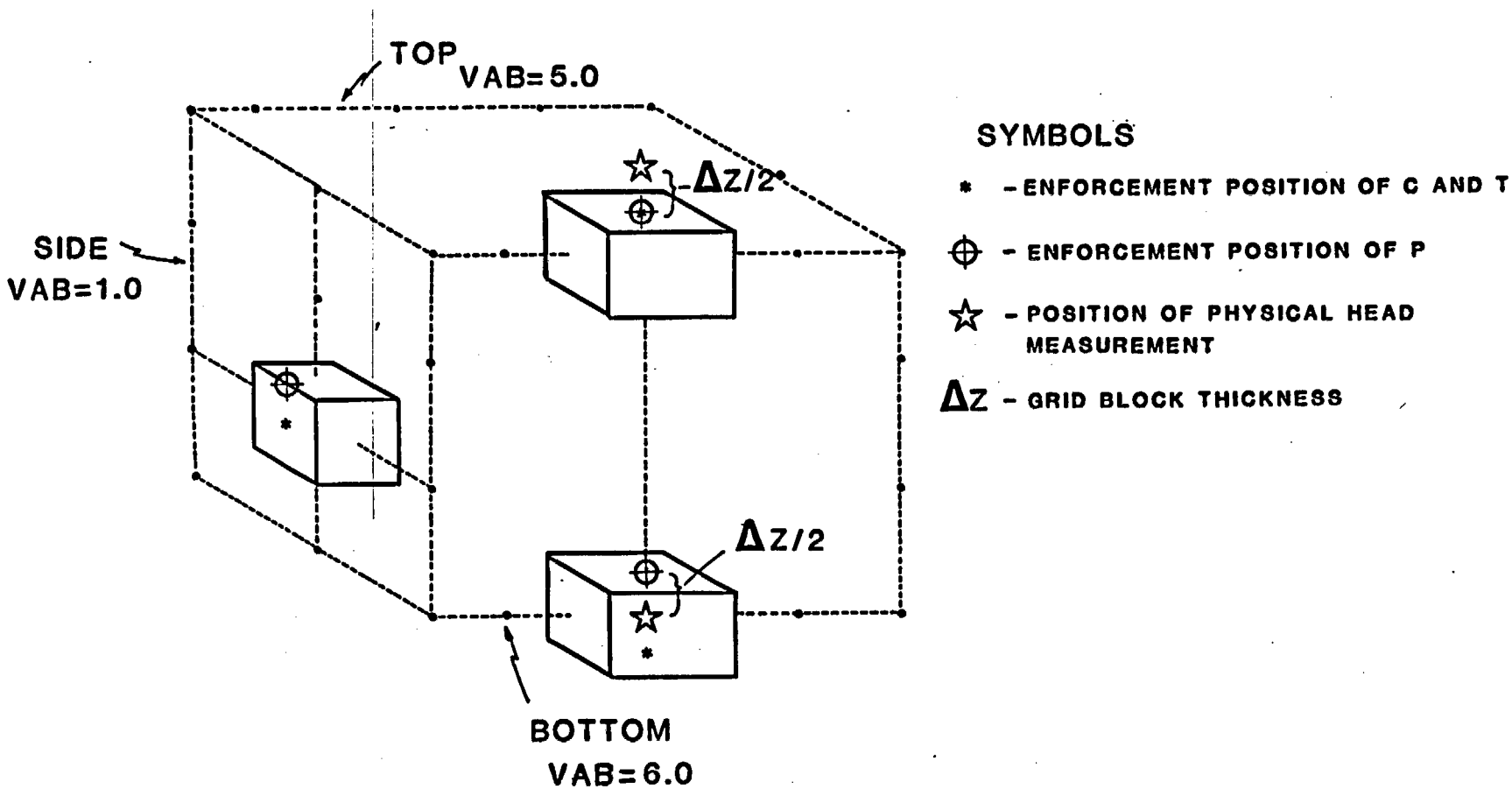


Figure 1. Positions of Aquifer Influence Functions (see text for explanations).

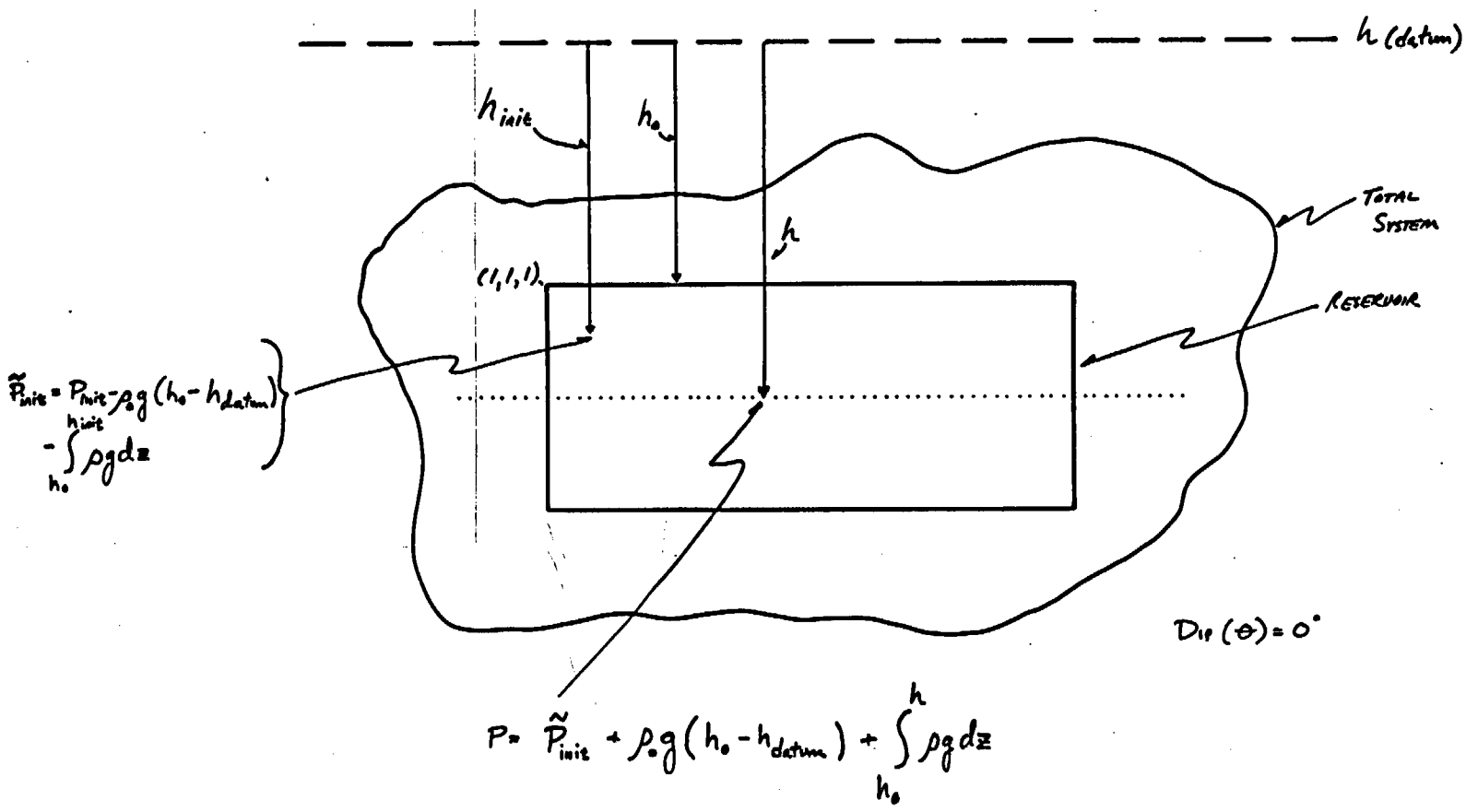


Figure 2. Initial Conditions and Pressure Calculations

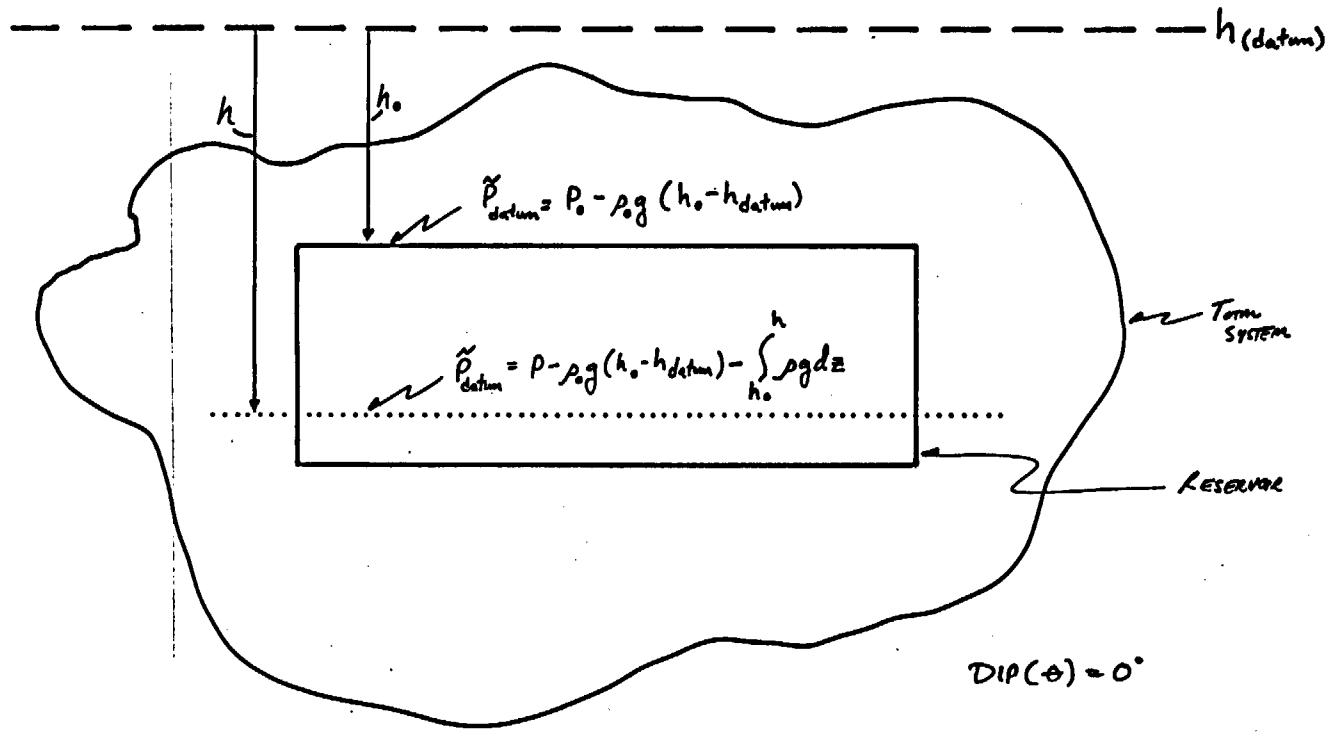


Figure 3. Calculation of P_{datum} when ITHRU=2 inside and outside of the grid.

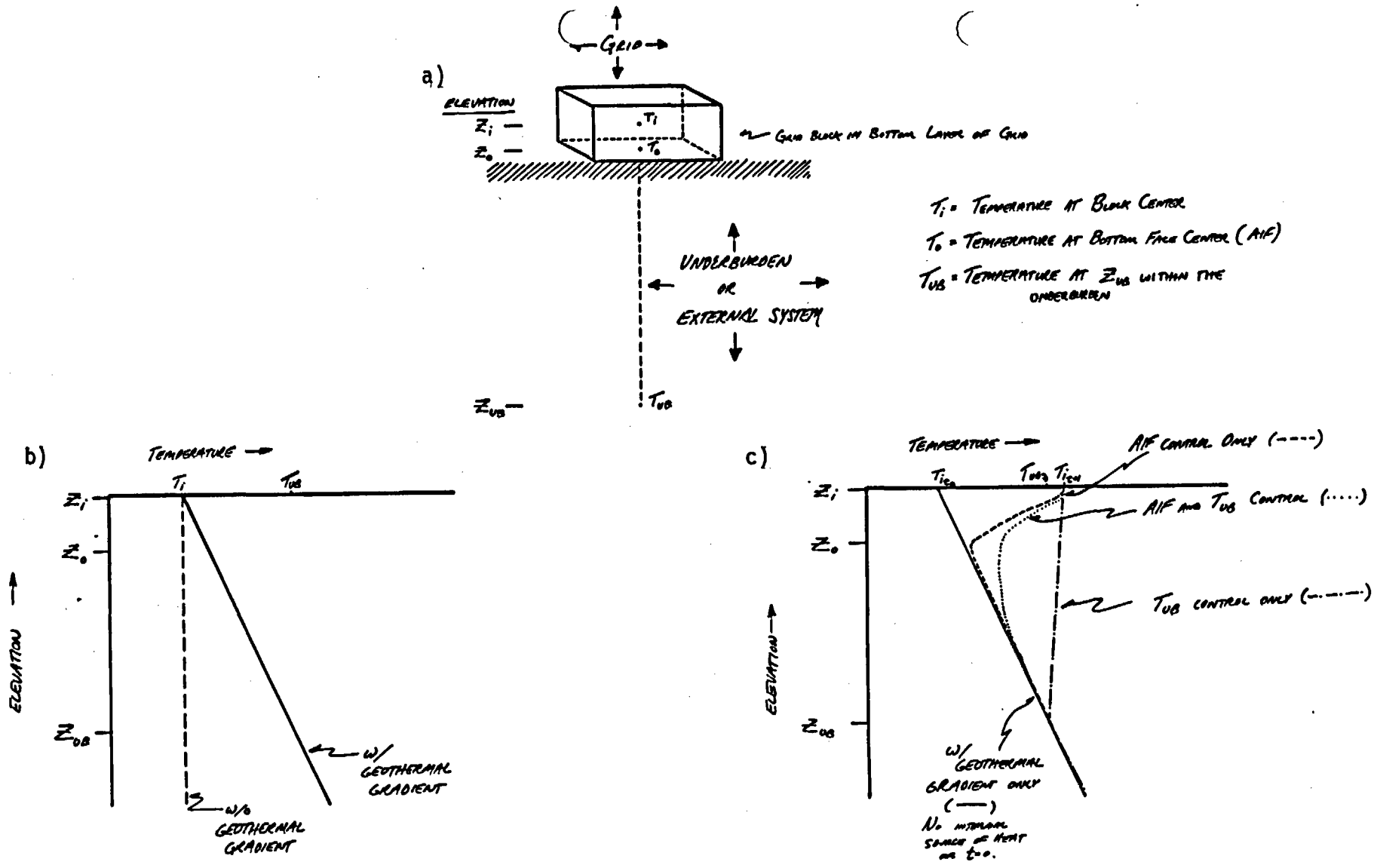
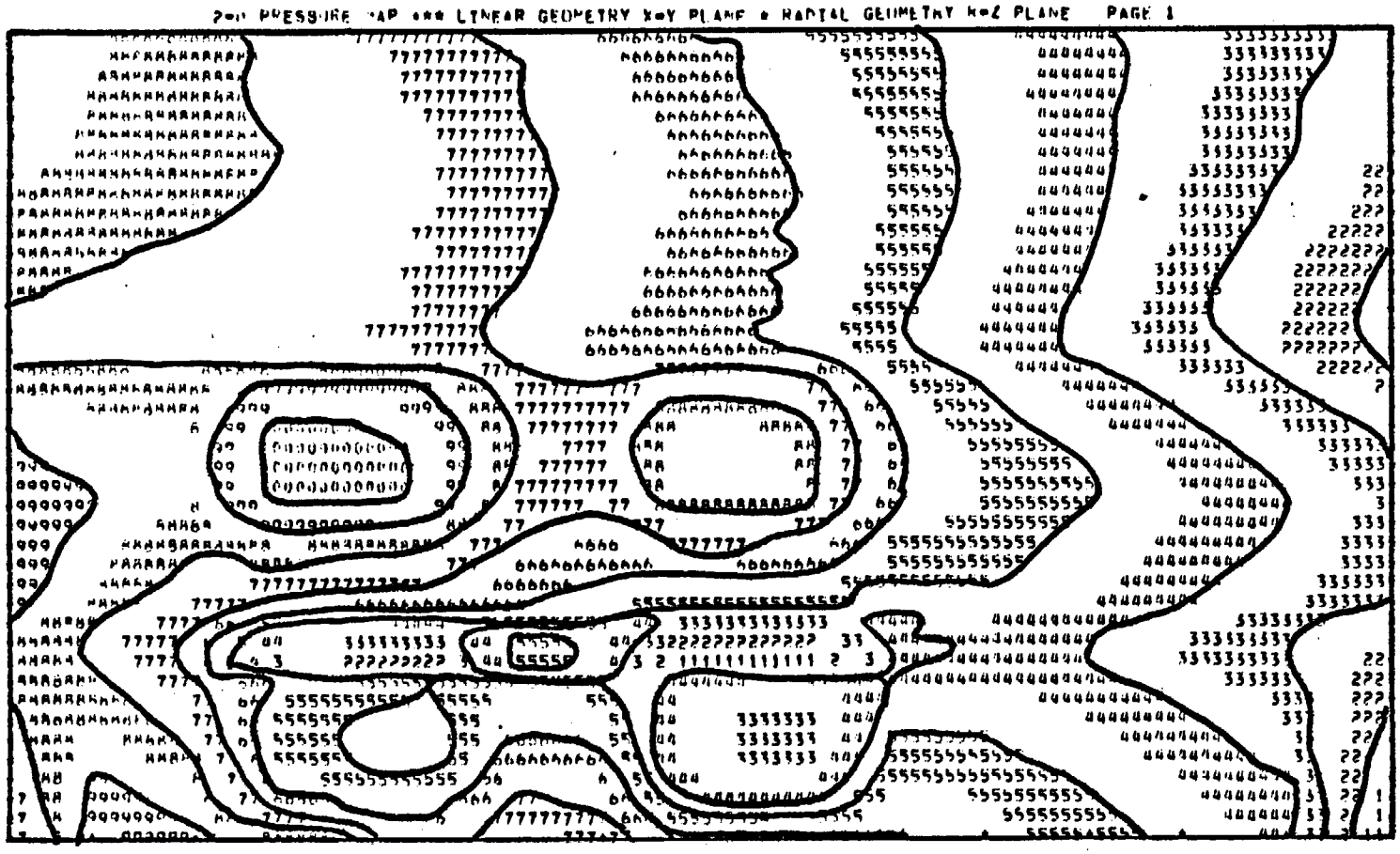


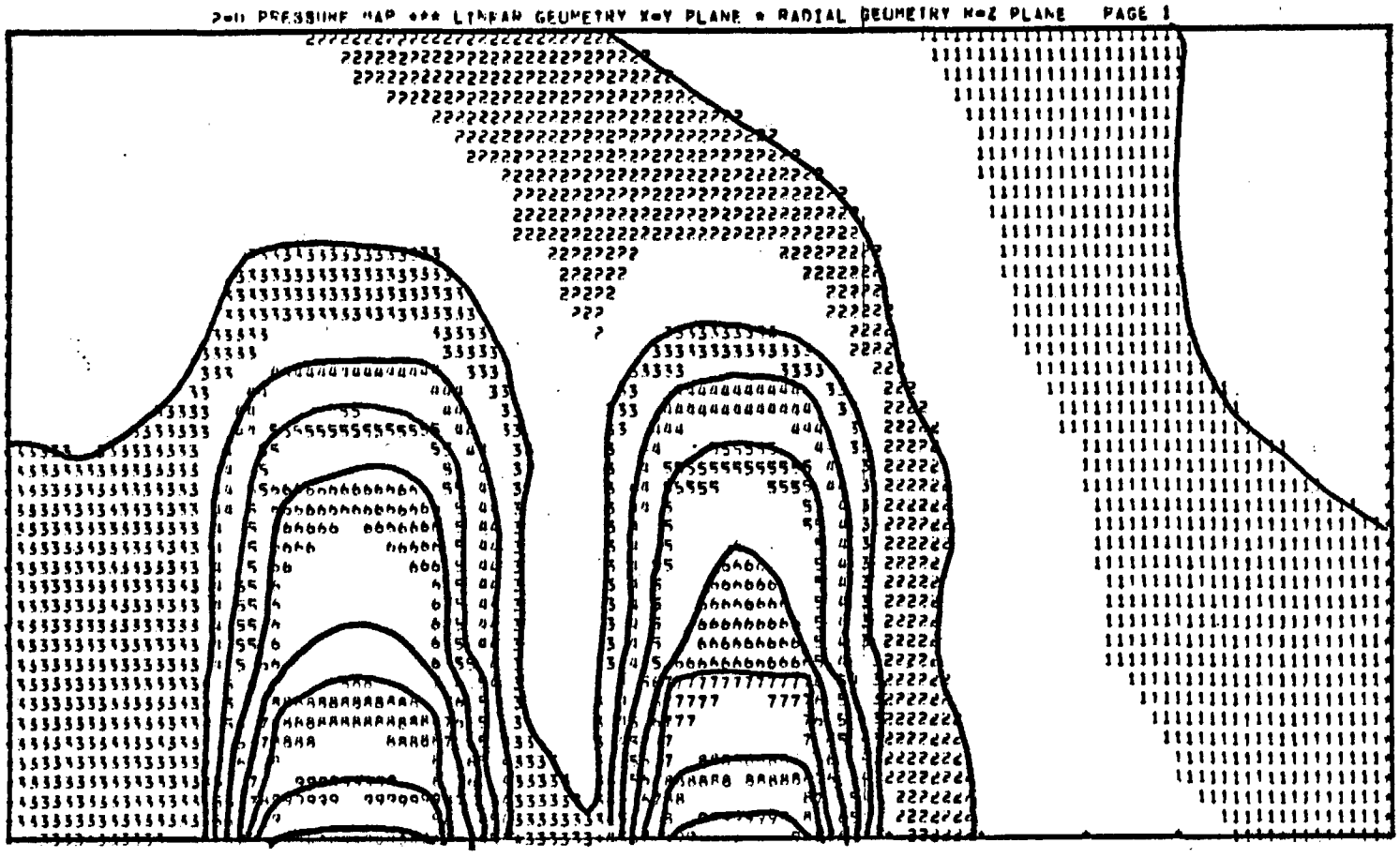
Figure 4. Temperature boundary conditions for basal blocks with their associated temperature profiles with internal sources of heat in the grid.

a) locations of the model temperatures for comparison
b) initial temperature profiles below the grid with and without a geothermal gradient
c) temperature profiles below grid for transient simulations w/internal heat sources



DEPENDENT VARIABLE RANGE	MAP CHARACTER		
0. = 1.134E+06			
1.134E+06 = 1.139E+06	1	1.189E+06 = 1.194E+06	6
1.139E+06 = 1.145E+06		1.194E+06 = 1.200E+06	
1.145E+06 = 1.150E+06	2	1.200E+06 = 1.205E+06	7
1.150E+06 = 1.156E+06		1.205E+06 = 1.211E+06	
1.156E+06 = 1.161E+06	3	1.211E+06 = 1.216E+06	8
1.161E+06 = 1.167E+06		1.216E+06 = 1.222E+06	
1.167E+06 = 1.172E+06	4	1.222E+06 = 1.227E+06	9
1.172E+06 = 1.178E+06		1.227E+06 = 1.233E+06	
1.178E+06 = 1.183E+06	5	1.233E+06 = 1.238E+06	0
1.183E+06 = 1.189E+06			

Figure 5. SWIFT Pressure at Datum plot with ITHRU = 0. Pressure is mapped in Pascal units.



DEPENDENT VARIABLE RANGE	MAP CHARACTER
0. - 1.149E+06	
1.149E+06 - 1.164E+06	1
1.164E+06 - 1.179E+06	
1.179E+06 - 1.194E+06	2
1.194E+06 - 1.209E+06	
1.209E+06 - 1.223E+06	3
1.223E+06 - 1.238E+06	
1.238E+06 - 1.253E+06	4
1.253E+06 - 1.268E+06	
1.268E+06 - 1.283E+06	5
1.283E+06 - 1.298E+06	
1.298E+06 - 1.313E+06	6
1.313E+06 - 1.328E+06	
1.328E+06 - 1.342E+06	7
1.342E+06 - 1.357E+06	
1.357E+06 - 1.372E+06	8
1.372E+06 - 1.387E+06	
1.387E+06 - 1.402E+06	9
1.402E+06 - 1.417E+06	
1.417E+06 - 1.432E+06	0

Figure 6. SWIFT Pressure at Datum plot with ITHRU = 2. This plot is realistic. The pressure distribution in Figure 5 is unrealistic. Pressure is mapped in Pascal units.