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Date: July 14, 1992

To: B.M. Butcher, J. Schreiber, and P. Vaughn (6342)

P.B. Davies Steve E.D. Gorham

From: P.B. Davies, S.W. Webb, E.D. Gorham (6119)

Subject: Feedback on "PA Modeling Using BRAGFLO -- 1992" 7-8-92 memo by J. Schreiber

As a follow-up to our discussions at the June 25th meeting, J. Schreiber's memo (attached) describes the configuration and rationale for repository/Salado modeling using BRAGFLO in the PA 1992 calculations. At B. Butcher's request, we have reviewed these descriptions and the following paragraphs summarize our feedback. You need to be aware that in order to respond in the very short time frame requested, this is only a brief review by those individuals that were available over the past 3 days. Therefore, this review does not cover the level of detail that should ideally be given and this review does not have input from a number of pertinent staff members. We feel that PA's effort to articulate model configuration and rationale and to incorporate feedback prior to starting simulations is a significant step forward in communications. We also feel that working through multiple iterations of this process in the months prior to calculations has the potential to significantly improve the calculations in future years. Our comments on the proposed configuration for this year are as follows:

1. The modified configuration for human intrusion scenarios is based on an "equivalent radial panel" scaled to match the initial excavated volume of a single panel. The Schreiber memo expresses concern that the 60.85 meter radius of this equivalent panel is small compared to the potential travel path distance in an actual panel (218 meters max.). Therefore, it has been suggested that the high permeability (and increased porosity) DRZ above and below the panel be extended outward to a radius of 96.78 meters. The stated rationale for this is 1) "to include some of the effect of the greater travel distances in an actual panel" and 2) to "include the DRZ above and below the pillars". There are two potential problems with this rationale. First, the original reasons for considering travel distance within an actual panel centered around the question of how much *waste* could be "accessed" by brine flow *within a panel* (Lappin et al., 1989; Marietta et al., 1989). Because there is no waste within the DRZ, extending the travel distance within the DRZ does not appear to address questions related to travel path length through waste within an actual panel. Second, the concept of "including the DRZ above and below the pillars" is confusing because other than a relatively short (roughly 1 meter) DRZ that occurs along room walls, this is no DRZ above or below the pillars. One might consider extending the DRZ in order to capture the potential increased gas storage volume if we had good information about the dimensions, porosities, and evolution of the DRZ. However, these

are poorly known and at this point do not provide a reasonable rationale for extending the DRZ. In summary, extension of the DRZ above the pillars has the effect of increasing pore volume in the DRZ to a level that cannot be substantiated by the available data. Therefore, we recommend that DRZ not be extended above the salt pillar.

2. The illustration of the model configuration is somewhat confusing in that it gives the appearance that the anhydrite interbeds start at the lateral edge of the DRZ and transition zones. Perhaps these schematics would benefit by showing how the geologic units fit into the model zones.

3. Why and how are the Culebra and the Unnamed Lower Member of the Rustler lumped in these calculations? The Unnamed Lower Member of the Rustler Formation is a dissolution residue at the contact between the Rustler and Salado. While this unit is a significant water-bearing unit in Nash Draw, it thins considerably and its transmissivities at the WIPP site are orders of magnitude lower than those in the Culebra. We do not see any good reason to lump these two units and suggest that unless there is some compelling reason not stated in the Schreiber memo as to why the Unnamed Member should be included, the Culebra Dolomite should be the only Rustler unit to be modeled explicitly.

4. Where does the 0.675 value for waste porosity (i.e. average disposal room porosity) come from? The initial porosity in the SANCHO closure calculations is 0.66. These calculations provide the basis for the creep closure porosity surface. The maximum porosity in F.T. Mendenhall's GRIDB.DAT porosity surface file is 0.565.

5. The permeability, porosity, and initial pressure are all specified in the document. What about the specific storage parameters? What are the values and what are they based on?

6. We (6119 and 6342) have not yet reached good closure on the question of the far field permeability distribution for the anhydrite interbeds. The original recommendation (model configuration and parameter distributions transmitted to PA 4-1-92 by E.D. Gorham) was to use only permeability values from a limited number of tests (3) in non-depressurized anhydrite. This approach assumed that the PA model for the 1992 calculations would be capable of including increased permeability due to fracture dilatation in response to elevated gas pressures. When it became apparent that fracture-based permeability changes will not be available in the '92 models, it was recommended that an attempt be made to crudely incorporate the effects of gas-driven increases in fracture permeability by specifying a much larger far-field permeability range for the anhydrite that included not only the non-depressurized tests, but also the group of tests in depressurized but substantially intact anhydrite and the group of tests in anhydrite that has experienced substantial fracturing in the DRZ (E.D. Gorham 6-15-92 memo). This approach was considered unrealistically conservative by performance assessment personnel in the June 25th meeting and a compromise was reached that 1) the performance assessment calculations will not attempt any representation of the interbed fracture process in the '92 calculations; 2) that explicit caveats will be placed visibly in the report that this potentially significant process was not included in the calculations; and 3) the field permeability for the anhydrite interbeds will be represented by the small group of tests in non-

depressurized anhydrite interbeds together with the much larger group of tests in depressurized but substantially intact anhydrite. While this compromise appears to be acceptable to most people, it should be recognized that this distribution is not without potential flaws that could perhaps be corrected if there were sufficient time to construct a new distribution that focused on capturing the uncertainty in whether or not some of the tests in the depressurized but substantially intact anhydrite have in fact experienced significant permeability enhancing deformation. Given the present time constraints, we suggest that the compromise distribution be used, but that it be recognized that this distribution is not without potentially important flaws.

7. Where does the DRZ porosity relationship [TZ poros + x(0.06-TZ poros)] come from and what is its purpose? We understand that in general terms, this is intend ed to relate sampled values of DRZ porosity with those from the transition zone, but there is not enough information in the Schreiber memo to fully understand this. Also, if sampled porosities between these zones are being related, shouldn't sampled permeabilities be related as well? At some point in future calculations, serious consideration should also be given to correlation of sampled permeability with sampled porosity.

8. What is the basis for the seal permeability and porosity? Are these values from recommendations from 6121?

9. We are pleased to see that the effects of depressurization of the Salado during the operation phase are being taken into account explicitly and that this appears to be a relatively straightforward task in the current PA model setup.

10. The specification of initial saturation conditions in the waste and especially in the DRZ is a difficult problem. The manual adjustment of saturations in the DRZ could lead to significant problems in correctly calculating brine mobility and gas storage volume within this zone. The approach proposed in the Schreiber memo is to start the DRZ fully brine saturated but at the end of the 20-year depressurization to manually reduce the brine volume to that which would be present prior to any adjustment (increase) of the DRZ porosity. This approach essentially assumes no substantial flow from the far field into the DRZ during the 20-year depressurization period. Given the presently specified range of anhydrite permeabilities, this is probably an unrealistic assumption. Given that this manual adjustment of the DRZ does not have a strong technical basis and that its effect is probably non-conservative (i.e. it produces less brine for gas generation and more open pore volume of gas storage), we recommend that the depressurization be run (which may produce some desaturation itself) with the specified DRZ porosity and permeability at the start of the run and that this manual saturation adjustment not be made. Another possible approach would be to not take credit for any increase in porosity in the DRZ, which we may have difficultly defending over a 10,000 year time frame.

11. The description of the relative permeability and capillary pressure curves looks good. The difficulty mentioned in defining the capillary pressure curve for a material at less than residual brine saturation is easily overcome if a maximum capillary pressure value is specified; this value can then be used if the saturation is below the brine residual

saturation value. Also, the last sentence seems to imply that a region can start out with residual saturation or higher, but the value can become below residual saturation during the calculation. We assume the only way this can happen is in the redefinition of the porosity in the DRZ regions and that it does not happen otherwise.

REFERENCES

Gorham, E.D. (6119). *Additional Suggestion for 1992 PA Calculations.* 6-15-92 Memorandum to B.Butcher and M. Tierney (6342).

Lappin, A.R., R.L. Hunter, D.P. Garber, P.B. Davies. 1989. *Systems Analysis, Long-Term Radionuclide Transport, and Dose Assessments, Waste Isolation Pilot Plant (WIPP), Southeastern New Mexico; March 1989.* SAND89-0462, Sandia National Laboratories, Albuquerque, New Mexico.

Marietta M.G., S.G. Bertram-Howery, D.R. Anderson, K.F. Brinster, R.V. Guzowski, H. Iuzzolino, R.P. Rechard. 1989. *Performance Assessment Methodology Demonstration: Methodology Development for Evaluating Compliance With EPA 40 CFR 191, Subpart B, for the Waste Isolation Pilot Plant.* SAND89-2027, Sandia National Laboratories, Albuquerque, New Mexico.

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PA Modeling Using BRAGFLO -- 1992

J. Schreiber, 7/8/92

Geometry

Human Intrusion Scenarios -- Axisymmetric cylindrical equivalent panel.

The equivalent panel will preserve the initial excavated volume and the initial excavated height of a panel. The panel as modeled will be a cylinder; it will include only the initial excavated volume, and not the pillars, as was done last year. The radius of the cylindrical panel is 60.85 m. The radius used last year is that of an enclosed panel (including pillars), 96.78 m. Since the maximum travel distance in a panel will be less this year owing to the smaller equivalent panel radius, it is desirable to increase the effective radius of the cylinder to simulate more closely the greater travel distances in an actual panel. The distance from the center of an actual panel to a far corner is 138 m, while the greatest travel distance in an actual panel (from panel center to the middle of the end of a panel, going around pillars) is 218 m. To include some of the effect of the greater travel distances in an actual panel, the high-permeability DRZ above and below the cylindrical panel was extended out to last year's radius of 96.78 m, which in effect will include the DRZ above and below the pillars. At the level of the waste, the DRZ does not extend laterally beyond the panel waste; the material beyond the 60.85 m radius of the panel, which can be thought of as the pillars, is treated as intact halite. From the top of Anhydrite a+b to the top of MB138, out to a radius of 96.78 m, is a composite region, the "Transition Zone", which is 9.24 m thick and is assumed to have the same properties as intact anhydrite. The mesh extends vertically from the bottom of the Castile brine reservoir to the top of the Culebra Member of the Rustler Fm, with the Unnamed Member lumped in with the Culebra.

Undisturbed Scenario -- Entire repository, rectangular geometry

The excavated volume of the entire repository is represented by a single rectangular region, and includes no pillars or panel seals. This mesh is essentially the same as the one used in the May 1992 RCRA calculations ("Case 3"). The mesh preserves the initial excavated volume of various regions and their original excavated heights. The panel seals and backfilled drifts between the repository and the Waste Shaft are lumped into a single region of high permeability. The four shafts are consolidated into a single shaft located at a distance from the repository equal to the distance to the actual Waste Shaft. To the north of the shaft is a region that represents the initial excavated volume of the experimental region. This mesh contains the same DRZ's and Transition Zones as the cylindrical panel mesh. These regions extend laterally 1 m beyond the waste to the south and 1 m beyond the experimental region to the north, and includes a 1-m-thick DRZ at the south end of the repository and a 1-m-thick DRZ at the north end of the experimental region. This mesh extends vertically from the top of the Castile Fm to the top of the Culebra Member of the Rustler Fm; the Culebra and Unnamed Members are lumped together. The thickness of the shaft seal will vary from 10 m to 50 m.

Material Properties

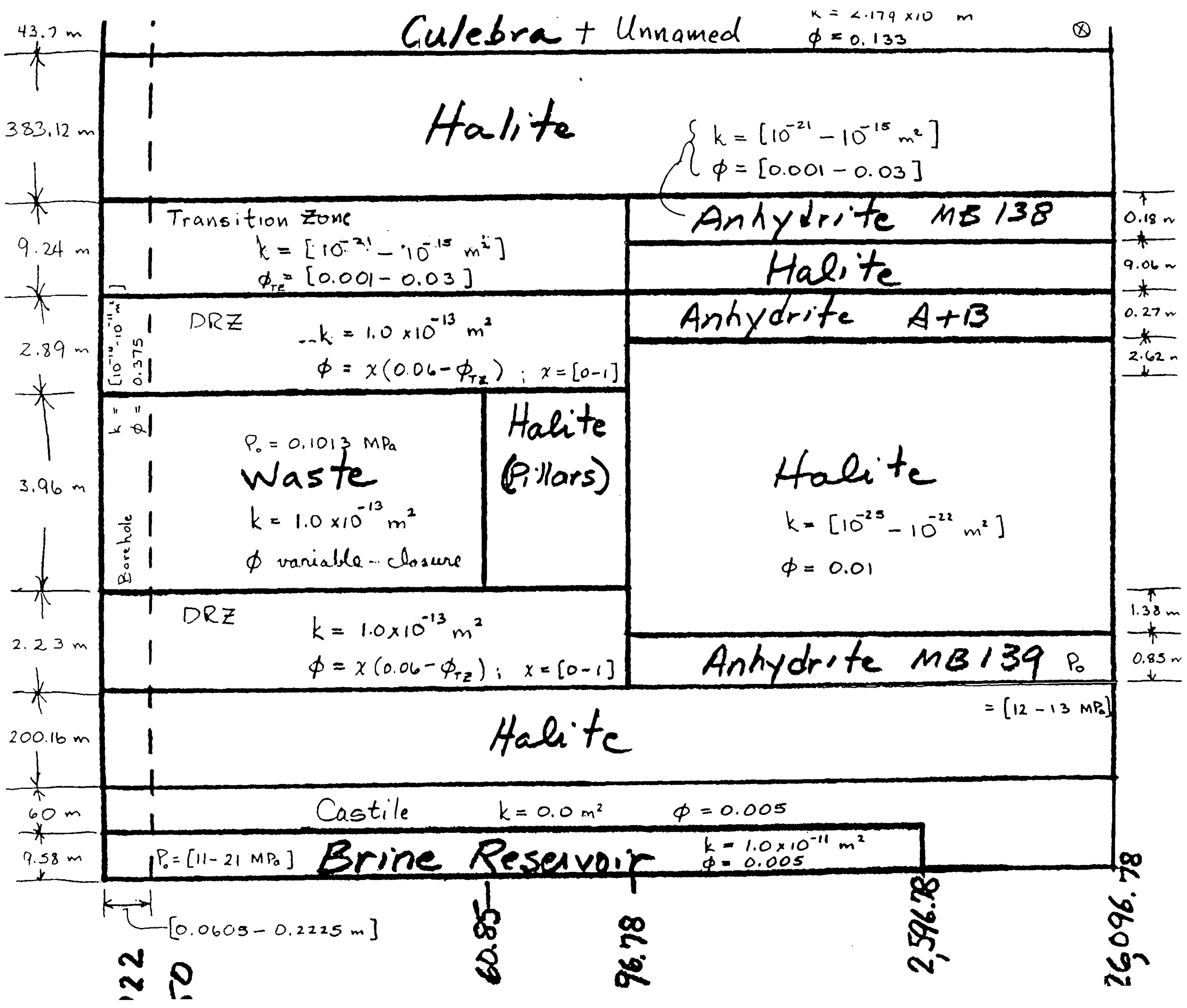
The initial porosity of the waste will be fixed at 0.675, as specified by the creep closure surface. Creep closure will be simulated to account for porosity changes over time, until a human intrusion occurs. After that time, the porosity of the waste will remain fixed at the level attained at that time. The halite DRZ immediately above and beneath the panel, as well as MB139 DRZ and Anhydrite a+b DRZ are all assumed to have identical properties. The permeability of this composite DRZ will be fixed at 1.0E-13 m^2. A range of permeabilities from 1.0E-15 to 1.0E-12 m^2 was originally proposed; however, these permeabilities are so high compared with permeabilities of surrounding materials and so close to the final waste permeability of 1.0E-13 m^2 that varying them will have no noticable effect. The Transition Zone properties will be identical to those of intact far-field anhydrite: permeabilities range from 1.0E-21 to 1.0E-15 m^2; porosities range from 0.001 to 0.03. Far-field anhydrite is assumed this year not to fracture; this effect is being ignored because it cannot yet be accurately simulated. Halite permeability will be sampled over a range of 1.0E-25 to 1.0E-22 m^2. Halite porosity will be set equal to the far-field anhydrite porosity, which is sampled, ranging from 0.001 to 0.03. The final porosity of the DRZ will vary, and will depend on the far-field anhydrite porosity: it will be calculated from [TZ poros + x(0.06-TZ poros)], where x ranges from 0 to 1. In the Undisturbed calculations, the seals & backfill, shaft, and experimental regions will have a porosity of 0.075 and a permeability of 1.0E-15 m^2. The DRZ adjacent to these three regions will have a permeability of 1.0E-15 m^2. The shaft seal permeability will vary, ranging from 3.3E-21 to 3.3E-20 m^2. The seal porosity will be 0.075.

Initial and Boundary Conditions

Initial pressure distribution will be calculated over a 20-year period (see Startup Procedure -- BRAGFLO 1992 PA). This 20-year startup calculation establishes the initial pressure distribution in all regions except the waste and DRZ. The pressure distribution at the beginning of the Startup Procedure will be hydrostatic everywhere (except in the waste and in the Culebra) relative to the pore pressure in MB139. A range of MB139 pressure from 12 to 13 MPa will be used. The initial pressure in the waste will be 1 atm (0.101325 MPa); the waste pressure will be reset to this value at the end of the startup. In the Culebra, the starting pressure will be 1.053 MPa, and the far-field pressure will be held at that value over the 10,020-year calculation. (This is the pressure measured in well H-1; it is the same value as used last year.) Note that the Culebra has a fixed-pressure boundary condition, whereas the rest of the mesh uses a no-flow boundary condition. The starting brine saturation will be 1.0 everywhere except in the waste. At the end of the 20-year startup, the waste will be assigned its sampled value of initial brine saturation, which will range from 0.0 to 0.14. The DRZ will start fully brine-saturated, but at the end of the startup time, the brine saturation will be adjusted so that the brine volume is the same after the porosity is adjusted. The porosity will be adjusted at that time from its starting value (volume average based on 0.01 for halite and the sampled value for intact anhydrite) to its final sampled value. Gas will be added to the DRZ to fill in the added porosity. The pressure in the DRZ will be reset to 1 atm at this time. In the undisturbed calculations, the seal & backfill, shaft, shaft seal, and experimental region will be initialized in the same manner as the waste. All of these excavated regions will be set to be fully saturated with gas at 1 atm pressure at the end of startup. In particular, the shaft seal will initially be fully saturated with gas at atmospheric pressure; this is more conservative with regard to RCRA compliance than assuming it is fully saturated with brine, because more gas can flow through.

Relative Permeability & Capillary Pressure

The Brooks-Corey relative permeability model will be used in 2/3 of the calculations and the van Genuchten-Parker model will be used in 1/3 of the calculations. An index parameter (0 or 1) will be sampled with these probabilities, so that either one model or the other will be used in any one calculation. Relative permeability parameters will be varied and will be the same for all materials except the waste, for which a fixed set of values will be used. Residual brine and gas saturations both will range from 0.0 to 0.4. The Brooks-Corey parameter, lambda, will range from 0.2 to 10.0. The van Genuchten-Parker parameter m will be calculated from m = lambda/(1 + lambda). Threshold capillary pressures will be determined from the correlation with permeability in all regions. The van Genuchten-Parker parameter Po will be calculated by equating the capillary pressure from each of the two models at an effective saturation of 0.5, and solving the expression for Po. In the intrusion borehole, the residual gas saturation will be set to zero, which makes the intrusion calculations run much more easily. In the waste, in the DRZ, in the intrusion borehole, and in all excavated regions in the Undisturbed Scenario mesh, the capillary pressure will be zero. This has proved to be necessary because the capillary pressure curves are not defined for imbibition into a medium that has less than residual brine saturation. So any regions where the brine saturation starts out or may become less than residual have to be modeled with zero capillary pressure.


Culebra + Unnamed
k = 2.179 x10 m
φ = 0.133
⊗
43.7 m
383.12 m
Halite
k = [10⁻²¹ – 10⁻¹⁵ m²]
φ = [0.001 – 0.03]
Anhydrite MB 138
0.18 m
Halite
9.06 m
Anhydrite A+B
0.27 m
2.62 m
9.24 m
Transition Zone
k = [10⁻²¹ – 10⁻¹⁵ m²]
φ_TZ = [0.001 – 0.03]
2.89 m
DRZ
k = 1.0 x10⁻¹³ m²
φ = χ(0.06 – φ_TZ) ; χ = [0–1]
Borehole
k = [10⁻¹⁴ – 10⁻¹¹ m²]
φ = 0.375
3.96 m
P₀ = 0.1013 MPa
Waste
k = 1.0 x10⁻¹³ m²
φ variable – closure
Halite (Pillars)
Halite
k = [10⁻²⁵ – 10⁻²² m²]
φ = 0.01
1.38 m
2.23 m
DRZ
k = 1.0x10⁻¹³ m²
φ = χ(0.06 – φ_TZ) ; χ = [0–1]
Anhydrite MB139
0.85 m
P₀ = [12 – 13 MPa]
200.16 m
Halite
60 m
Castile k = 0.0 m² φ = 0.005
9.58 m
P₀ = [11– 21 MPa]
Brine Reservoir
k = 1.0x10⁻¹¹ m²
φ = 0.005
[0.0605 – 0.2225 m]
22
60.85
96.78
2,596.78
26,096.78

BRAGFLO 1991 DISTURBED CALCULATION

00-04 LOCAL 00000000

```
GENMESH  C-5.11VV 09/17/91
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POSTLHS  3.5 VAX   9/20/91
ICSET    C-1.02VV 09/20/91
ALGEBRA  C-2.12VV 09/20/91
BRAGFLO  1.20      9/27/91
POSTBRAG 2.0VV    10/15/91
ALGEBRA  C-2.15VV 06/19/92
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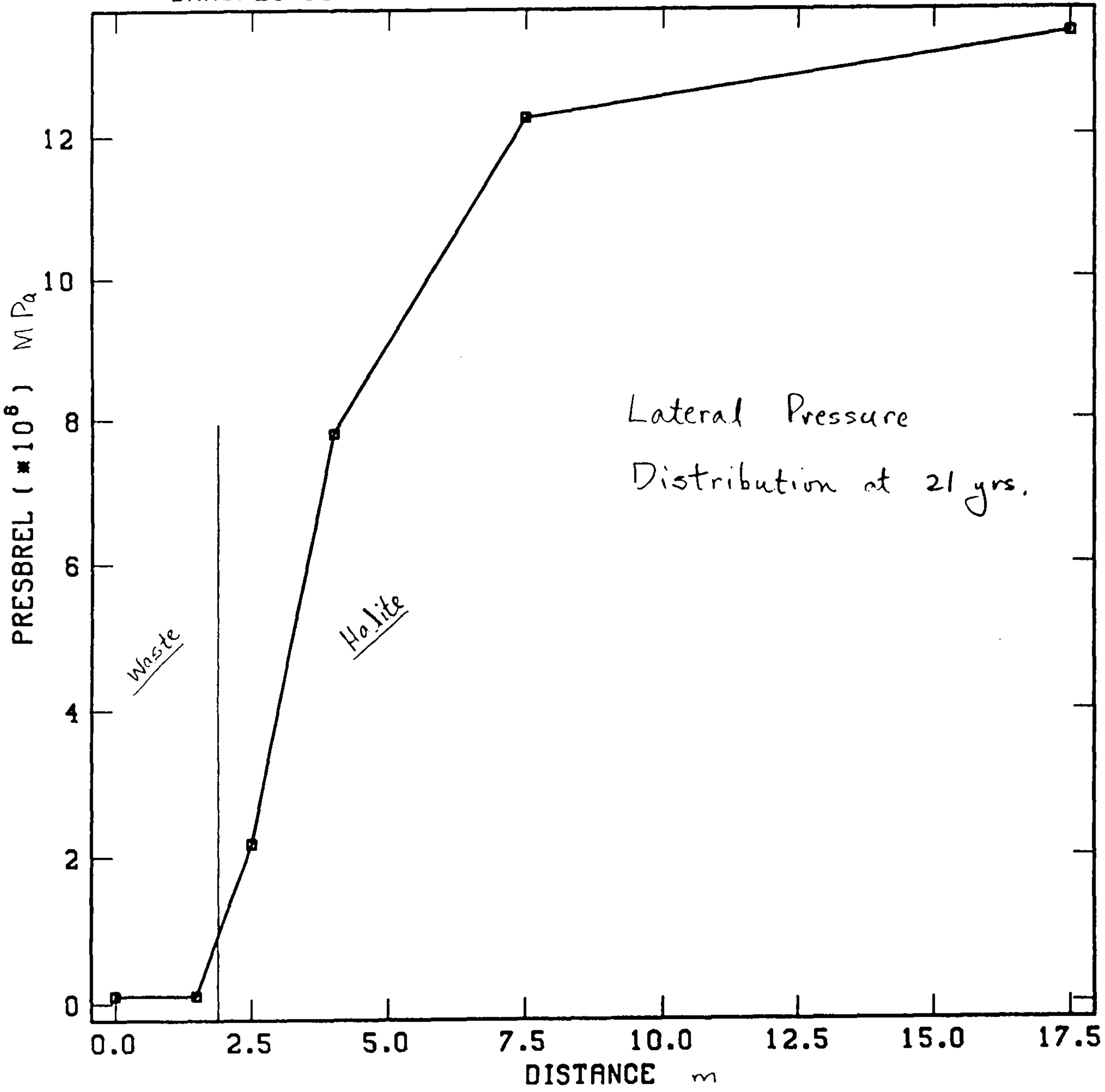

Lateral Pressure Distribution at 21 yrs.

Elements 249..134

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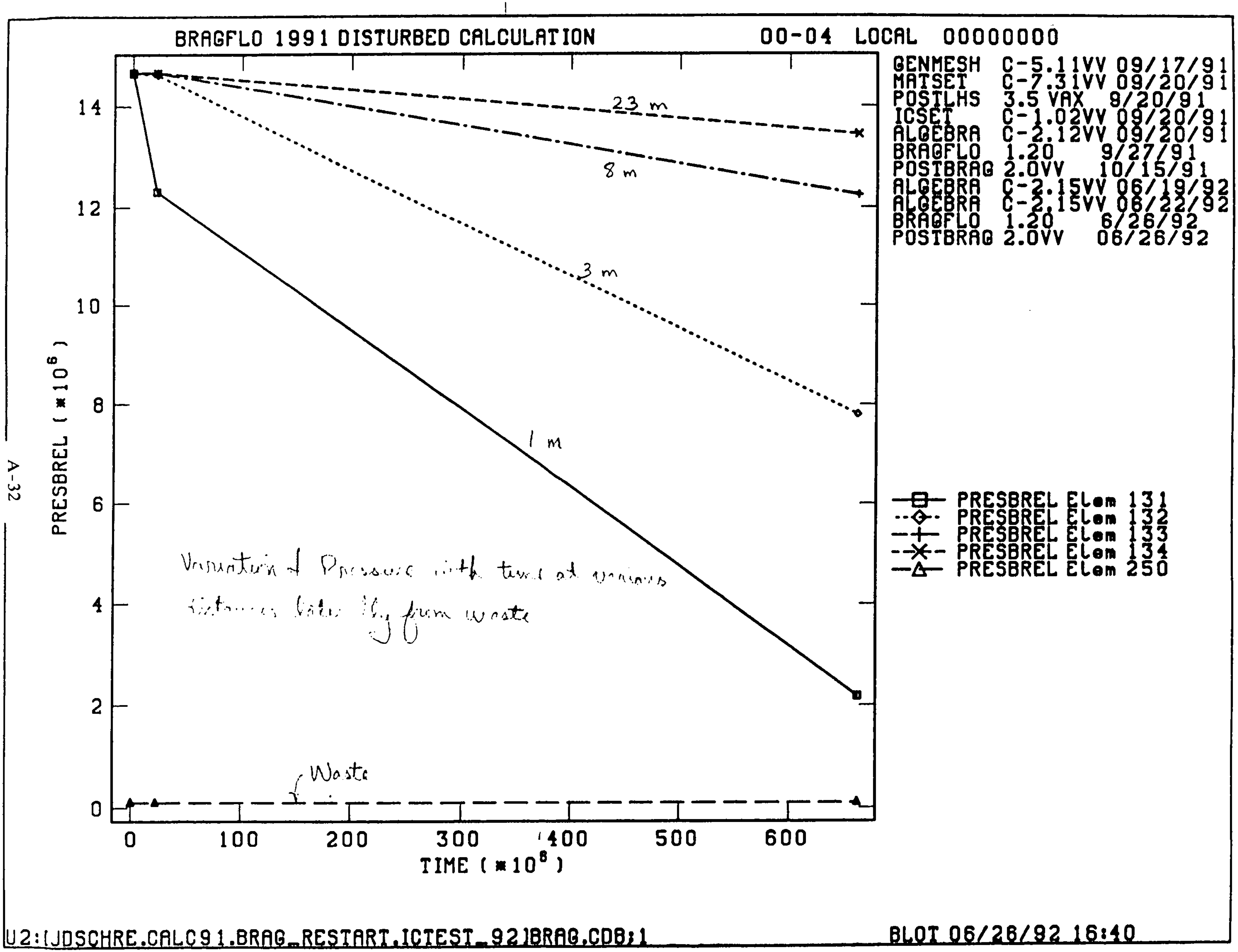
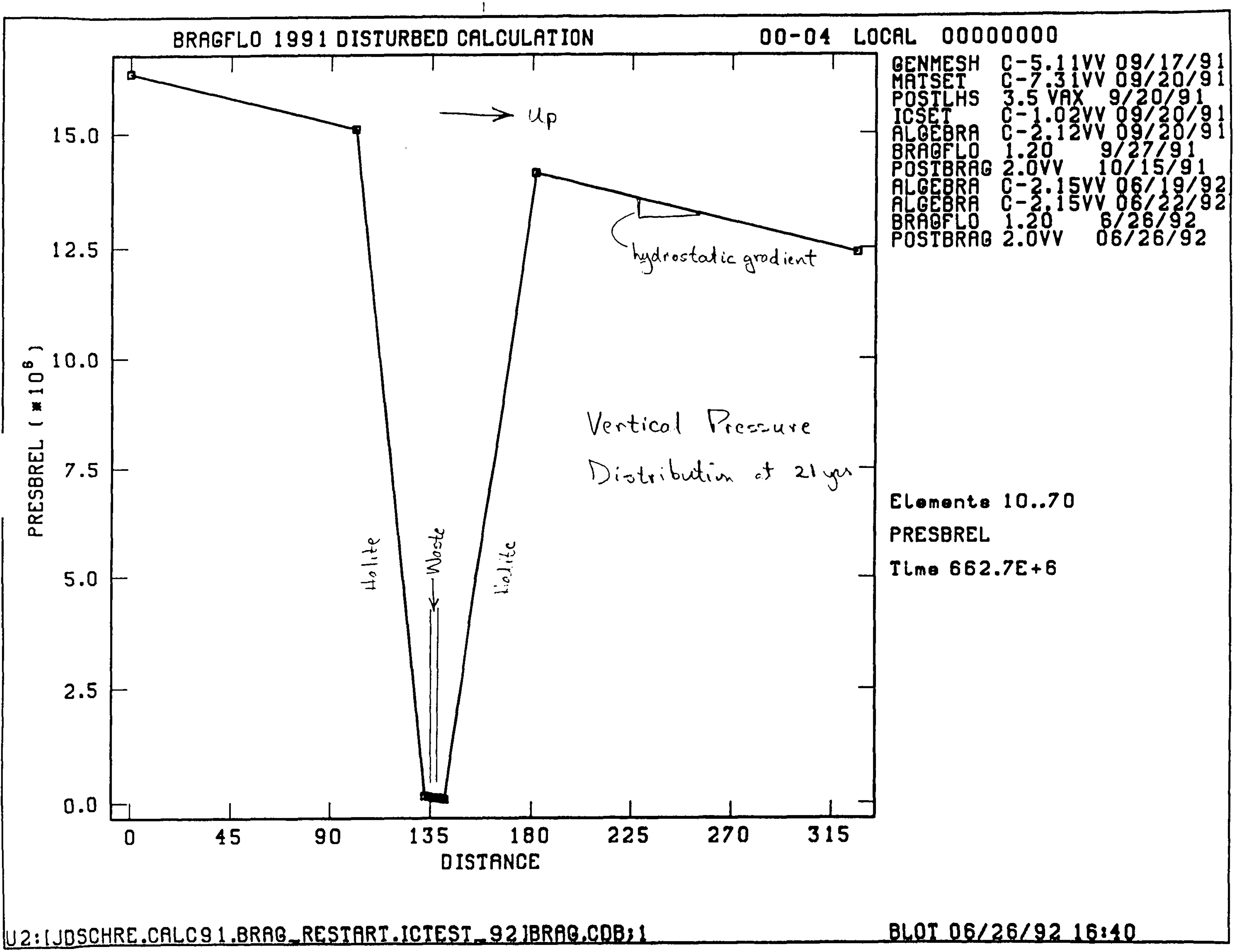


Variation of Pressure with time at various distances laterally from waste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POSTLHS 3.5 VAX 9/20/91
ICSET C-1.02VV 09/20/91
ALGEBRA C-2.12VV 09/20/91
BRAGFLO 1.20 9/27/91
POSTBRAG 2.0VV 10/15/91
ALGEBRA C-2.15VV 06/19/92
ALGEBRA C-2.15VV 06/22/92
BRAGFLO 1.20 6/26/92
POSTBRAG 2.0VV 06/26/92
PRESBREL (*10⁶)
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
45
90
135
180
225
270
315
DISTANCE
Up
hydrostatic gradient
Vertical Pressure Distribution at 21 yrs
Halite
Waste
Halite
Elements 10..70
PRESBREL
Time 662.7E+6
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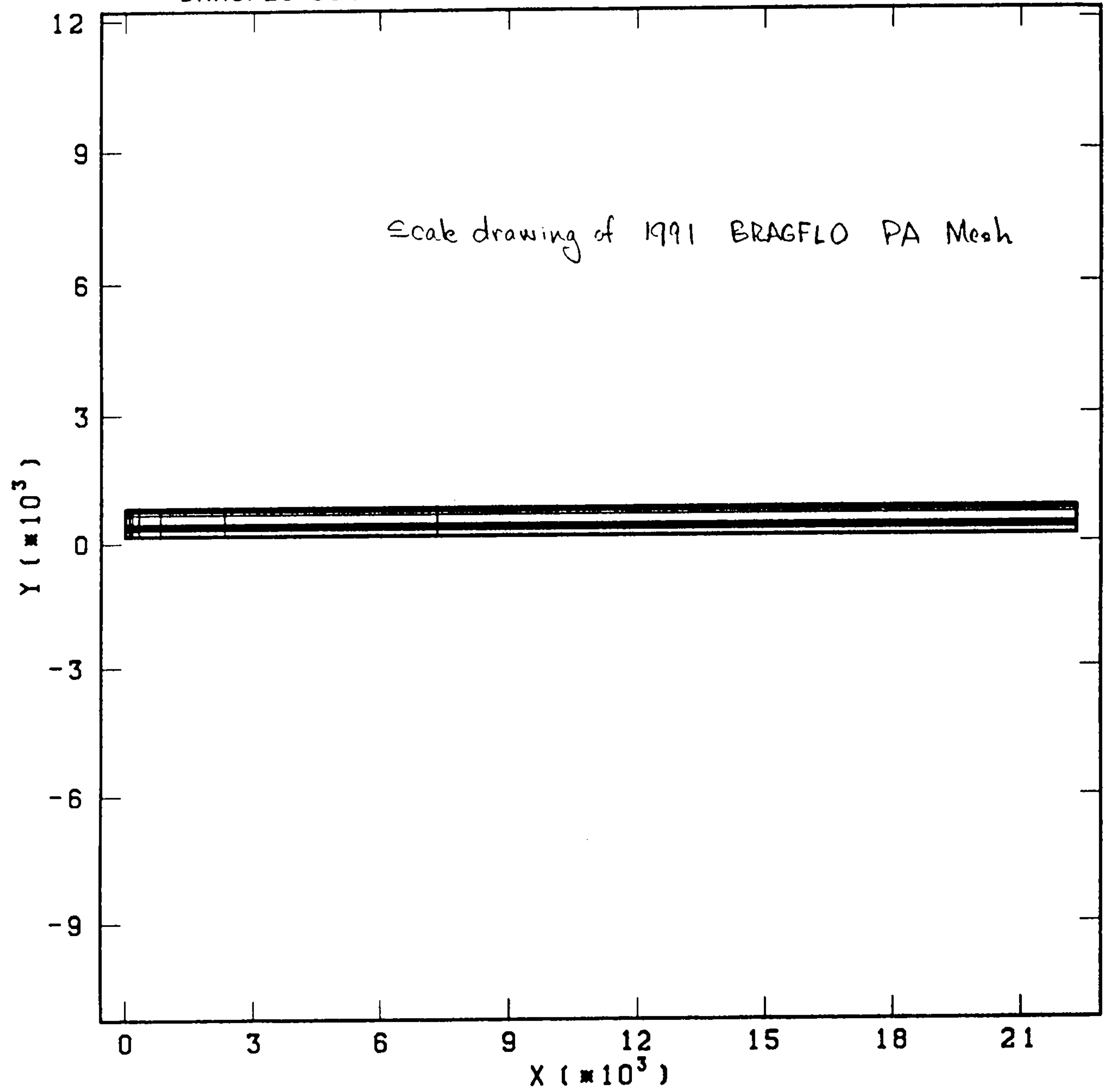

Scale drawing of 1991 BRAGFLO PA Mesh

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BRAGFLO  1.20      9/27/91
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POSTBRAG 2.0VV    06/26/92
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NO Deformation

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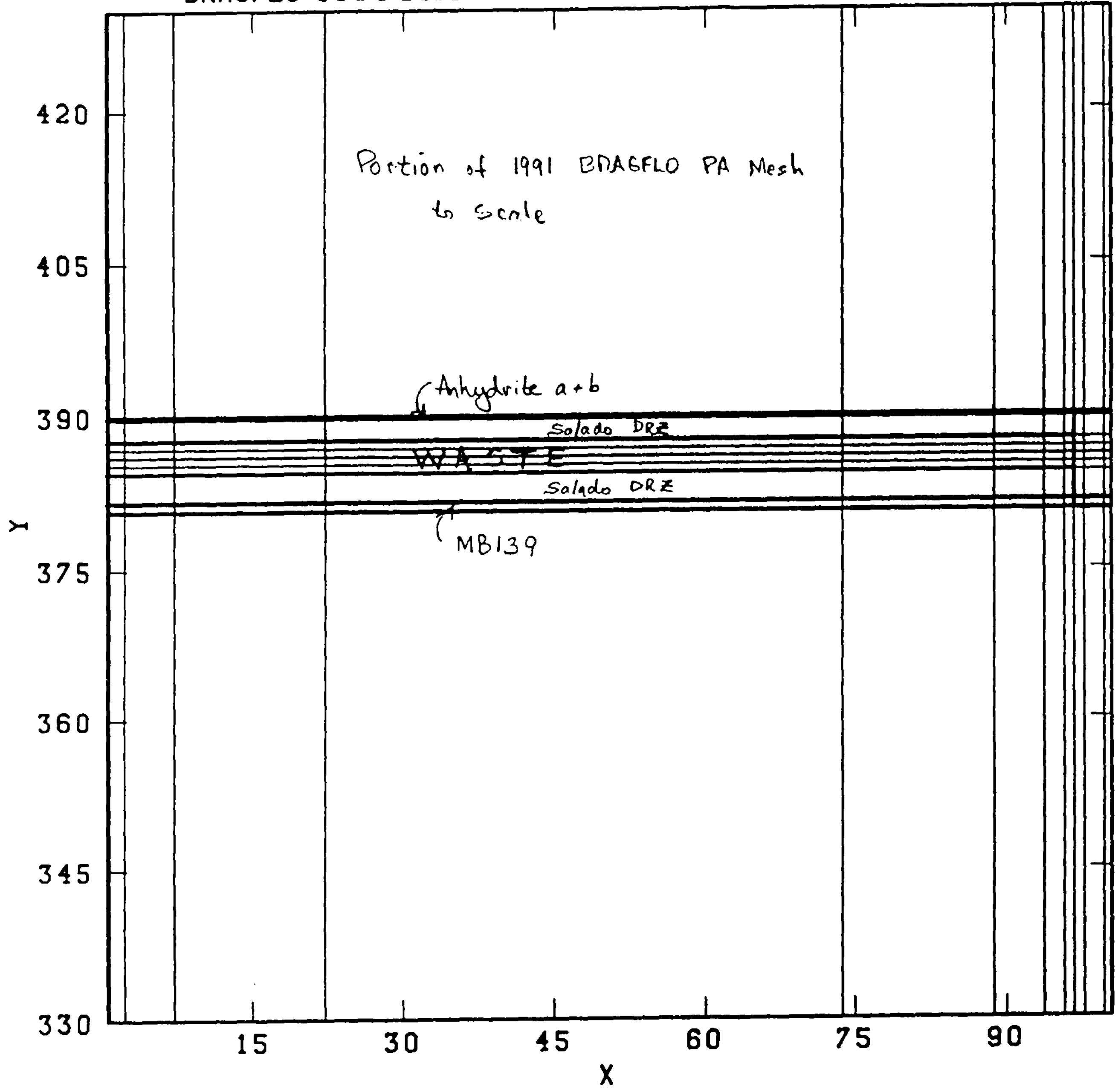

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POSTBRAG  2.0VV    06/26/92
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NO Deformation

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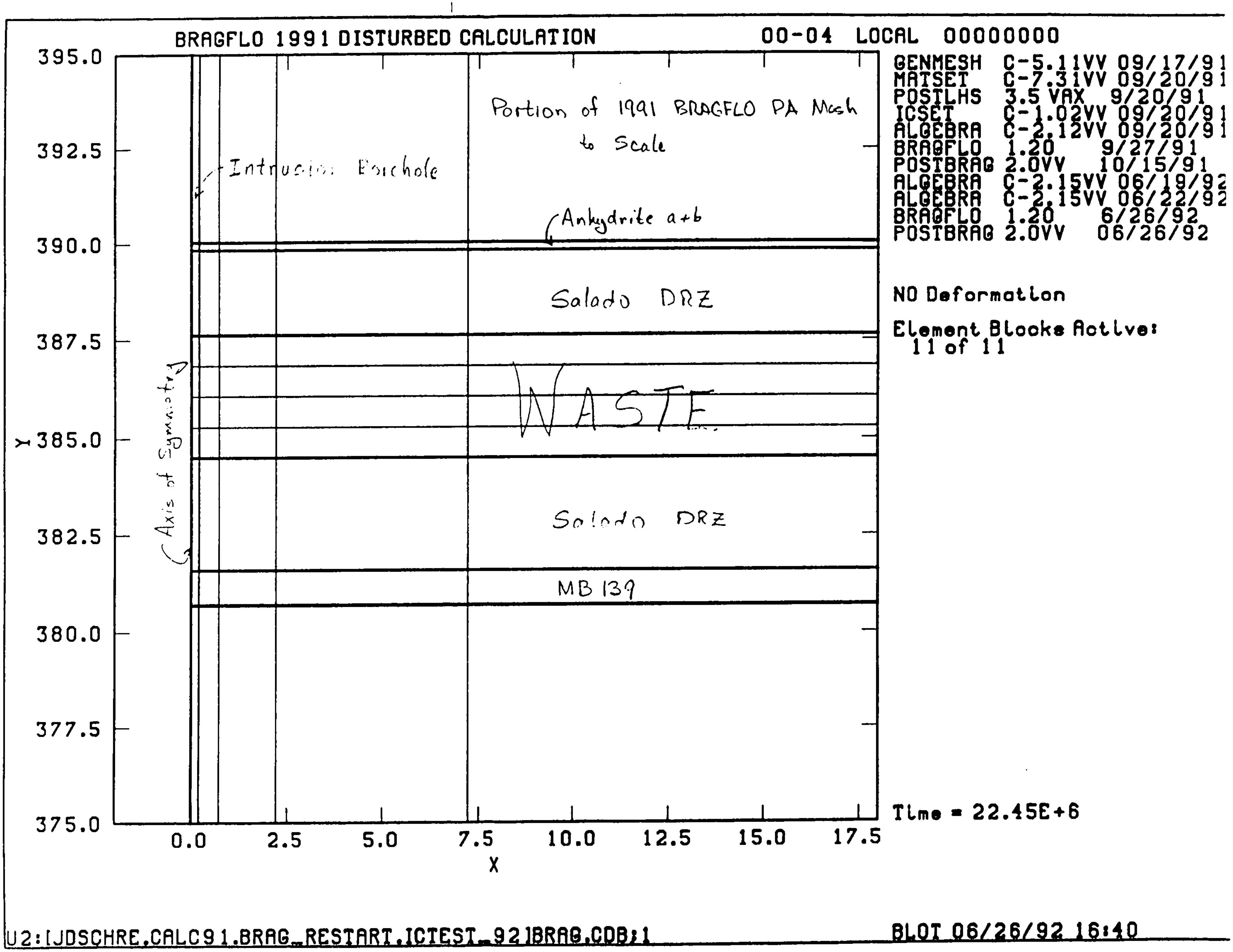
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BRAGFLO 1.20 6/26/92
POSTBRAG 2.0VV 06/26/92
NO Deformation
Element Blocks Active:
11 of 11
Portion of 1991 BRAGFLO PA Mesh to Scale
Intrusion Borehole
Anhydrite a+b
Salado DRZ
WASTE
Salado DRZ
MB 139
Axis of Symmetry
395.0
392.5
390.0
387.5
385.0
382.5
380.0
377.5
375.0
Y
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2.5
5.0
7.5
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15.0
17.5
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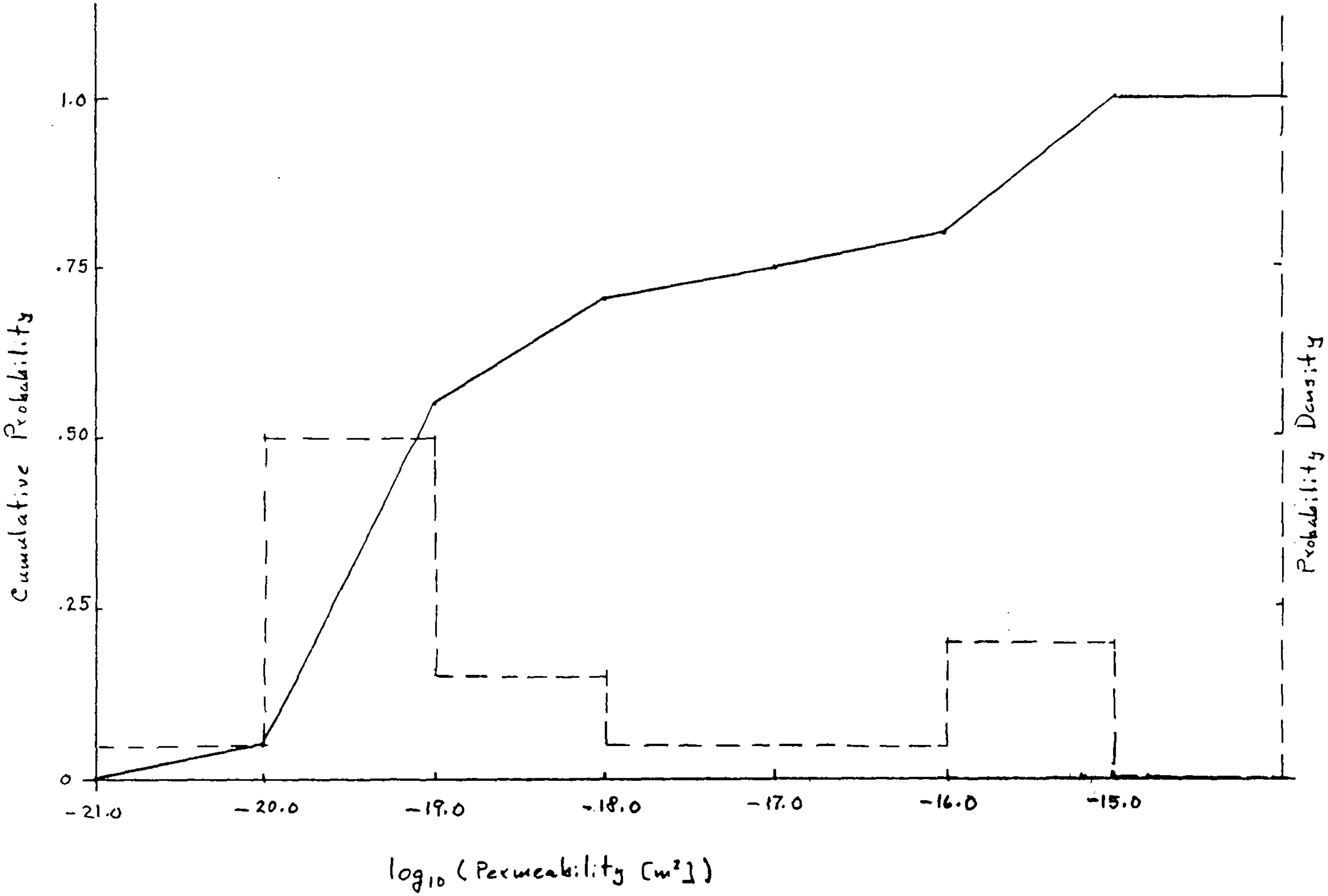

1992 Undisturbed Anhydrite Permeability