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Contaminant Transport Model Validation: The Oak Ridge Reservation, Oak Ridge, Tennessee

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CONTAMINANT TRANSPORT MODEL VALIDATION: THE OAK RIDGE RESERVATION

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ABSTRACT

In the complex geologic setting on the Oak Ridge Reservation, hydraulic conductivity is anisotropic and flow is strongly influenced by an extensive and largely discontinuous fracture network. Difficulties in describing and modeling the aquifer system prompted a study to obtain aquifer property data to be used in a groundwater flow model validation experiment.

Characterization studies included the performance of an extensive suite of aquifer tests within a 600-square-meter area to obtain aquifer property values to describe the flow field in detail. Following aquifer testing, a groundwater tracer test was performed under ambient conditions to verify the aquifer analysis. Tracer migration data in the near-field were used in model calibration to predict tracer arrival time and concentration in the far-field. Despite the extensive aquifer testing, initial modeling inaccurately predicted tracer migration direction. Initial tracer migration rates were consistent with those predicted by the model; however, changing environmental conditions resulted in an unanticipaed decay in tracer movement.

Evaluation of the predictive accuracy of groundwater flow and contaminant transport models on the Oak Ridge Reservation depends on defining the resolution required, followed by field testing and model grid definition at compatible scales. The use of tracer tests, both as a characterization method and to verify model results, provides the highest level of resolution of groundwater flow characteristics.

1. INTRODUCTION AND SCOPE

Groundwater flow and contaminant transport computer models have been used on proposed and existing below-ground waste disposal sites throughout the nation and on the Oak Ridge Reservation (ORR) for pathways analyses. To date, the accuracy of such models to reliably simulate groundwater flow and transport has not been rigorously demonstrated by comparison of model predictions with aquifer tracer test behavior. Consequently, pathways analyses in the fractured geologic media on the ORR may inaccurately represent natural site conditions and may contain significant error.

Oak Ridge National Laboratory staff conducted a field experiment to acquire data for input to perform a computer model validation. The objective of this exercise was to demonstrate the predictive accuracy of groundwater contaminant transport modeling in the saturated zone on ORR. The results of the exercise provide insight into the interpretation of model results for regulatory decision making. The results also provide insight regarding the utility of site characterization studies commonly used as model input.

Prior to conducting the model validation test, consideration was given to results from past geohydrologic investigations in similar geologic settings on ORR and in the area immediately surrounding the test site. Studies of the test results suggest that generally vertically upward head conditions exist and that shallow groundwater discharge is to the nearest surface drainage feature. This knowledge contributed to the selection of the model validation test site and to the position of the test in the groundwater column.

This report is a comprehensive summary of the model validation experiment. It documents the predictive accuracy of one existing groundwater flow and contaminant transport computer model in the geohydrologic environment of a limited portion of ORR. The report also evaluates the utility of commonly acquired hydrologic data, as well as the interpretations of those data, to meet model input requirements.

The model validation study was a lengthy and multifaceted process. It consisted of test planning through detailed geohydrologic site characterization, numerical model refinement, and tracer test performance for model calibration and validation. Each of the major subtasks within the model validation study is discussed as follows: model validation test planning (Sect. 3), site data collection (Sect. 5), tracer test (Sect. 6), and modeling (Sect. 7).

2. TEST DESCRIPTION

The model validation field experiment is a groundwater tracer test. The test is a subset of site characterization studies being conducted on a site in west Bear Creek Valley on ORR for the proposed disposal of low-level nuclear waste. Interpretations of tracer test data are used to establish parameter values for input to groundwater flow computer models in the calibration of those models. In addition, tracer test data were used to evaluate the utility of various site characterization studies commonly used in pathways analyses.

Golder Associates, Inc., was contracted by Martin Marietta Energy Systems, Inc., staff to provide technical assistance in the performance of this project. Golder Associates was to plan and execute field tests for the purpose of providing data for validation of contaminant transport computer model(s) and to perform and document the computer model validation under MMES supervision. Contract deliverables included: (1) documentation of the results of contaminant transport model validation and (2) the calibrated model. This report summarizes the activities that constituted the model validation test. Details of the test can be found in Golder Associates, Inc. (1988).

3. MODEL VALIDATION TEST PLANNING

The model validation test consisted of three stages. Before the tracer test was conducted, a computer simulation of tracer migration was performed using data collected from the larger Bear Creek Valley site characterization activities. The purpose of this simulation was to test conceptual models of site flow and to determine model sensitivity to various flow field parameters. This exercise provided an estimate of the extent of site testing required to calibrate the model for the tracer test.

The second stage of the validation test was conducted in the near-field, approximately 15 m (50 ft) from the tracer injection point. Measured tracer concentration, migration rate, and direction data from this second stage were used in the solution of the equations governing groundwater flow and contaminant transport. These parameter values were then used as model input parameters for flow and transport model calibration. The final test stage was to use the calibrated contaminant transport model to predict tracer concentration, arrival time, and location at a far-field location, approximately 30 m (100 ft) from the tracer injection point.

The test was conducted in the spring when, because of the high precipitation, the phreatic surface was relatively high and maximum hydraulic gradient existed. Planning included the selection of a test site, selection of appropriate test monitoring equipment, and selection of a tracer.

3.1 SITE SELECTION

Figure 1 shows the locations of active and proposed waste disposal sites on ORR. Site characterization activities are being conducted on a proposed site in west Bear Creek Valley on ORR for the disposal of low-level nuclear waste. Figure 2, a topographic map of the west Bear Creek Valley site, shows the location of the model validation test area (in pocket).

Criteria for model validation site selection included the following: First, it was desirable to conduct the model validation field test under ambient conditions, i.e, to select a site with a relatively high hydraulic gradient (relative to the overall site). Second, it was desirable to conduct testing near a groundwater discharge location (a stream) that could be monitored for tracer in the event that the monitoring well field missed the tracer. Third, the test area had to be small enough to allow tracer detection to occur under ambient conditions in a reasonable period of time but large enough to constitute a viable model validation. Fourth, the site had to be representative of similar sites on ORR.

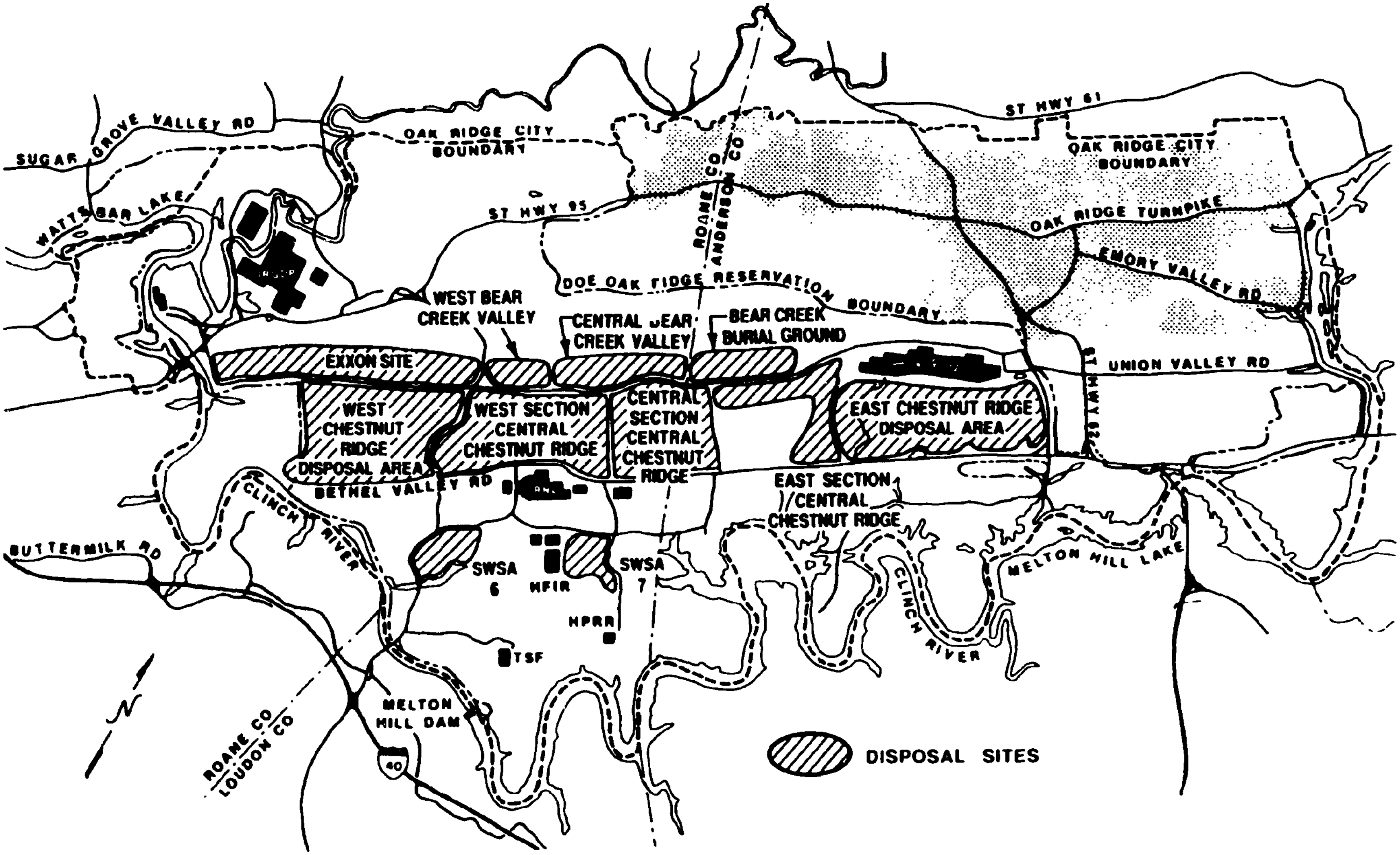

Fig. 1. Active and proposed waste disposal sites on the Oak Ridge Reservation.

A detailed map of the model validation tracer test site is shown in Fig. 3 (in pocket). The site meets all the above criteria. The local hydraulic gradient appears to be relatively high with few irregularities, the creek to the west provides a likely groundwater discharge point for the tracer, and the site is geologically representative of other sites on ORR.

3.2 TRACER AND MONITORING EQUIPMENT SELECTION

Tracer selection was one of the principal components in the test planning. The selection criteria included: (1) an easily detectable tracer, (2) an environmentally nonhazardous tracer, (3) a readily available tracer, (4) a readily soluble tracer, (5) physical properties similar to those of water, (6) a nonsorbing tracer, and (7) a tracer that could be remotely detected with minimum disturbance to the groundwater system. The expenses involved in monitoring equipment for tracer detection were also evaluated. Dyes, ion-specific tracers, and radioactive tracers were considered.

The tracer selected for the test was Rhodamine WT, a dye that can be detected in very small concentrations with the use of a fluorimeter. Rhodamine WT is environmentally safe, is readily available, and has physical properties similar to those of water. Monitoring equipment for dye detection is relatively inexpensive, readily available, and easy to install and maintain.

Sampling equipment for the tracer test consisted of 8 dedicated automatic samplers and a peristaltic pump. Automatic samplers were programmed to sample at 2-h intervals, which allowed for good definition of change in dye concentration over time for input to model calibration. As the tracer test progressed, automatic samplers were periodically relocated from those wells that continually lacked tracer. Periodic modifications were made in the rate of sampling as tracer concentration varied. Because of the large number of detection wells in the well field, some were sampled manually with the use of a peristaltic pump.

Samples were analyzed in the field with a Perkin Elmer fluorimeter, Model 5B, which is capable of detecting Rhodamine WT at concentrations as low as 0.1 parts per billion (ppb); the visual detection limit is 400 ppb.

4. REGIONAL AND SITE GEOLOGY

The Oak Ridge area is underlain by Cambrian and Ordovician age rock units. Table 1 is a generalized stratigraphic column of bedrock formations at ORR. Structural deformation during the Appalachian Orogeny resulted in the development of northeast trending imbricate thrust sheets, the differential weathering of which formed the Valley and Ridge Physiographic Province. A generalized geologic cross section of ORR is shown in Fig. 4. The regional strike is N 45 to 65 E degrees; and the dip is typically 30 degrees southeast, varying from 20 to more than 45 degrees locally.

Bear Creek Valley is underlain by the six formations that comprise the Middle to Late Cambrian Conasauga Group. The valley is bordered on the northwest by Pine Ridge, underlain by the Rome Sandstone, and bordered on the southeast by Chestnut Ridge, underlain by the Knox Group Dolomite. The Rome through Knox rock units form a major portion of the Whiteoak Mountain thrust sheet, so called because of their position upon the Whiteoak Mountain Fault Zone to the northwest. Lee and Ketelle (1988) described the geology of the west Bear Creek Valley site.

The model validation tracer test site is located on the uppermost Maryville Limestone near the contact with the overlying Nolichucky Shale. The Maryville is characterized by oolitic, intraclastic, and thin-bedded limestone interbedded with dark gray shale typically containing thin, planar and wavy-laminated, coalesced lenses of light gray limestone and calcareous siltstone. Fine-grained glauconite often occurs at the tops of the thin-laminated limestone lithology. The presence of oolites and intraclast size and orientation suggest the Maryville represents event-driven paleodeposition. However, the lateral discontinuity of many Maryville lithologies indicates that event deposition was of an extremely localized nature.

Small- and intermediate-scale structural features are ubiquitous in the Maryville. Small-scale structural features are limited to fractures and joints. Bedding-plane fractures occur with a frequency of 0 to 10 fractures per foot, and many show evidence of dip-slip displacement. Fracture surfaces often contain slickensides and secondary calcite, chlorite, and pyrite remineralization. Additional fractures in more competent lithologies (i.e., limestone) are oriented normal to bedding and do not cross lithologic boundaries. As such, they are typically only several inches long and extend for undetermined lengths parallel to bedding. Bedding-normal fracture orientation data were obtained from several excavated pits as part of the larger site characterization study. Analysis of those data indicates the presence of two orthogonal fracture sets, oriented roughly parallel and normal to geologic strike. These results are consistent with previous reports of extension fracture orientation in Melton Valley on ORR.

STRATIGRAPHIC COLUMN OF CAMBRO-ORDOVICIAN ROCKS, WHITE OAK MOUNTAIN THRUST BLOCK, OAK RIDGE, TENNESSEE

Age	Group	Formation/Unit	Description	Thickness (ft)
MIDDLE ORDOVICIAN	CHICKAMAUGA (Och) [b]	Unit H [a]	Thin interbedded limestone and calcareous siltstone. Gray, olive, buff, and maroon.	>270
		Unit G	Limestone and siltstone in thick beds. Limestone fine- to medium-grained, nodular. Siltstone dark gray with vague limestone interbeds.	290
		Unit F	Laminated to thin-bedded calcareous and shaley siltstone. Maroon and olive gray.	20
		Unit E	Limestone and siltstone in thick beds. Limestone fine- to medium-grained, nodular and amorphous. Siltstone dark gray with limestone laminae.	300
		Unit D	Limestone. Medium-grained and stylolitic. Nodular and bedded chert.	140
		Unit C	Limestone and siltstone in thick beds. Limestone nodular and micritic. Siltstone calcareous and dark gray. Nodular chert.	95
		Unit B	Siltstone. Massive maroon and gray with limestone in thin, even beds.	250
		Unit A	Limestone and siltstone in thick beds. Dark to light gray, purplish to maroon. Nodular and bedded chert.	300
LOWER ORDOVICIAN	KNOX (OCk)	NEWALA Fm.	Medium-bedded dolostones and limestones with variable chert content, scattered chert matrix limestones. Abundant maroon mottling.	900 (est)
		LONGVIEW Fm.	Dense massive chert, bedded chert, and dolomoldic chert observed in residuum.	50–100 (est)
		CHEPULTEPEC Fm.	Dolostone, fine- to medium-grained, light to medium gray, medium to thick bedded, sandy near base.	500–100 (est)
UPPER CAMBRIAN		COPPER RIDGE Fm.	Dolostone, medium to thick bedded, fine to coarse crystalline, medium to dark gray. Chert varieties include massive, cryptopoan, and oolitic.	900–1300 est

Table I. Generalized stratigraphic column of bedrock formations on the Oak Ridge Reservation

STRATIGRAPHIC COLUMN OF CAMBRO-ORDOVICIAN ROCKS, WHITE OAK MOUNTAIN THRUST BLOCK, OAK RIDGE, TENNESSEE (Continued)

Age	Group	Formation/Unit	Description	Thickness (ft)
MIDDLE CAMBRIAN	CONASAUGA (Єc)	MAYNARDVILLE Fm.	Upper (Chances Branch Mbr.) – limestone and dolomitic limestone in thick massive beds.	140
			Lower (Low Hollow Mbr.) – dolomitic limestone in thick massive beds. Light gray to buff.	200
		NOLICHUCKY Fm.	Upper – shale and limestone in thin to thick beds. Shale dark gray or maroon. Limestone light gray, oolitic, wavy-bedded, or massive.	60–140
			Lower – shale and limestone in medium to thick beds. Shale dark gray, olive gray or maroon. Limestone light gray, oolitic, glauconitic, wavy-bedded, and intraclastic.	430–450
		MARYVILLE Fm.	Limestone and shale or siltstone in medium beds. Limestone light gray, intraclastic, or wavy-bedded. Shale or siltstone dark gray.	320–410
		ROGERSVILLE Fm.	Shale and argillaceous limestone. Laminated to thin-bedded, maroon, dark gray, and light gray.	80–110
		RUTLEDGE Fm.	Limestone and shale in thin beds. Limestone light to olive gray. Shale gray or maroon.	100–120
		PUMPKIN VALLEY Fm.	Upper – shale and calcareous siltstone. Laminated to very thin-bedded. Shale reddish brown, reddish-gray, or gray. Calcareous siltstone light gray or glauconitic.	130–150
			Lower – shale and siltstone or silty sandstone. Thin-bedded. Shale reddish-brown or gray to greenish gray. Siltstone and silty sandstone light gray.	175
LOWER CAMBRIAN		ROME Fm. (Єr)	Sandstone with thin shale interbeds. Sandstone fine-grained, light gray or pale maroon. Shale maroon or olive gray.	Unknown

[a]Chickamauga Group stratigraphic subdivisions reflect those identified at the Oak Ridge National Laboratory site. Other formation names are consistent with regional stratigraphic nomenclature.
[b]Group name abbreviations are those commonly used on geologic maps and cross sections in the region.

Table 1 (continued)

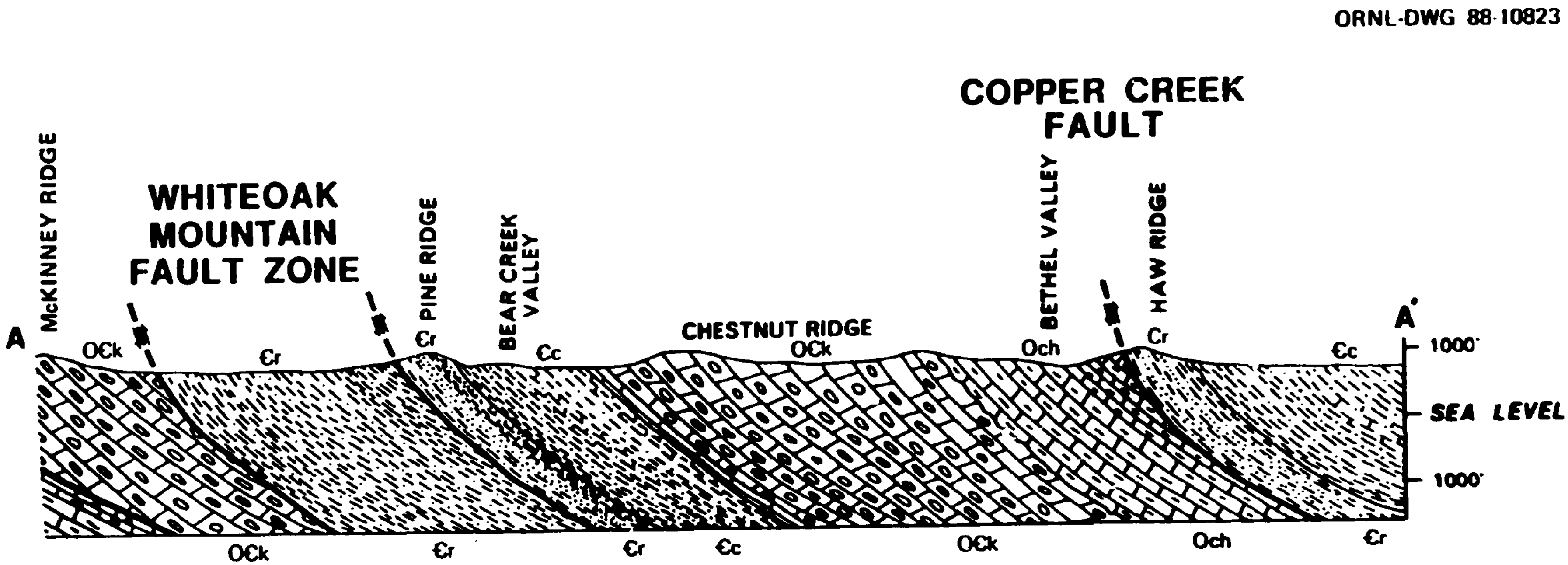

Fig. 4. Generalized geologic cross section of the Oak Ridge Reservation.

Numerous intermediate-scale structural features are identified in the Maryville. These features are recognized as (1) folded bedding considered to be drag folds, (2) heavily fractured beds resembling fault gouge, and (3) discreet shear fractures, with high- and low-angle orientation with respect to vertical. Both drag folds and fault gouge extend from several inches to several feet vertically, while shear fractures exhibit small to undetermined bedding offset. The effect of these intermediate-scale structural features on the geohydrologic system is discussed in Sect. 5.2.

Like the entire Conasauga Group, thin residual, alluvial, and colluvial soils develop above the Maryville at the tracer test site. The soils are underlain by a comparatively thick saprolite zone that varies from 2 to 6 m (7 to 20 ft) thick. The saprolite is composed of weathered bedrock that has lost its rock cement but retained its bedding features. Its upper portions can be readily penetrated with a hand auger. The saprolite/bedrock interface is gradational because of decreasing weathering with depth but is typically defined at the depth of machine auger refusal.

5. SITE DATA COLLECTION

To develop the necessary level of understanding of the site geology and the geohydrologic system, an extensive data acquisition program was undertaken. Data acquisition proceeded incrementally such that later-stage information built upon early-stage information. Data acquired from the site are presented below in the sequence of their acquisition. Throughout the remainder of this report, reference to the map of the validation tracer test site (Fig. 3) is recommended.

5.1 ROCK CORING

Three core holes were drilled on or adjacent to the model validation tracer test site: GW-404, GW-455, and GW-471. They were drilled for the dual purposes of providing geologic control on the site and for subsequent straddle packer testing of the geohydrologic system. The results of rock core logging and packer testing were used to design the tracer test location and well field.

A total of 164 downhole m (539 downhole ft) of rock was logged from the three core holes—with emphasis on identifying formational contacts and lithologic or structural features indicative of groundwater flow.

5.2 GEOHYDROLOGIC TESTING

Three test methods were used to characterize aquifer properties at the model validation site: packer tests, pump tests, and slug tests. This section describes the estent of these tests.

5.2.1 Packer Testing

One of the methods employed in the tracer test area to characterize the geohydrologic system was a system of downhole straddle packers. The principal advantage of the straddle packer testing system is that specific stratigraphic intervals can be isolated for testing and compared with packer test results from adjacent intervals. In the system used for this test, packer data are entered directly into a portable field computer that (1) allows preliminary test analysis while the test is in progress and (2) plots the results immediately following each test.

Packer testing began in core hole GW-404. To acquire the most comprehensive data possible and to obtain benchmark hydrologic data, the entire depth of GW-404 was tested at a 3.6-m (12-ft) interpacker spacing. Review of packer testing results suggested the presence of anomalously high hydraulic conductivity in test GW-404-5. Reexamination of the rock core indicated the presence of a zone of structural deformation that consisted of small drag folds, high-angle shears, and fault gouge in this interval. The identification of this interval ultimately dominated subsequent site testing and tracer test design.

Packer test results in core holes GW-455 and GW-471 are similar to those for GW-404. The zone of deformation noted in GW-404 was identified in the same stratigraphic interval, at different depths, in both GW-455 and GW-471. The deformation in the latter two holes, however, resulted in the inability to completely isolate the zone with the packer equipment. Partial packer testing of the zone confirmed, however, its anomalously high hydraulic conductivity.

Packer test data were later analyzed in the laboratory to determine the hydraulic conductivity and to estimate the static hydraulic head for each packer test interval.

5.2.2 Pump Testing

Two pump tests were performed in selected intervals of the shallow aquifer system at the tracer test site. The objective of the pump tests was to better define the aquifer properties and to quantify the aquifer anisotropy. In addition, values for bulk hydraulic conductivity, storativity, and vertical leakage components were obtained, as well as semi-quantification of potential hydraulic boundaries.

5.2.2.1 Site selection and pump test design

On the basis of the packer test results from core holes GW-404, GW-455, and GW-471, it was determined that considerable evidence supported the hypothesis that geologic structure and stratigraphy strongly influence the groundwater system. It was therefore decided to conduct a tiered pump test of specific stratigraphic intervals. Four observation wells, equidistant from the central pump wells, were oriented parallel and perpendicular to the geologic strike. Each observation well consisted of three individual wells. The deep well was constructed at the known depth of the zone of deformation with high hydraulic conductivity. Each intermediate-depth well was constructed at a shallower depth in a stratigraphic interval of low hydraulic conductivity. Each shallow well was constructed at the phreatic surface. Two individual pumping wells, in the center of the observation well field, were constructed just below the water table and in the same stratigraphic interval as the deep observation wells. Two separate pump tests were made—one in the shallow water table zone and the other in the zone of deformation. The location of the pump test site was selected to intercept the zone of deformation at depths of less than 30 m (100 ft) and to use the pump test wells as monitoring wells for the tracer test.

5.2.2.2 Pump test drilling and well construction

Two pumping wells and twelve observation wells were installed for the pump test. Well drilling employed once-through water rotary techniques (1) to reduce damage to the borehole walls, (2) to prevent high air pressure associated with air-rotary drilling from opening flow pathways between wells, (3) and to remove all possible drill cuttings to minimize well development. At the desired depth, a bentonite gel slurry was circulated through each hole to remove any remaining drill cuttings. This process was immediately followed by the circulation of clean potable water through the hole to remove any remaining gel. All wells were constructed of 2.5-to 5-cm-diam (1- to 2-in.-diam) schedule 40 polyvinylchloride (PVC) screen and riser. In addition, wells were constructed in the zone of deformation with high hydraulic conductivity in core holes GW-455 and GW-471 as far-field observation points.

5.2.2.3 Well development

The objective of well development is to remove sediment associated with well drilling and installation and to provide effective hydraulic connection between the rock formation and the well screen. Pump test wells were developed by air-lift techniques with either compressed air or nitrogen, pumping with a submersible pump, or hand bailing. Wells were generally developed until the well produced representative formation water. Water developed from the wells was considered to be representative when values of specific conductance, pH, and visual clarity remained relatively stable. Wells were developed for a minimum of 4 hours (h) or until water representative of the formation was produced. Several wells of low yield often required purging until dry and then repurging after many hours or days. In general, a minimum of three well volumes was removed from each well completed in intervals possessing sufficient yield characteristics.

5.2.3 Slug Testing

The objective of slug testing was to obtain values for in situ horizontal hydraulic conductivity. Slug tests were performed on all the deep and intermediate pump test observation wells, on the two pumping wells, and in core holes GW-455 and GW-471. Pump tests were not performed on the shallow pump test detection wells because of their general low yield. Slug test results are in close agreement with those obtained from packer testing.

5.3 TRACER TEST WELL FIELD DESIGN AND INSTALLATION

The review of the data acquired from site testing indicated that the tracer test should be conducted in the shallow groundwater system, just below the water table. Hydraulic conductivity values in the shallow pump test wells were slightly higher than in the deep wells. Thus, conducting the test at the water table was considered to more closely simulate a leak scenario.

Drilling and well installation of the tracer injection and detection wells were completed in four stages. To use existing pump test wells most efficiently as tracer detection wells, tracer test injection well (GW-484) was placed upgradient from the pump test wells. The first-stage tracer detection wells, GW-479 through GW-483, were drilled with the same wash rotary drilling techniques and well development procedures used for the earlier pump test wells. These wells were planned as near-field tracer detection wells to acquire tracer migration rate and direction data for use in contaminant transport model calibration. On the basis of site geohydrologic testing results, wells GW-480 and GW-482 were located in the anticipated downgradient flow direction from GW-484; and GW-479 and GW-483 were located as background wells. The anticipated tracer migration direction based on site geohydrologic testing is shown in Fig. 3. GW-481 was drilled along the geologic strike from the injection well to test the hypothesis that geology has a strong influence on groundwater flow direction.

6. TRACER TEST

Rhodamine WT dye tracer was pumped into GW-484 on Wednesday, April 20, 1988. Following the removal of approximately 10 liters (L) of standing water from the well, 10 L of 40% Rhodamine WT solution was injected continuously from 11:25 to 11:37 a.m. After tracer injection, 3.8 L (1 gal) of deionized water was pumped into well to flush the remaining tracer from the injection tube. Monitoring began immediately after tracer injection.

The tracer was first detected 7 h after injection at 1.4 ppb in well GW-481. The presence of the tracer in GW-481 and its absence in GW-473 and GW-474—in the anticipated path of tracer migration—corroborated the pretest hypothesis of the geologic influence on flow and prompted the second stage of detection well drilling and construction. The second and subsequent stages of drilling differed from the first-stage drilling and well construction. To impose minimal effect to the groundwater system, the second and subsequent stages of drilling consisted of soil auguring to refusal with no well development.

Wells GW-485 through GW-489 were constructed from 2 to 12 days after tracer injection. The tracer was detected in only GW-486 and GW-487, and the highest concentration (9090 ppb) was identified 22 days after injection in GW-487. Tracer detection in only these wells clearly showed that the anticipated tracer migration direction, on the basis of site geohydrologic testing, differed from the actual direction by approximately 35 degrees. Tracer migration was proceeding in a direction parallel to the geologic strike, exactly as predicted by the conceptual hypothesis. Tracer absence in any other detection wells indicated also that the migration pathway was extremely narrow.

Wells GW-490 through GW-494 comprise the third stage of the well construction, 26 days after injection. The purpose of these wells was to provide the final data for calibration of the groundwater flow and contaminant transport models. Tracer was found in GW-493 at concentrations similar to those found in GW-487. Wells GW-491 and GW-492 contained significantly lower concentrations. Tracer detection at these wells represents 17.4 m (57 ft) of migration along a pathway parallel to geologic strike in a plume less than 3 m (10 ft) wide.

7. GROUNDWATER FLOW AND CONTAMINANT TRANSPORT MODELING

The objective of groundwater flow and contaminant transport modeling is to evaluate the model's ability to accurately simulate tracer migration at the test site on the basis of site data and to predict the tracer arrival time and concentration at a distant site location. This objective was accomplished by using the data acquired on tracer migration in the near-field to perform model calibration. The calibrated model was then used to predict tracer arrival time and concentration in the far-field.

The model selected for validation was the Golder Groundwater Package, a finite-element model prepared by Golder Associates, Inc., staff. This model was selected because Golder Associates staff is familiar with this package and because it is fundamentally similar to other publicly available models used widely in site modeling.

In the latter phases of site hydrologic testing, a finite-element mesh was generated. This mesh incorporated those hydrologic and geologic site characteristics that affect flow. The mesh element size is smaller near the well field, where more data exist and coarsens toward the site perimeter where less or no data exist. The initial mesh generation oriented the mesh elements 35 degrees southwest of the geologic strike (N 205 degrees) on the basis of the shallow-pump test analysis.

A western constant head boundary was established at the 258-m (848-ft) mean sea level contour in the flood plain of the creek. An eastern no-flow boundary was established at the divide of the adjacent topographic high. Prescribed head boundaries were established in the north and south on the basis of interpolation of piezometer data.

7.1 MODEL CALIBRATION

The initial model calibration involved adjustment of those parameters for which the least data were available (anisotropy and prescribed head). Model calibration required that assumed values be made for these parameters to simulate field conditions. Tracer detection in only those wells located along the strike from the injection well (N 240 degrees) indicated that the predicted direction of tracer movement, based on site hydrologic data, was inaccurate. To reconcile site hydrologic data with observations of tracer migration, the finite-element grid was divided into two material properties. The northern material retained the hydraulic conductivity value obtained from shallow pump testing, and the southern material was assigned progressively lower hydraulic conductivity values until the model-generated plume mimicked the tracer plume. To match field observations of tracer migration direction, six orders of magnitude (10^6) adjustment to the value of hydraulic conductivity was required in the southern material property.

The use of imaginary material properties to simulate tracer migration direction introduced problems of plume drift to the south and plume migration significantly faster in the model than in the field. To correct these problems, the finite-element grid orientation was adjusted to parallel the geologic strike. Continued adjustments to porosity and longitudinal dispersivity values and the maintenance of the two material properties eventually produced model calibration that simulated tracer behavior in the field. The solute transport model was considered to be calibrated when it closely simulated field tracer observations.

7.2 MODEL VALIDATION

The calibrated solute transport model was allowed to run for 40 days into the future to simulate the tracer concentrations at various locations in the far-field. On the basis of the calibrated model output, a location was selected at a distance of 33.5 m (110 ft) from the tracer injection point where the model validation detection wells were to be positioned. Wells GW-495 through GW-499A were constructed at 1-m (3-ft) intervals at the model-predicted location. The model predicted that on May 25, 1988, the concentration at the model validation well field would be 1300 ppb.

At the time this report is written, mid-September 1988, the tracer has not yet been detected in any model validation wells. The tracer arrival time predicted by the contaminant transport model used in the validation test was grossly inaccurate. Efforts to understand the cause for this disappointing result continue. Those efforts are discussed in Sect 8.

8. ACTIVITIES FOLLOWING MODELING

In late June 1988, when it was clear that the tracer was not present in the validation well field, and additional drilling was begun to locate the tracer. To investigate the possibility that the tracer had migrated to the south of the observed direction along the geologic strike, wells GW-499B through GW-499F were drilled as a southern continuation of the model validation wells. Sampling in these wells for nearly 2 weeks showed no tracer, but its absence allayed the concern that the tracer had bypassed the model validation well field.

Lack of tracer detection for an extended period of time beyond the final model calibration wells prompted the drilling of additional wells to confirm that the tracer had not migrated in a completely unexpected direction. Four new wells, GW-499G through GW-499J, were drilled along the geologic strike midway between the validation well field and GW-493, the final model calibration well. After several days, the absence of the tracer in these wells prompted the drilling of six more wells, GW-499K through GW-499P, 3.3 m (15 ft) southwest of GW-493 along the strike.

Tracer was identified in well GW-499M immediately after drilling, and GW-499N and GW-499O showed tracer several days later. The highest tracer concentration was in GW-499N, directly along the strike from the injection well and GW-493. Several days after tracer detection in GW-499N, tracer was detected in GW-499G. At the time this report is written, small concentrations of tracer are present in GW-499G and GW-499I. The continued presence of significantly higher tracer concentrations in GW-493 indicates that the tracer did not deviate from its original direction but rather that it stalled dramatically from its earlier migration rate.

The presence of tracer in GW-499M through GW-499O substantiates the conceptual model that geology is a dominant influence on groundwater flow and transport under ambient conditions. It is envisioned that hydrology is the dominant influence in the rate of flow evidenced by decreasing flow rate with decreasing hydraulic gradient. Evidence supporting geology as the dominant influence in the direction of flow is the narrow tracer plume paralleling the geologic strike.

9. DISCUSSION

The results from this test indicate that at the scale of the test, on this site, and in this geologic setting, the selected finite-element groundwater flow and contaminant transport models do not simulate field observations. One major factor in model selection was that it is representative of other models widely used in site modeling. While minor differences exist in these models, the physical and mathematical principles governing porous media flow and transport are the same. In addition, the numerical interpretation of field data for model input may not realistically represent natural conditions. Significant improvement in our ability to numerically represent field data is required before improved model output can be achieved. Without improvements in the interpretation of site data for model input, model output results cannot be adequately evaluated.

Some question remains regarding the applicability of results from this test (which was conducted at a very small scale) to modeling in larger sites. The scale at which modeling simulates field observations cannot be reliably addressed from from results of this study. However, one factor in tracer test site selection is that the site was representative of other locations on ORR. As such, results of this test may reasonably be applied to other similarly sized sites on ORR.

The test results indicate that the sophisticated data acquisition techniques employed in site testing and the use of standard techniques for interpreting those data for describing the direction of migration were not representative of the natural flow field. Data were collected under conditions that are not representative of natural site conditions and at a scale that camouflaged the controlling influences on flow and transport.

After validation postmortem detection wells GW-499B through GW-499P were drilled, depth-to-water data were obtained from all the existing wells. To avoid potential tracer contamination of the well field during the test, no depth-to-water data were obtained. Analyses of these data clearly show a strong hydraulic gradient in the direction of tracer migration, along the strike. Had these data been available prior to the tracer test, the model finite-element grid mesh would have been in the proper orientation and the model-predicted tracer migration direction would have more closely simulated field observations.

Hydrologic data were acquired from the site while stressing the hydrologic system (pumping). Under conditions of stress induced by pumping, the hydrologic component of the system overrode the geologic component. During the tracer test, when the geohydrologic system was under ambient conditions, the geologic component dominated.

Analysis of the tracer migration rate indicates that the rate has now diminished from 80 cm/day (2.8 ft/day) at the beginning of the test to essentially zero migration. The apparent explanation for the decreasing migration rate is a diminished hydraulic gradient due to low precipitation. This explanation is supported by a nearly 60-cm (2-ft) lowering of water levels at the site since initiation of the tracer test.

An explanation for the direction of tracer migration was sought from the site rock core. The thin to medium interbedded limestones and calcareous siltstones [3 to 4.5 m (10 to 15 ft) thick] are punctuated regularly by thick [60- to 120-cm (2- to 4-ft)] clean silty shales. Detailed analysis of these rocks suggests that the comparatively erosion-resistent clean silty shales form slight bedrock highs. Some confidence exists that the shale beds that form the northern and southern boundaries of the tracer plume have been identified. Tracer has apparently moved within a minor—but commonly occurring—trough of erosion-prone silty limestones between the shale beds.

Rock fractures have long been considered to have a substantial effect on groundwater flow on ORR. Fracture analysis on the larger Bear Creek Valley site and elsewhere on ORR consistently show the presence of two dominant extension fracture sets oriented roughly parallel to the geologic strike and dip respectively. It is considered likely that fractures influenced the tracer migration direction. However, in the hydrologic discharge location of this test, the absence of tracer migration down dip suggests that the contribution of fracturing to flow is secondary to lithology and larger scale regional geologic structure.

Hydrologic data were acquired from the site at scales of 39 m (12 ft) and greater of aquifer thickness. Many, if not all, of the packer tests were conducted across the lithologic boundaries, which apparently control flow. Pump testing analyzed even greater thicknesses of the aquifer. The scale of these tests was too large to adequately resolve the geologic characteristics controlling flow.

Additional modeling with a different model, SEFTRAN (1987), and a different approach to the problem formulation has been conducted. Results of this modeling have more closely simulated field observations using credible material property values in the finite-element grid, which suggests that the finite-element approach to site modeling is appropriate. Moderate improvements to previous model validation predictions have been achieved.

10. CONCLUSIONS

This study included comprehensive, detailed, geologic and geohydrologic characterization to define and quantify the factors that control local groundwater flow.

Site characterization and tracer test behavior indicate that groundwater flow directions in the shallow flow system are dominated by small-scale (1-m) interbedding of limestone and shale and intermediate-scale (hundreds of meters) to regional-scale (hundreds of kilometers) geologic structure.

The model validation experiment consisted of three steps: (1) establishing a grid for use in numerical model application, (2) calibrating the model to site conditions based on early time-tracer-migration data, and (3) predicting far-field tracer migration rate and concentration. The validity of the model was then judged on the basis of the accuracy with which the model prediction matched the tracer behavior in the far-field portion of the test.

Modeling assumed steady state aquifer conditions, which were not met during the tracer test because of lack of significant rainfall for a period of weeks to months after the dye injection. The initial dye migration rates observed in the tracer test were consistent with the model-predicted rates; however, lack of rainfall resulted in water table decline and aquifer gradient reduction with an accompanying unanticipated slowdown of tracer movement. This observation indicates that short-term and seasonal variations in aquifer conditions strongly influence local, shallow-zone groundwater flow.

Despite the higher than average density of aquifer characterization tests performed, the initial modeling efforts inaccurately predicted the tracer migration direction. The site hydrologic test interpretation—and therefore the initial model grid—assumed that groundwater flow at the site was controlled by the hydraulic gradient determined from an initial well array. As the tracer test progressed, additional tracer detection wells were constructed, which provided a higher resolution of the local geology and water table gradient. The site characterization testing scale and the dominantly hydrologic, rather than geologic, interpretation of the test data are considered to have led to the inaccurate model predictions.

The tracer test was performed in a groundwater discharge area with weak upward vertical head conditions observed between bedrock and water table aquifer zones. The tracer was injected into the surficial aquifer zone and migrated with the water table gradient showing very little lateral or vertical dispersion.

The results of the tracer test are consistent with the larger scale conceptual model that has evolved for the Bear Creek Valley site through the Low-Level Waste Disposal Development and Demonstration site characterization studies. The results of the site characterization and modeling efforts indicate that flow in the shallow aquifer is controlled by geologic features on the order of 1-m thickness, which are not accommodated by conventional numerical models.

Successful model use on ORR depends on defining the resolution required for any application, followed by field testing and model grid definition at compatible scales. Where high resolution is required, very detailed tests and fine model grids will be required. The groundwater tracer test performed in this study demonstrated the strong control of geologic conditions on groundwater flow. The use of tracer tests—to both characterize sites and verify model results—provides the highest level of resolution of groundwater flow characteristics.

11. REFERENCES

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Ward, S., B. H Lester, and J. Mercer 1987. *SEFTRAN: A Simple and Efficient Two-Dimensional Groundwater Flow and Transport Model, Version 2.5*, GeoTrans, Inc., Herndon, Va., December.

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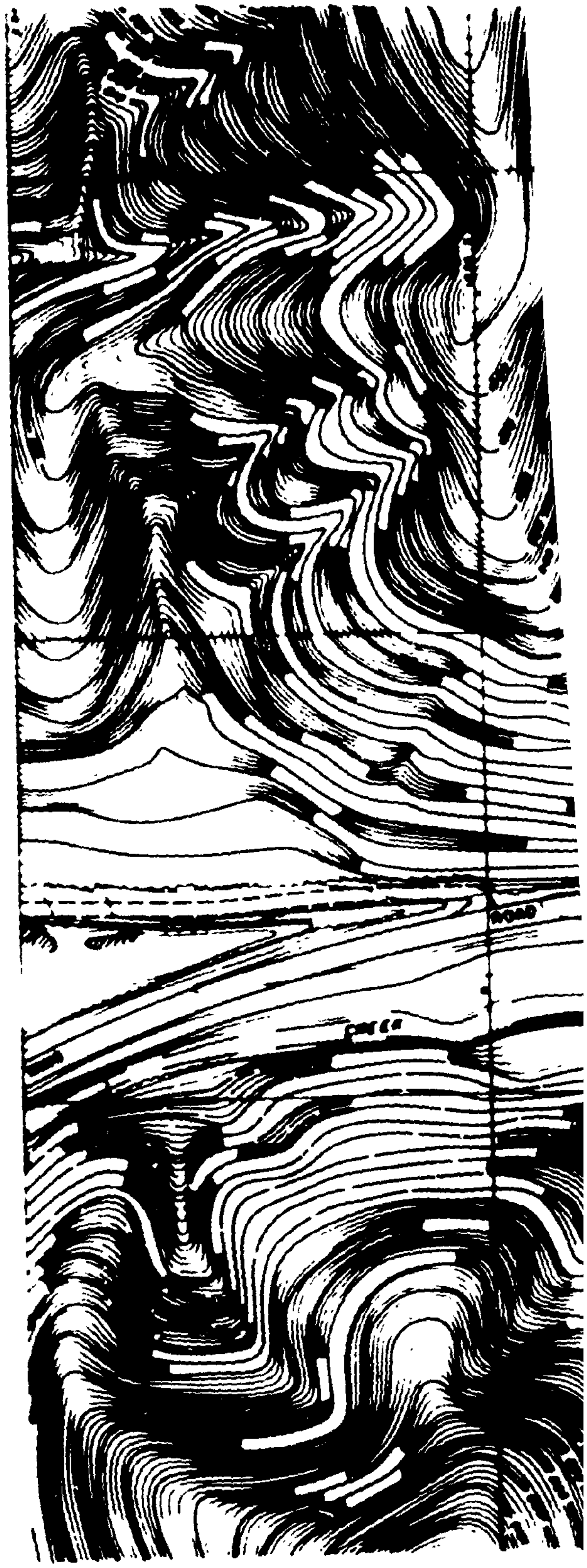
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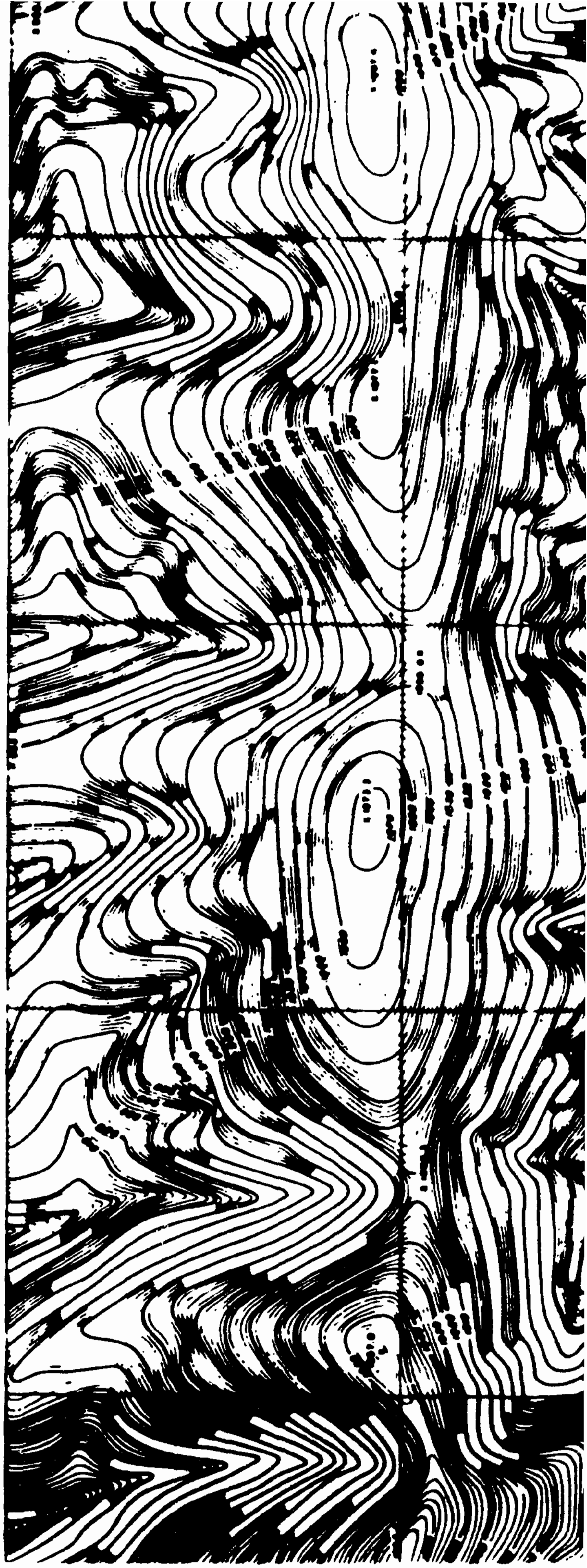

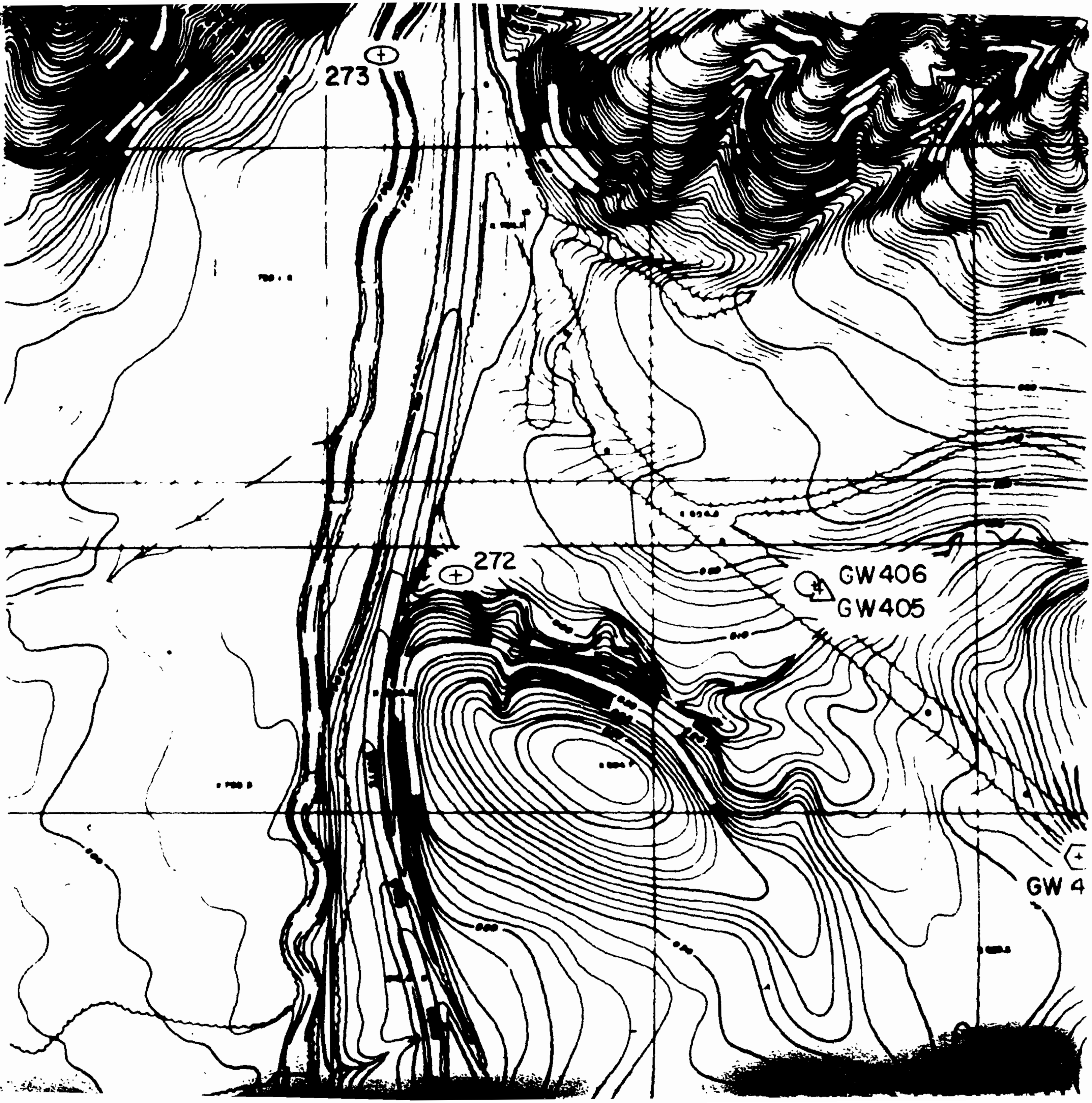
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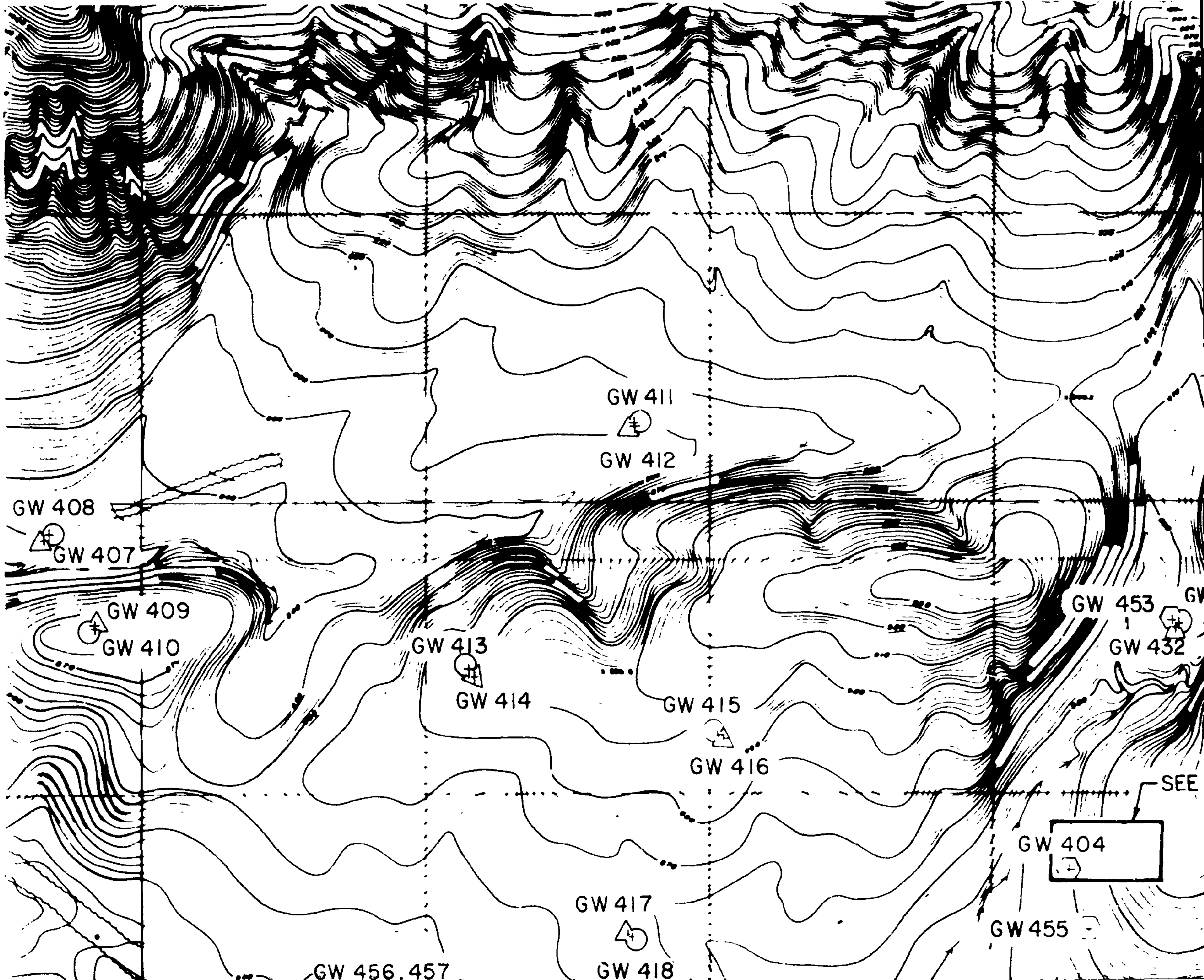
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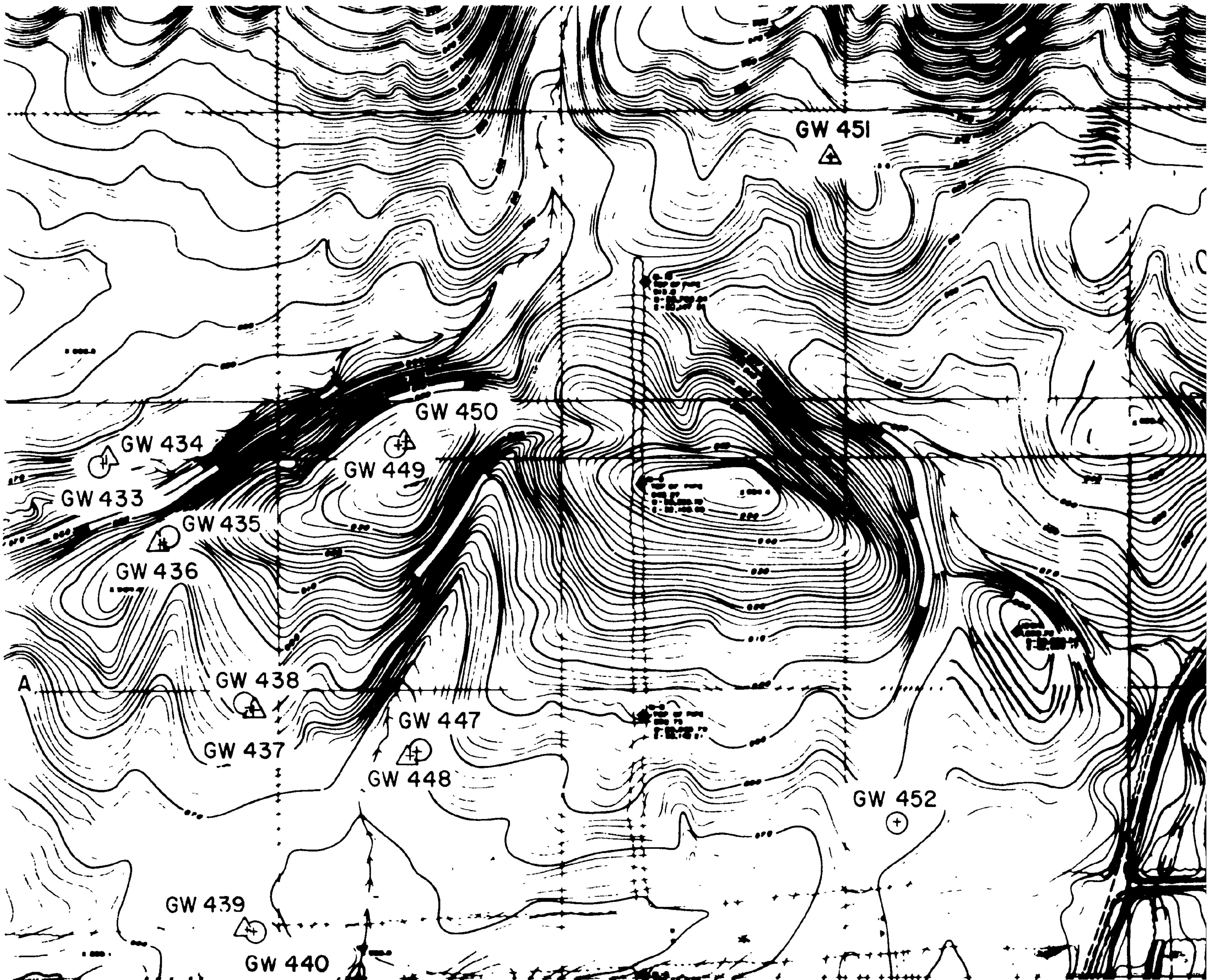
GW 455



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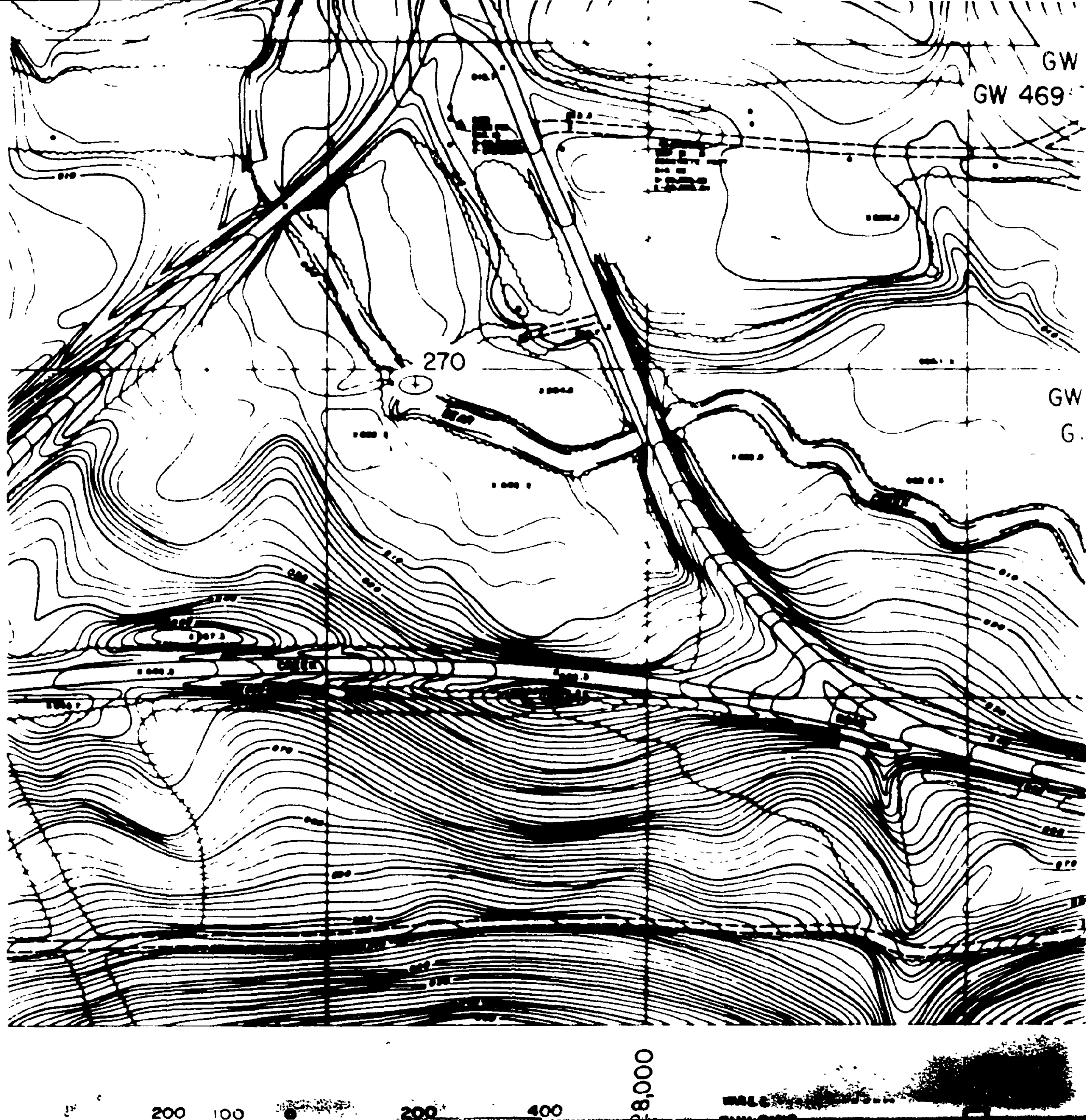
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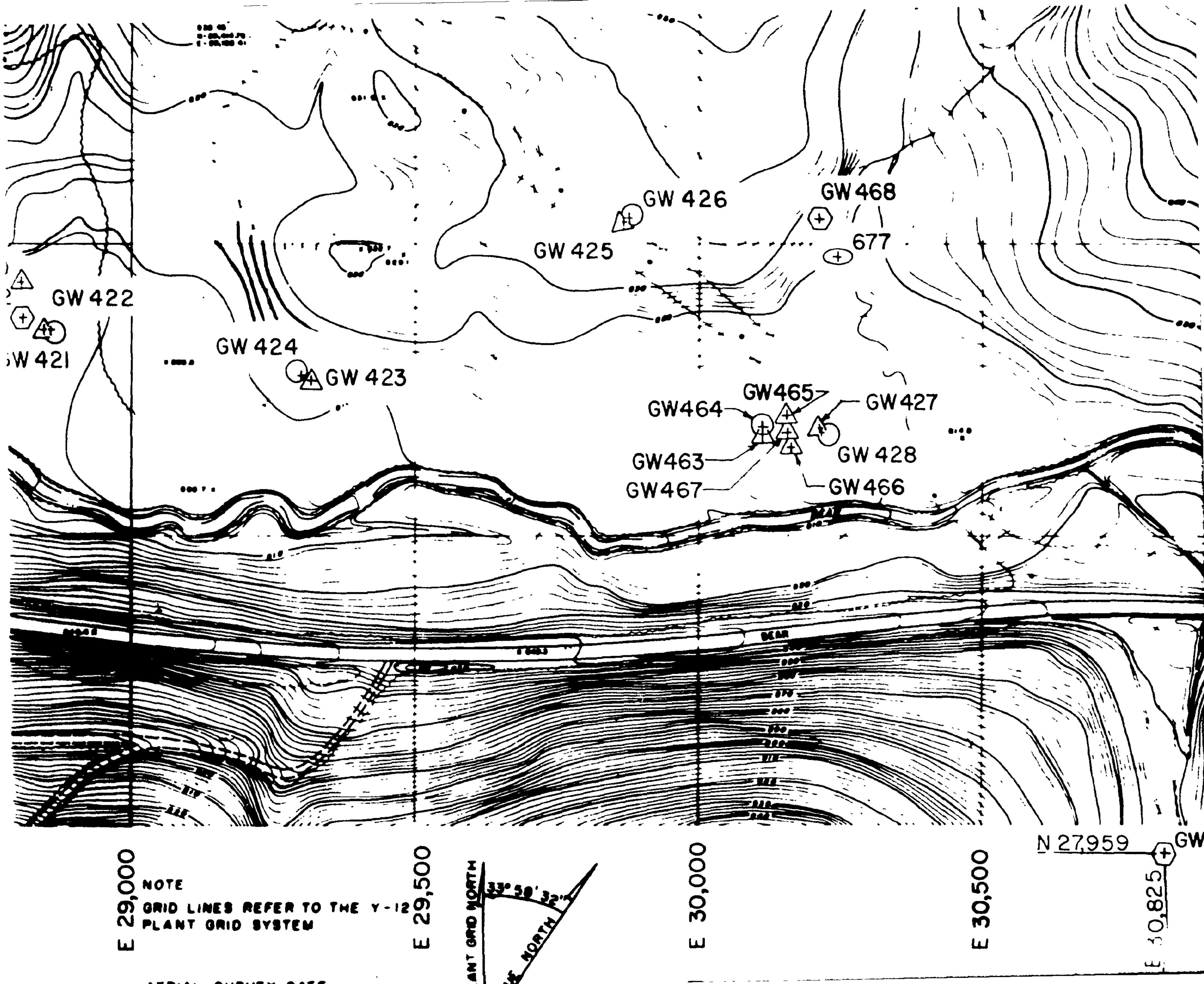
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GW 422
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GW 424
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GW465
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GW427
GW 428
GW463
GW467
GW466
N 27,959
E 29,000
E 29,500
E 30,000
E 30,500
E 30,825
NOTE
GRID LINES REFER TO THE Y-12 PLANT GRID SYSTEM
33°58'32"
NORTH

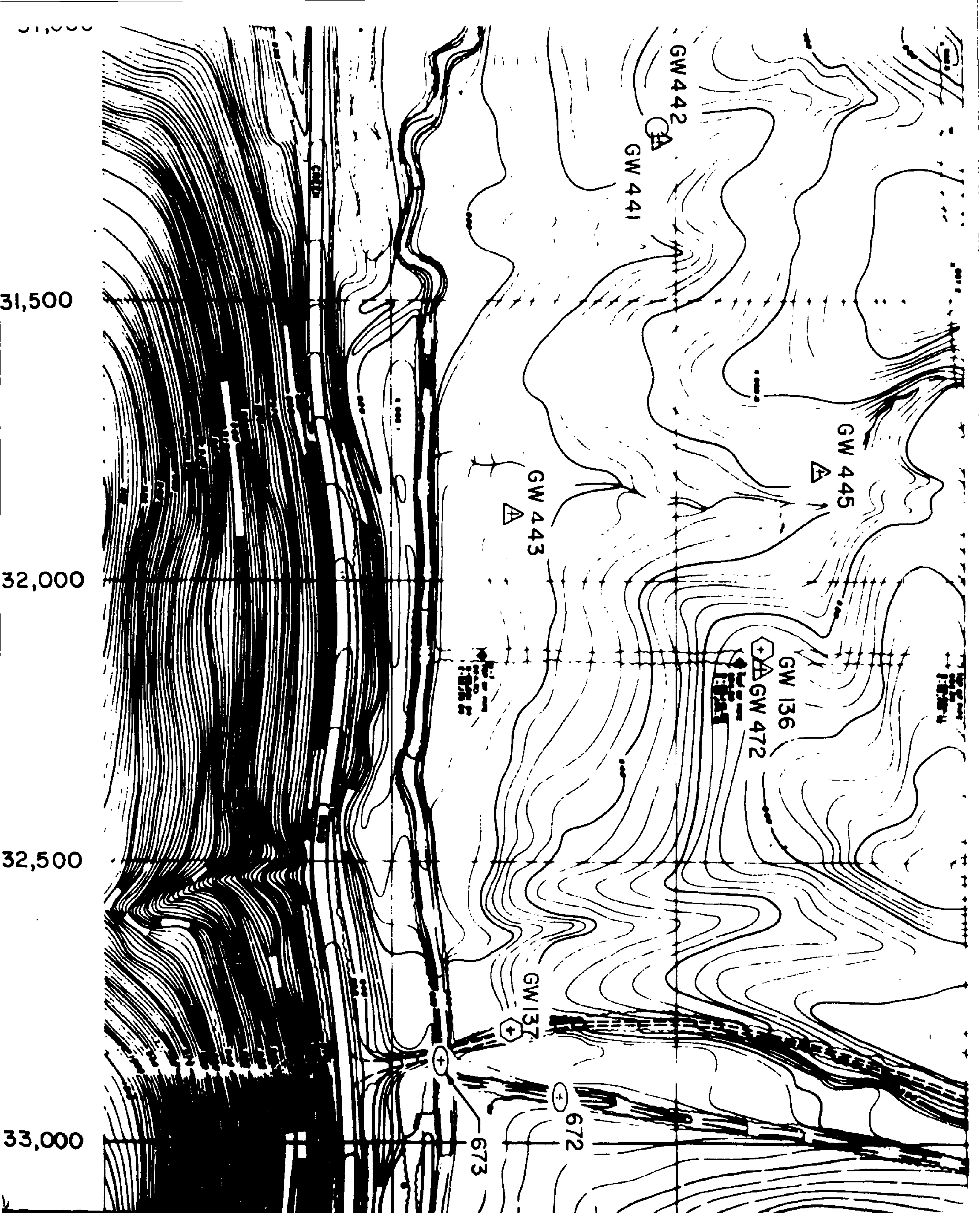
E 31,50(

E 32,00

E 32,50

E 33,00

FIG.
WEST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GW 442
GW 441
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GW 445
GW 136
GW 472
GW 137
672
673

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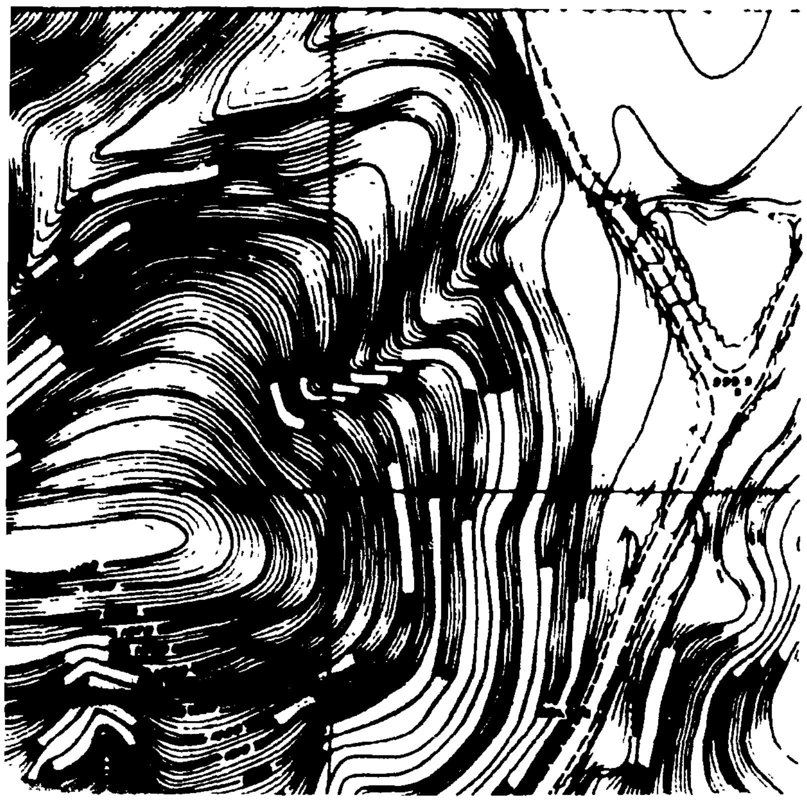
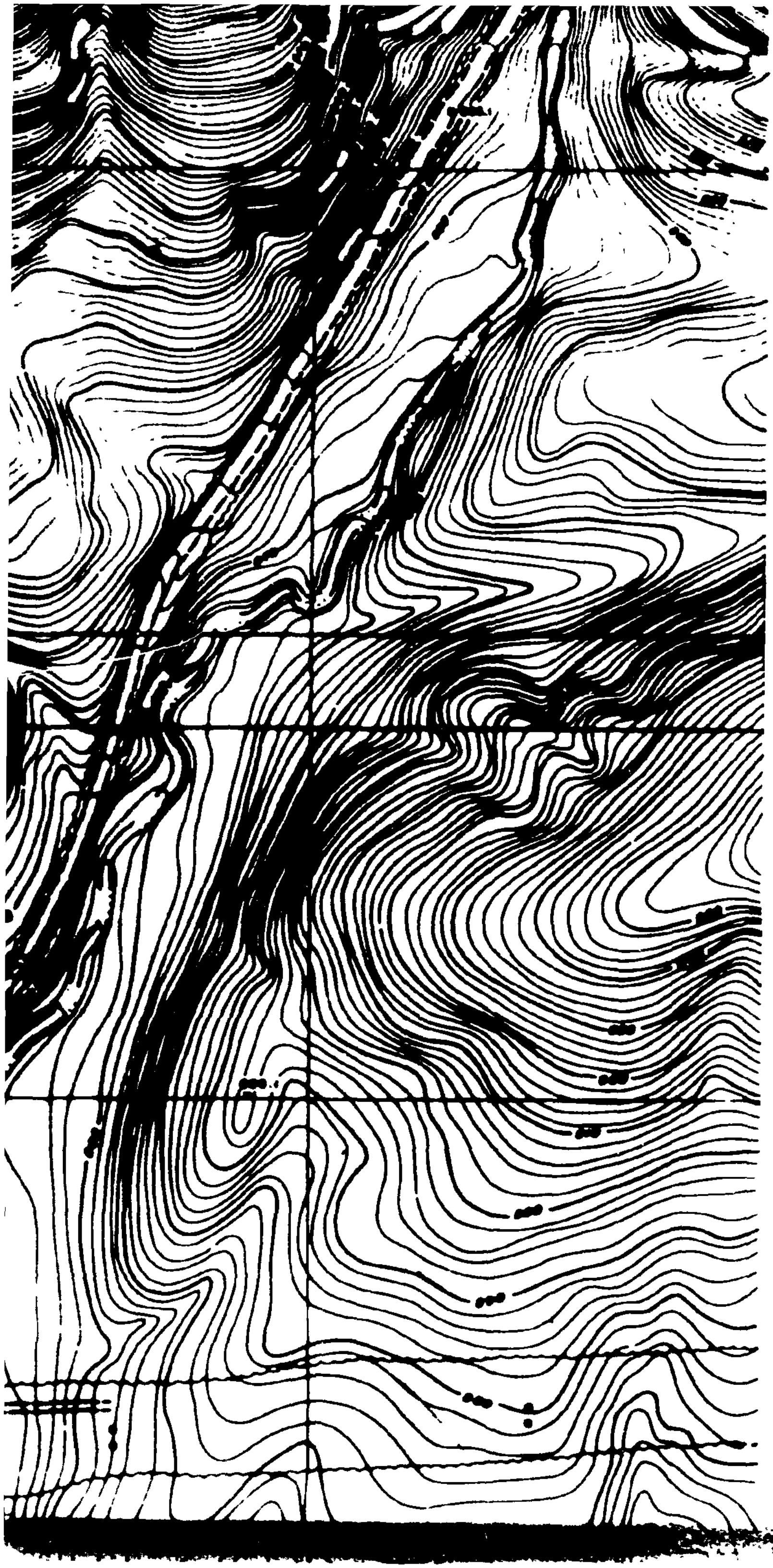


BEAR CREEK VALLEY WELL SURVEY DATA

WELL NO.	AS BUILT COORDINATES NORTHING	AS BUILT COORDINATES EASTING	ELEVATIONS GROUND	T/PROT. CASING	T/STEEL CASING	T/PVC CASING	MEASURE POINT
GW-136	29147.48	32120.20	855.81		856.34	858.53	858.[illegible]
GW-137	28712.00	32796.00	832.88		836.11		
GW-138	27959.00	30825.00	838.78		842.03		
GW-400	29926.99	28651.66	838.77	839.40	939.78		844.59
GW-401	29438.48	28709.57	834.80	835.27	835.97	836.24	837.64
GW-402	28869.60	28805.33	807.96	811.40		811.06	811.40
GW-403	29520.96	30479.75	835.43		837.12	839.22	838 45
GW-404	29870.29	30636.05	852.30		852 81		
GW-405	30323.58	28253.08	813 79	816 19		815.51	
GW-406	30330.43	28247 33	813.90	816.90		815.94	
GW-407	30434.65	28628.24	832.17	834.45		834 22	
GW-408	30442.79	28837.92	832.33	834 80		834.50	
GW-409	30289.30	28916.54	875.49	877.96		877.74	
GW-410	30283.26	28916.09	875.49	878.00		877.75	
GW-411	30637.33	29868.24	862.16	864.45		864.25	
GW-412	30625.76	29868.66	862.60	864 17		864.05	
GW-413	30211.02	29578.32	891.22	893.70		893.15	
GW-414	30199.96	29585.74	891.72	893 92		893.53	
GW-415	30099 66	30018.45	894.39	896 76		896.59	
GW-416	30096.84	30022.85	894 64	896.73		896.66	
GW-417	29758 11	29855.75	867.33	869.50		869.16	
GW-418	29752 14	29862 24	866.98	869 09		868 69	
GW-419	29473.36	29425.25	834.66	836 66		836.29	
GW-420	29473 57	29439 80	835 07	837.42		837 11	
GW-421	28850 04	28843 60	808 32	810 03		809.77	
GW-422	28849.53	28855.92	807.42	809.46		809.09	
GW-423	28762.24	29314.19	814.27	816.58		816.39	
GW-424	28773 84	29299.44	814.33	816.51		816.28	
GW-425	29037 15	29867 41	841 27	843.46		842 96	
GW-426	29042 81	29872 19	841 47	843 62		843 22	



GW-427	28682.11	30210.83	815.96	818.16		817.79	
GW-428	28678.78	30217.99	815.97	818.42		817.84	
GW-429	*29521.94*	*30471.44*	*835.40*	*837.42*		*837.16*	
GW-430	29522.24	30463.95	834.87	837.24		836.87	
GW-431	30289.41	30828.81	862.78	865.09		864.86	
GW-432	30283.78	30821.16	862.08	864.68		864.43	
GW-433	30390.62	31191.70	869.29	871.23		870.76	
GW-434	30397.54	31195.83	869.49	871.82		871.43	
GW-435	30253.45	31298.11	902.46	904.66		904.25	
GW-436	30250.71	31291.04	902.23	904.31		904.03	
GW-437	29960.52	31457.62	891.09	893.26		892.99	
GW-438	29967.91	31456.01	891.53	893.71		893.25	
GW-439	29582.44	31447.29	868.28	870.26		870.05	
GW-440	29580.31	31453.12	868.18	870.49		870.13	
GW-441	28967.71	31214.63	836.54	838.44		838.09	
GW-442	28967.06	31206.30	837.21	840.03		839.29	
GW-443	28713.58	31880.90	827.75		829.37		
GW-444	------- ABANDONED -------		------	------	------	------	
GW-445	29250.20	31805 46	842.15	842.20		846.53	
GW-446	------- ABANDONED -------		------	------	------	------	
GW-447	29893.72	31744.64	872.64	875.15		874.25	
GW-448	29885.85	31730.31	872.23	874.08		873.86	
GW-449	30422.63	31713.87	934.21	936.58		935.82	
GW-450	30430.33	31726.04	933.84	935.86		935.47	
GW-451	30919.40	32478.64	928.77	931.46			
GW-452	29767.95	32590.72	872.73	874.98		874.79	
GW-453	30298.35	30814.34	862.27	862 60	863.59 *		
GW-454	------- ABANDONED -------		------	------	------	------	
GW-455	29765.95	30676 25	853.44			855.75	855.75
GW-456	29621 30	29259 87	842.73	842 92*		844.88	
GW-457	29621.30	29259 87	842 73	842.92*		845.36	
GW-458	29581.22	29261.56	842 72	843 13		844.68	
GW-459	29581.22	29261.56	842 72	843 13		845.18	
GW-460	29601.91	29210.49	840.22	840.33		842.15	
GW-461	29601.91	29210.49	840.22	840.33		842.55	
GW-462	29601.15	29260 50	842.46	842.89		843.32	
GW-463	28679.66	30111.11	815.19			816.87	
GW-464	28680.53	30111.26	815.80			817.32	
GW-465	28788.36	30154.55	816.50			817.74	
GW-466	28650.90	30161.30	816.63			817.84	
GW-467	28678.88	30159.43	816.36	818.97		818.89	818.97
GW-468	29840.14	30210.77	826 19	829.53	829.12		829.63
GW-469	29440.48	28678.32	833.76	835.32		834.40	835.32
GW-470	28935.46	28882.98	808.63	811 [illegible]		810.57	811.01
GW-471	29875.29	30721.63	864.14			865.18	
GW-472	29145.47	32157.27	856.69	859.25			859 25
GW-473	29980.16	30737.60	868.60			868 93	
GW-474	29980.64	30743 32	868.87			870 03	
GW-475 A	29880.60	30737.81	868 63		869 07	870 20	

E 33,

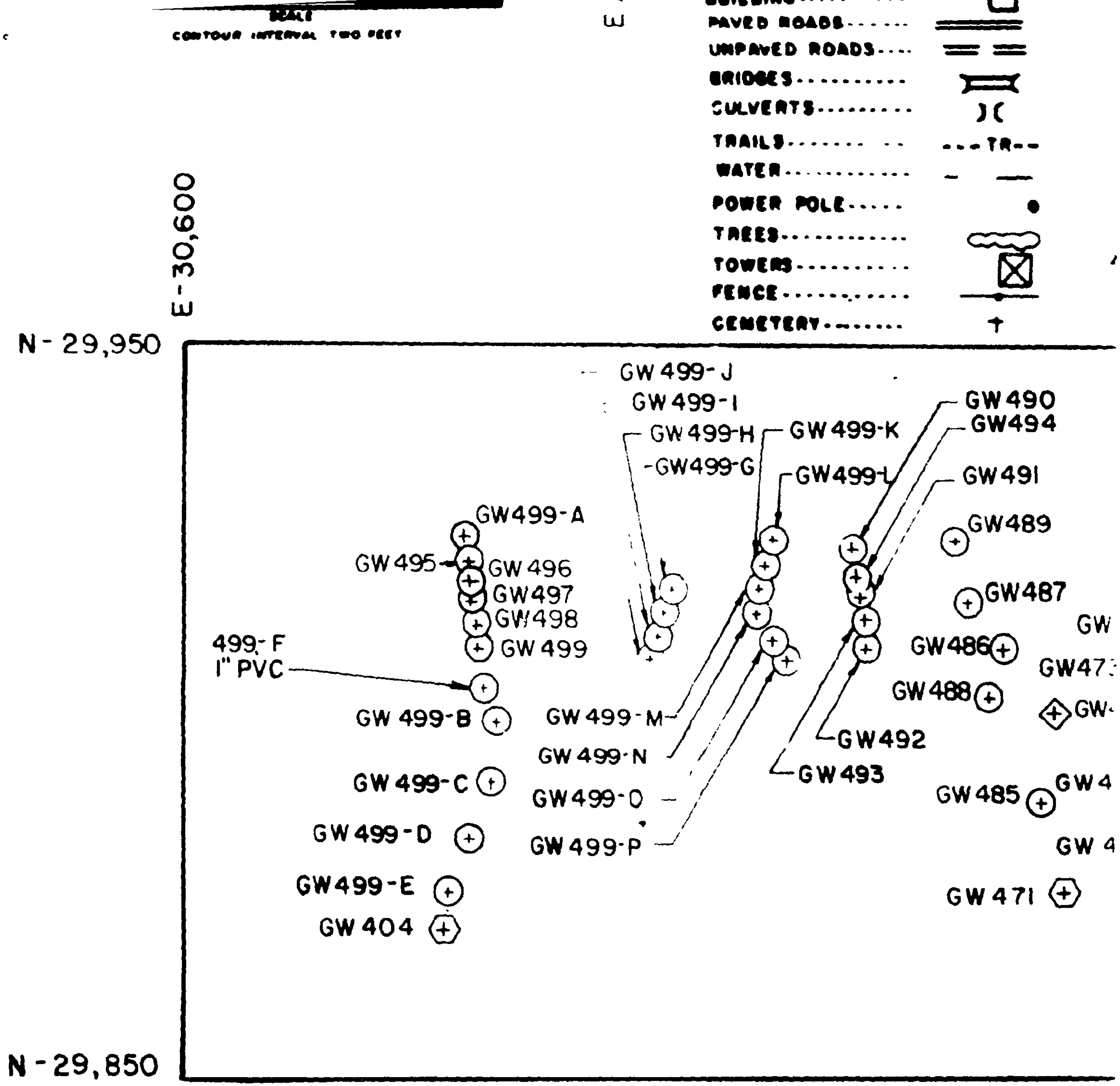
AR CREEK VALLEY SITE

GW-499K	29913.73	30680.58	859.44		862.32
GW-499L	29922.96	30681.85	859.62		862.26
GW-499M	29916.41	30679.56	859.39		862.35
GW-499N	29913.23	30679.66	859.32		862.27
GW-499O	29910.03	30681.70	859.20		862.03
GW-499P	29907.35	30683.35	859.37		860.07
LL/HAZ-13	30640.63	32192.72	916.34	918.83	918.61
LL/HAZ-14	30236.57	32157.15	932.47	935.09	934.95
LL/HAZ-15	29779.90	32153.06	878.41	880.00	879.89
WEIR 270	28967.56	27638.24	804.31 (CORNER OF CONC.)		
WEIR 272	31142.40	27584.70	802.66 (C/L OF CREEK @ BRIDGE)		
WEIR 273	30350.62	27698.64	808.11 (TOP OF WEIR)		
WEIR 672	28799.20	32920.15	831.23 (TOP C/L CONC.)		
WEIR 673	28582.92	32836.06	825.39 (N E SPILLWAY)		
WEIR 677	28975.18	30247.42	819.01 (TOP OF CONC)		

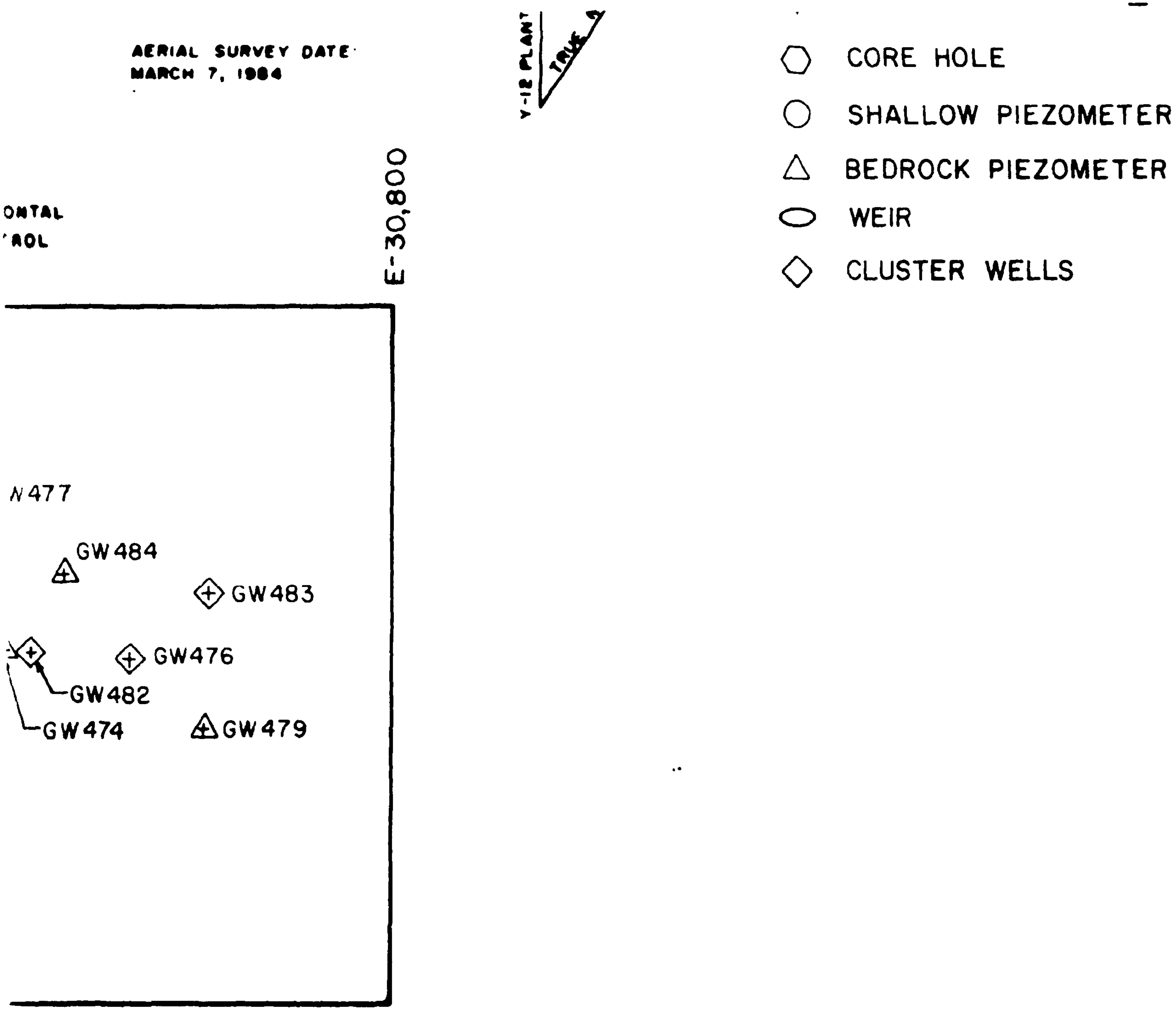
NOTES: 1) T/STEEL CASING OR T/PVC CASING REPRESENTS THE "NOTCH" OR "MEASURE POINT" LOCATED ON THE INNER CASINGS OF THESE WELLS

2) * INDICATES ELEVATION TAKEN AT TOP OF CONCRETE (NO PROTECTIVE CASING FOR THESE WELLS)

3) # INDICATES ELEVATION TAKEN AT TOP OF ELBOW

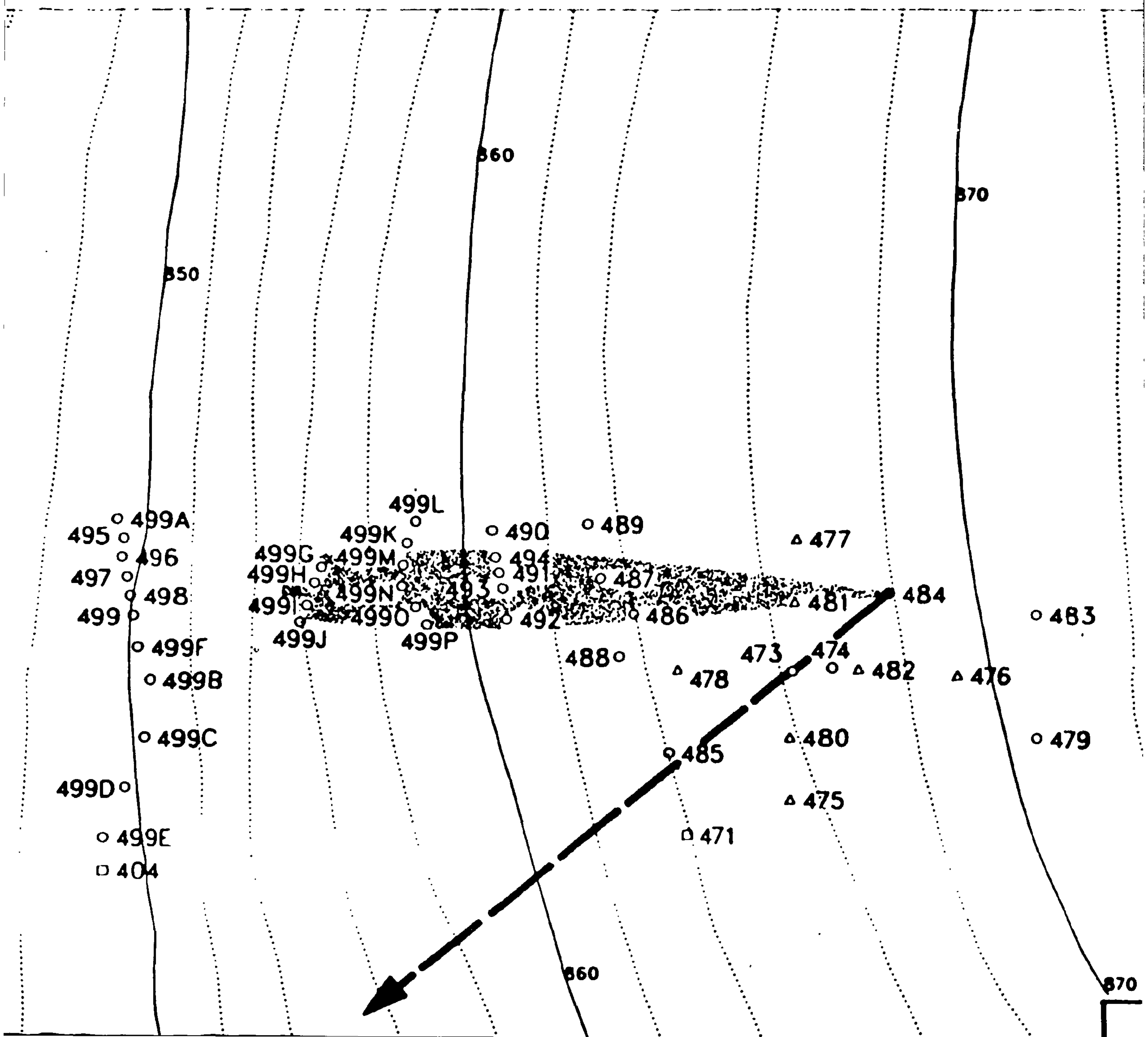


INSET A
SCALE: 1" = 20'



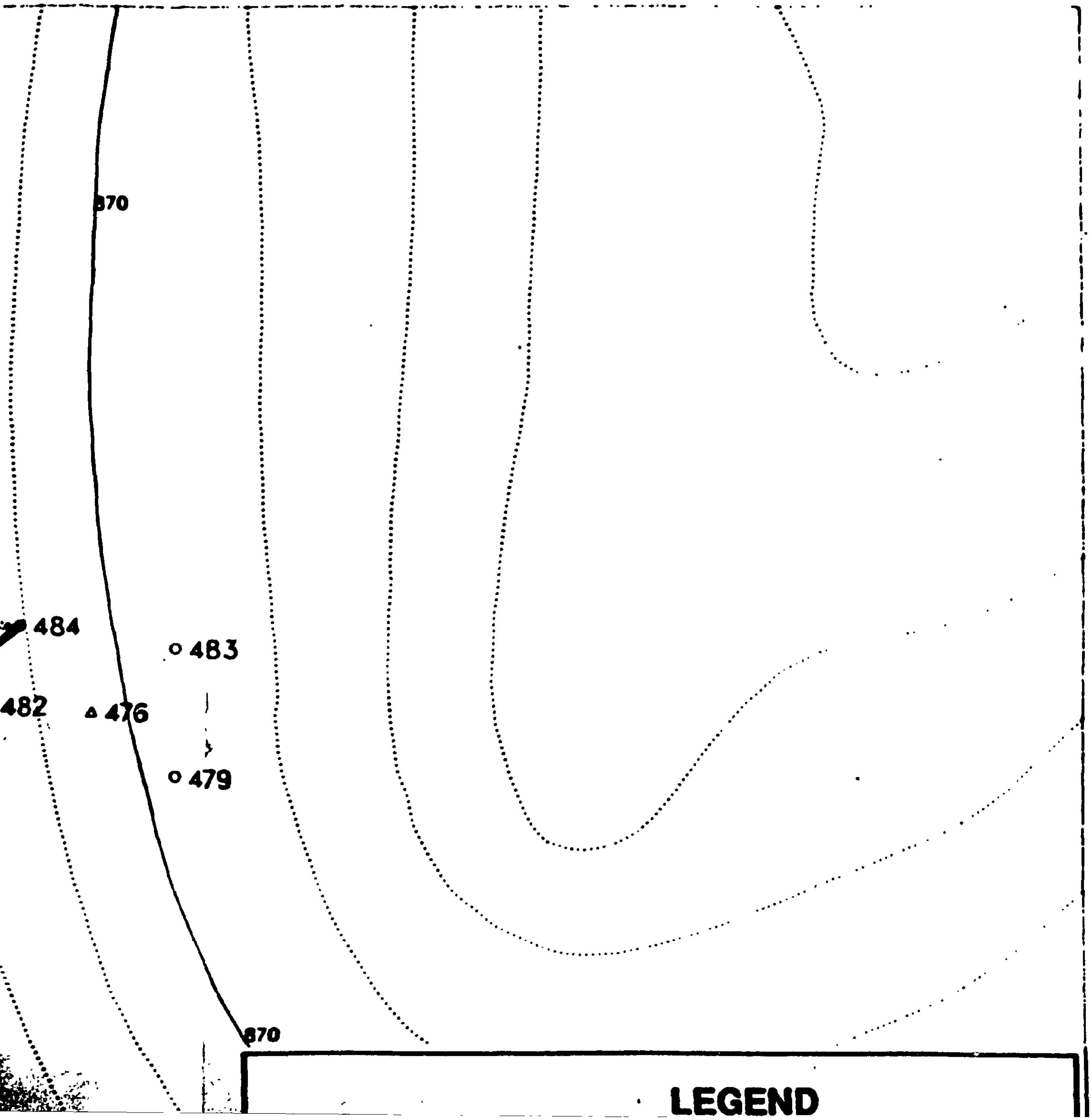
AERIAL SURVEY DATE
MARCH 7, 1984
Y-12 PLANT
TRUE
ONTAL
ROL
E-30,800
CORE HOLE
SHALLOW PIEZOMETER
BEDROCK PIEZOMETER
WEIR
CLUSTER WELLS
N477
GW484
GW483
GW476
GW482
GW474
GW479

FIG. 3
MODEL VALIDATION TEST SITE

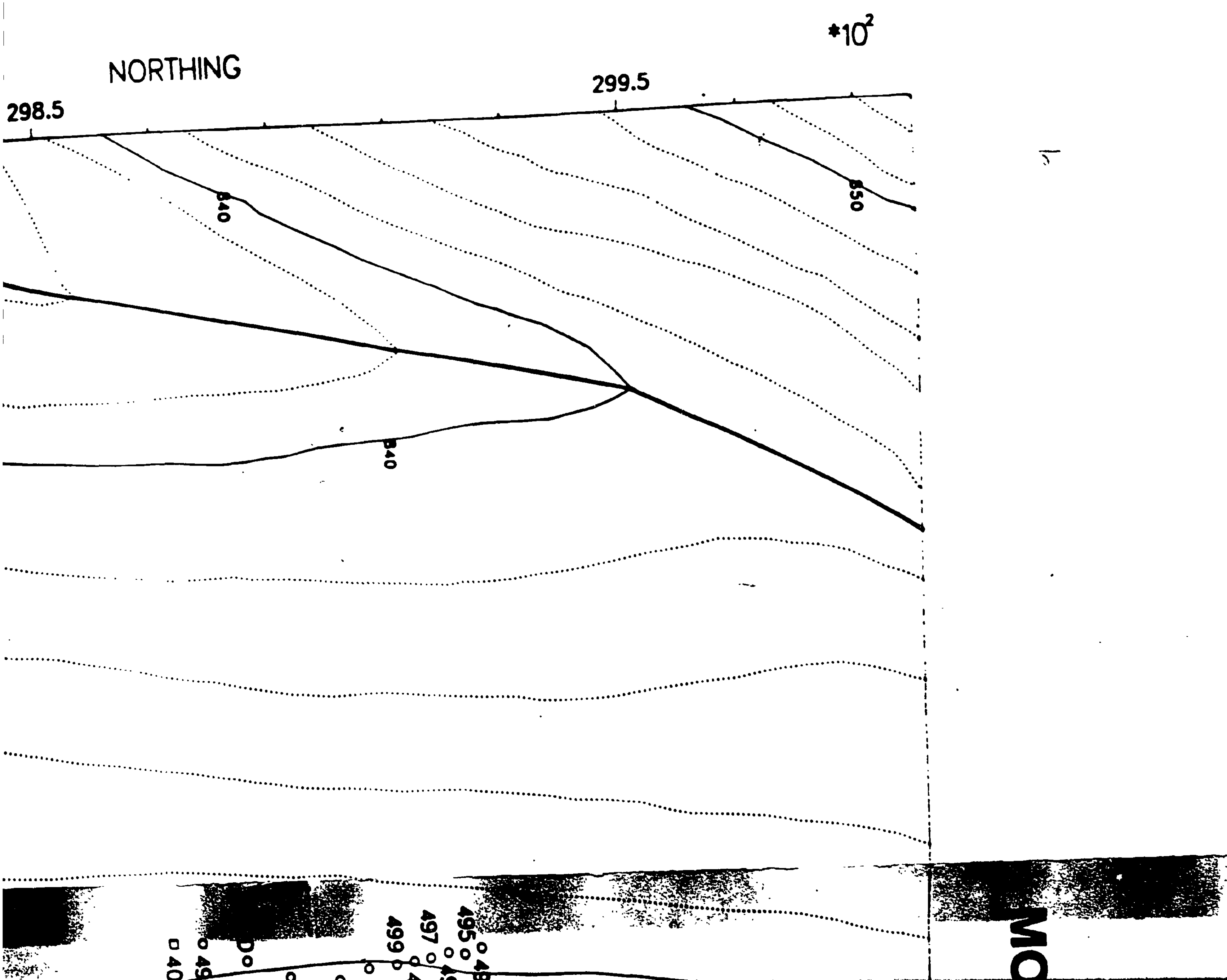


ORNL-DWG 88-14197

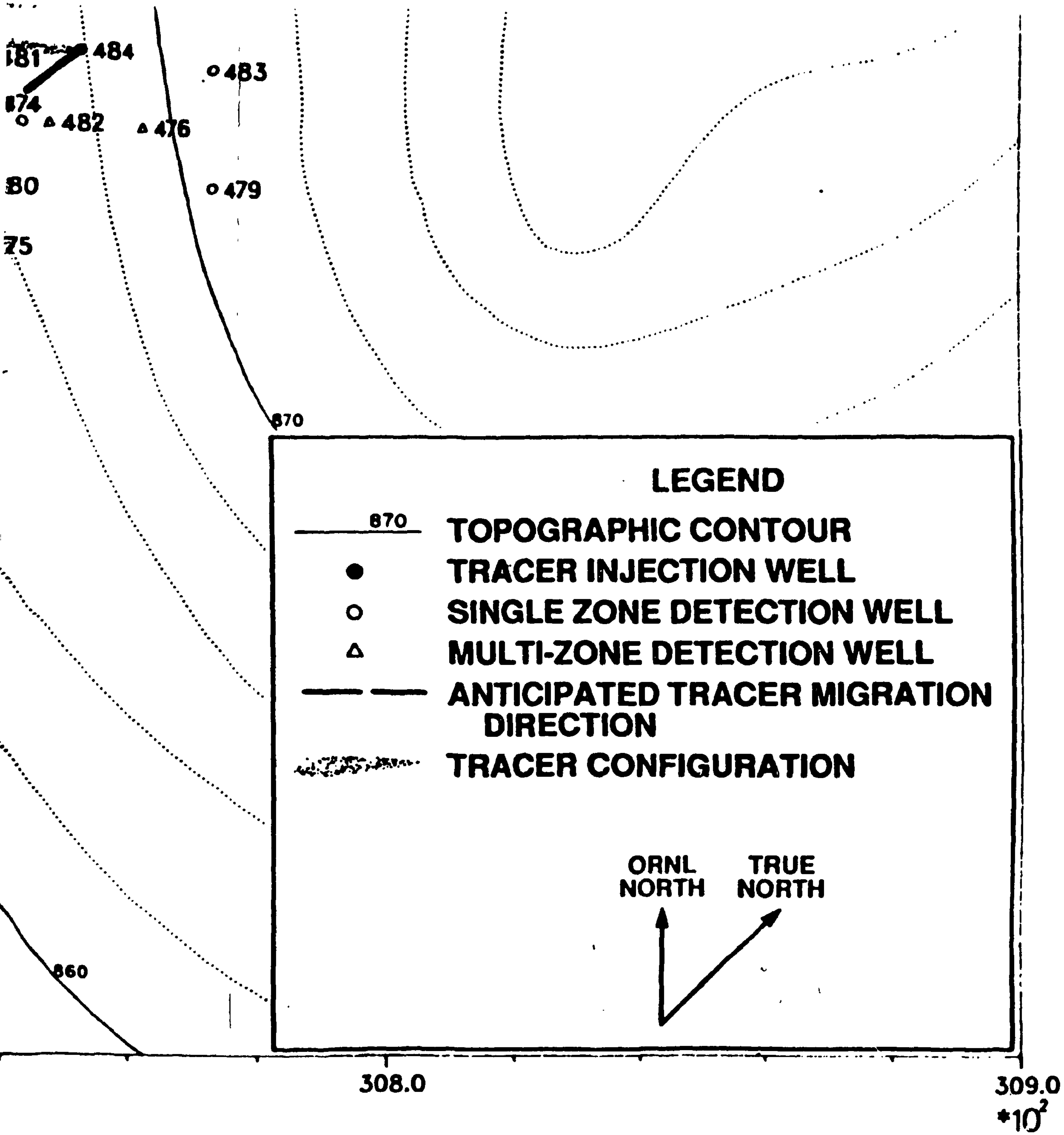
ITE



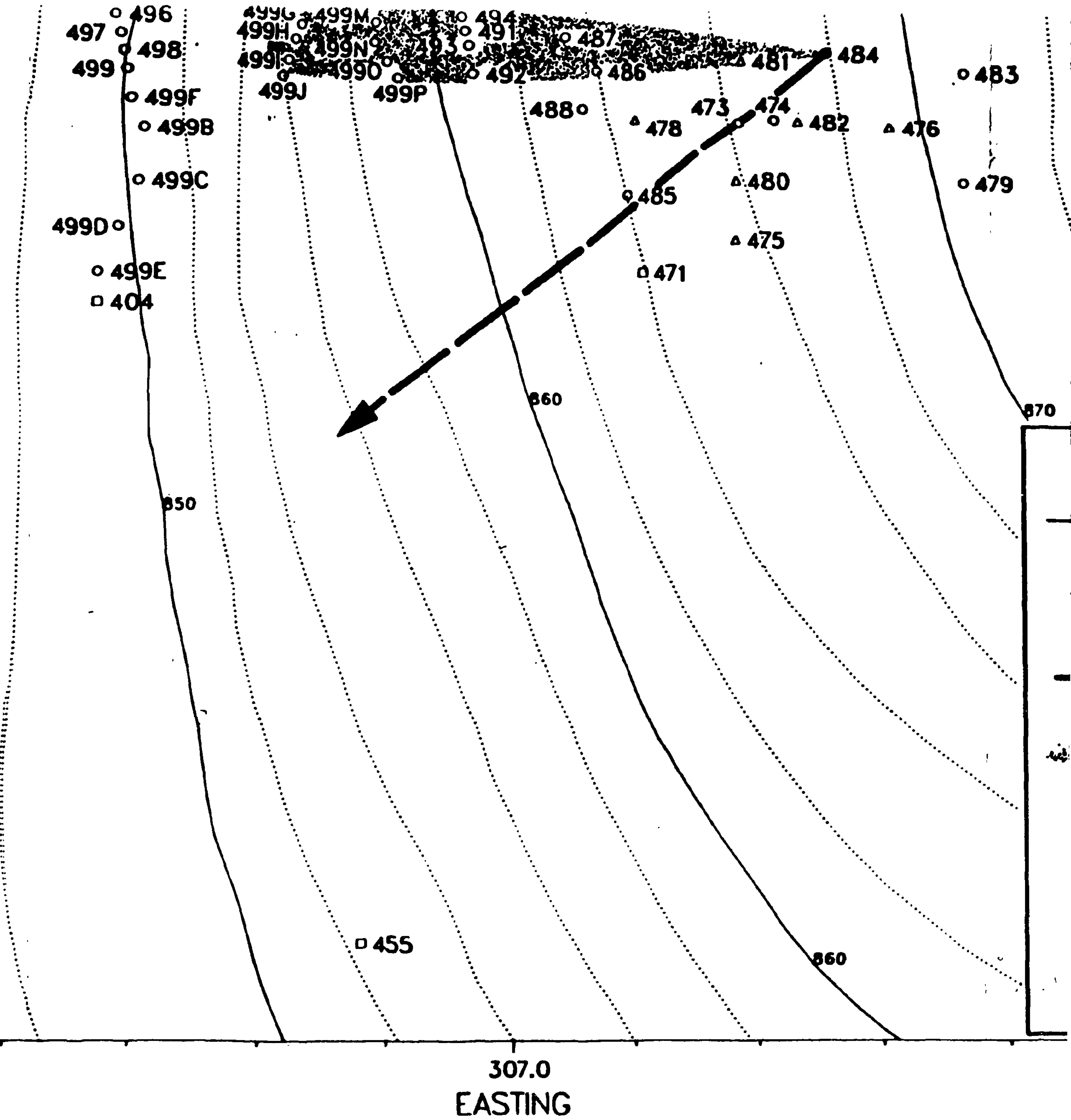
LEGEND



*10²
NORTHING
298.5
299.5
840
850
840
499
497
495



484
483
482
476
479
870
860
LEGEND
870 TOPOGRAPHIC CONTOUR
TRACER INJECTION WELL
SINGLE ZONE DETECTION WELL
MULTI-ZONE DETECTION WELL
ANTICIPATED TRACER MIGRATION DIRECTION
TRACER CONFIGURATION
ORNL NORTH
TRUE NORTH
308.0
309.0
*10^2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499F
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499C
499D
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499M
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499N
499I
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499P
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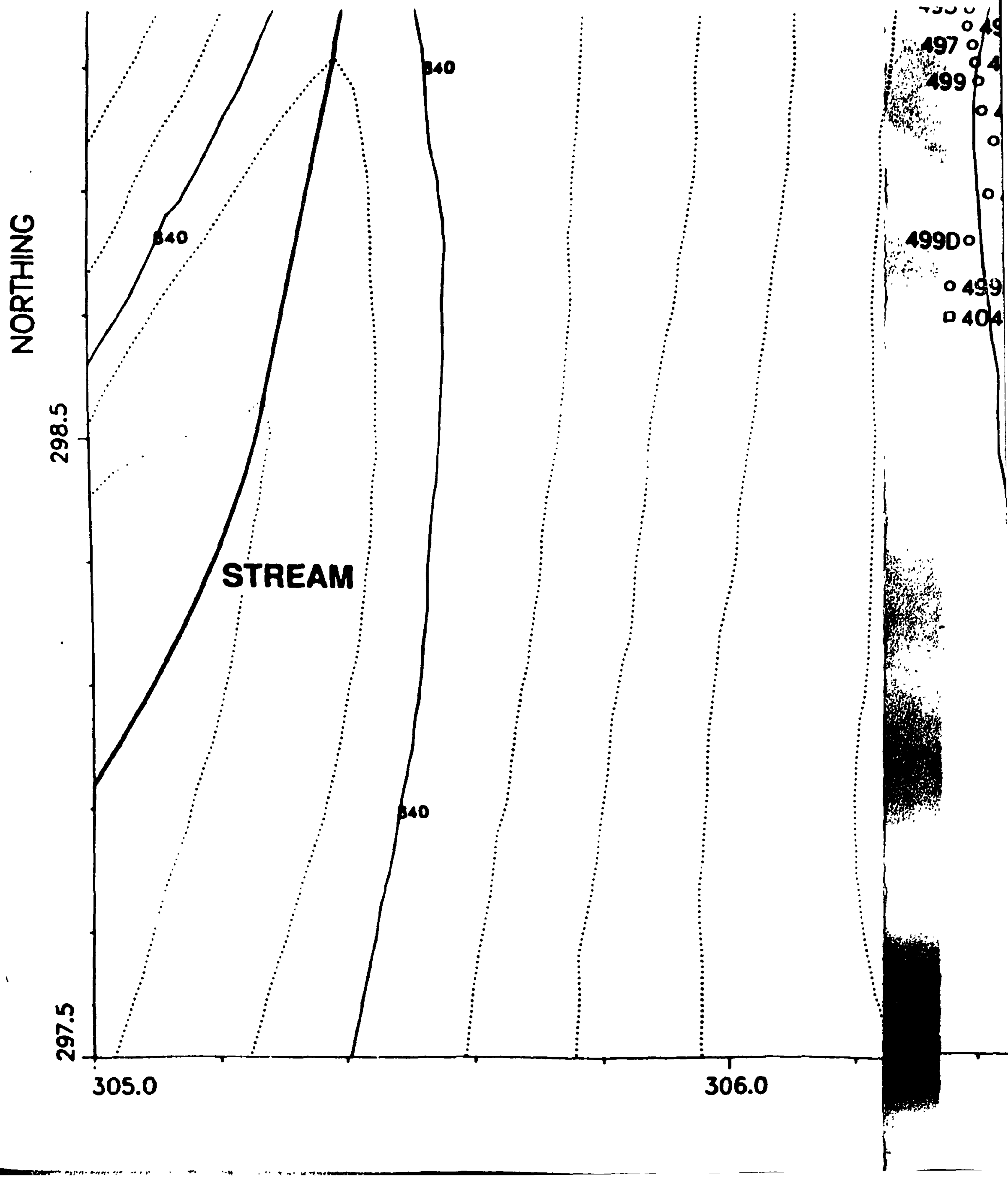
455
850
860
870
307.0
EASTING



NORTHING
298.5
297.5
305.0
306.0
840
840
840
STREAM
497
499
499D