Chapter 2. Model Preparation

I. Method

The modeling method included the formulation of a conceptual model, the approximation and discretization of the conceptual model into a mathematical model, and the solution of the mathematical model using the USGS computer programs, MODFLOW (McDonald and Harbaugh 1988) and MODFLOWP (Hill, 1990).

II. Conceptual model

The conceptual model is a simplification of an interpretation of the natural system. Such a simplification was necessary in order to construct a numerical problem solvable by MODFLOW and MODFLOWP. The conceptual model consists of three layers. Layer 1 is the Eocene Wasatch sand lens layer and was modeled explicitly. Layer 2 is the Eocene Wasatch / Upper Tongue River confining bed, which was modeled implicitly, meaning that it filled the space between the top and bottom layers, but was represented solely by a vertical hydraulic conductivity in the formulation of the model. Layer 3 is the Paleocene Wyodak coal seam of the Tongue River Member of the Fort Union Formation, which was modeled explicitly.

II.a. Model layers

II.a.1. Sand lens layer

The sand lens layer was developed about the Wasatch Sand Lens. The location of the Wasatch Sand Lens and its proportions are known to a high degree of certainty based on data, as described in section III.1. Since MODFLOW requires each layer to be continuous over the model area, layer 1 was extended arbitrarily from the sand lens to the boundaries of the model. The hydraulic conductivity of this layer was manipulated to approximate the undifferentiated Wasatch Formation material outside of the sand lens.

II.a.2. Implicit confining layer

Separating the coal, below, from the sand lens layer, above, is a confining layer. Based on the observation of driller's logs, this layer consists of undifferentiated Wasatch Formation material. As such it acts to hinder flow between the coal and sand lens layers.

II.a.3. Coal layer

Two interpretations of coal structure are supported by the data. The first is of one continuous coal seam, parted in the north and parted in the south, but unparted through the center of the study area. Alternatively, the layer of coal above the southern parting may pinch out, and not reconnect with the main body of the coal (Figure 2-1). A clear distinction can not be made between these two scenarios due to the correlation procedure, as discussed in section III.1.

II.b. Starting head gradients

A northwest gradient in the coal and sand lens layers was indicated for the study area both from raw head data and from previous studies in the area (Peacock, 1997a). The head in the sand lens layer is slightly higher than that of the coal layer.

II.c. Boundaries

The full-seam coal-line boundary, or cropline, in keeping with the conceptual model and in the interests of numerical stability, was designed as a specified head boundary. This eastern edge contains clinker, which is highly porous and permeable. Clinker in contact with the coal acts, in effect, as would a standing body of water, by flowing into the model as demanded (Peacock, 1997a).

The full-seam coal-line boundary was designed by overlaying the modflow grid and the full seam coal line, and determining on which side of the line the cells of the model fell.

The other three boundaries of the model are at a sufficient distance from the model stresses to not be reached by drawdowns in any of the layers over the time period of transient simulation. Thus they are modeled as specified head boundaries.

In order to determine the size of the model domain necessary for transient simulation, a first order approximation of the effects of the stresses on the system was made. A Theis solution was calculated with aquifer transmissivity of 840 square feet/day and a storativity of 0.00025. The coal was modeled as homogeneous and isotropic with a hydraulic conductivity (K) of 14 feet/day, which is on the order of the long axis of the K ellipse as calculated for the coal. The pumping from the Marquiss coal bed methane well field was approximated by one well pumping at a rate of 504 gallons/minute over a period of three years. The results are shown in figure 2-2. The model boundaries were constructed accordingly.

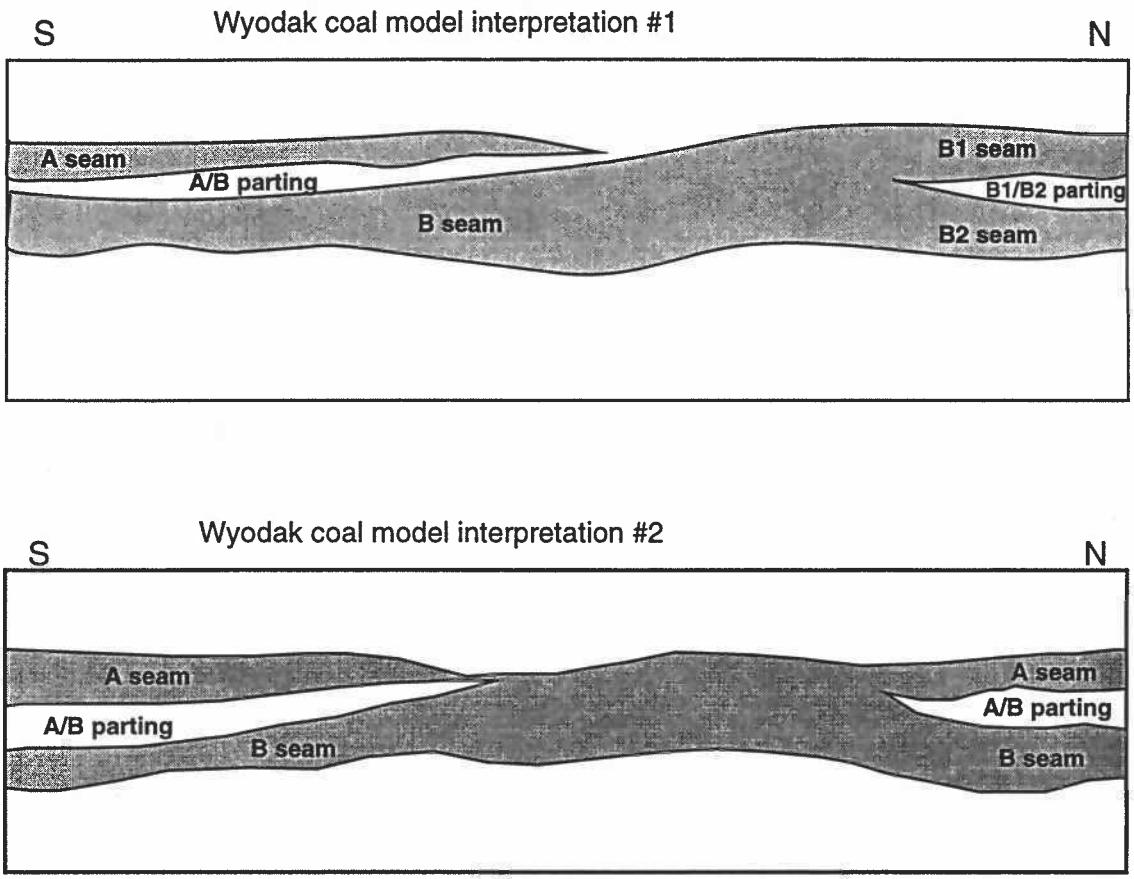

Figure 2-1. Idealized north-south cross sections through the study area of two coal structure interpretations which are indistinguishable from the data as analyzed in this study. Highly vertically exagerated.

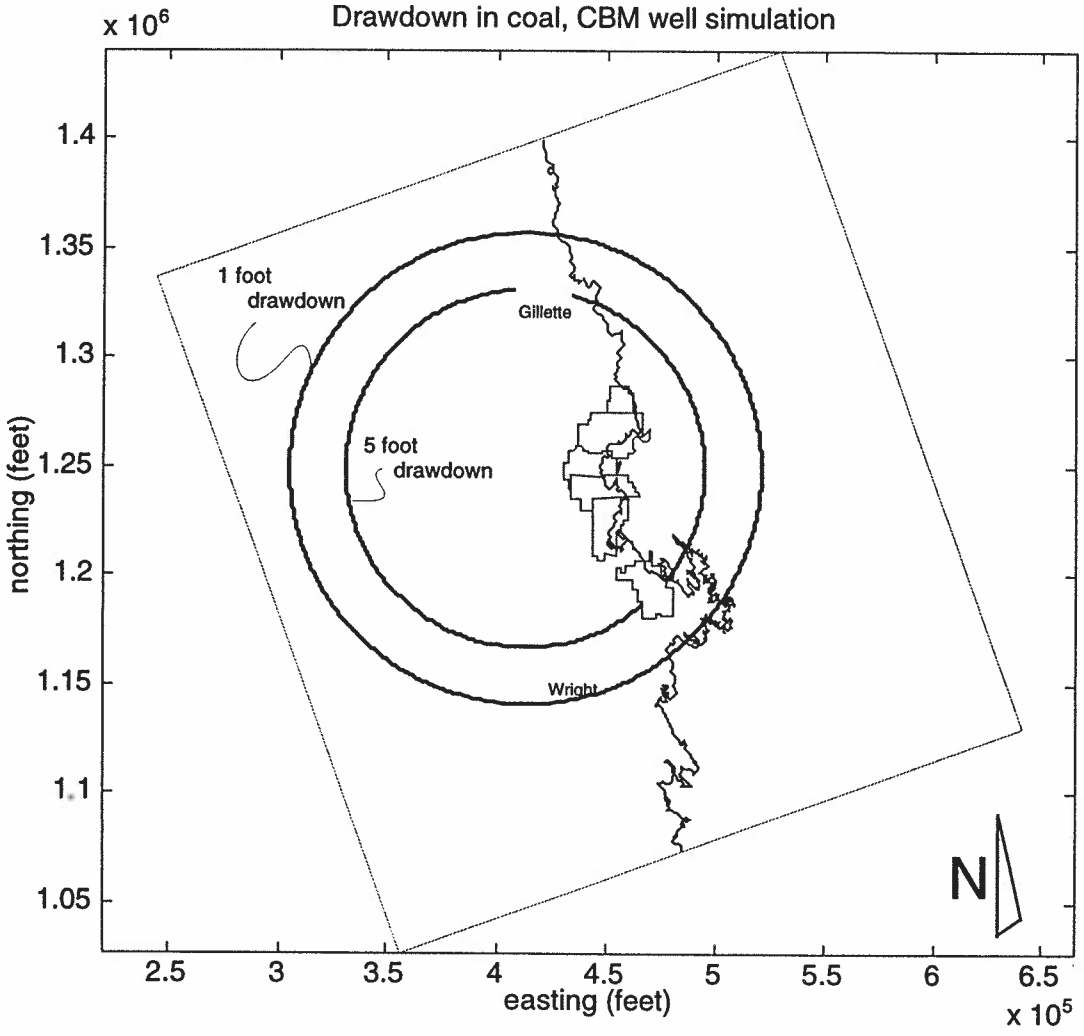

Figure 2-2 . Drawdown from aquifer stress simulation with transmissivity=840 feet^2/day and a discharge of 504 gal/day over 3 years from coal bed methane wells. Mine permits and cropline shown for orientation. Modflow model boundary shown as gray rectangle.

II.d. Anisotropy

The coal was determined, by two long-range aquifer pump tests conducted by the Bureau of Land Management (BLM), to have a two to one horizontal hydraulic conductivity anisotropy in the N27W direction (Kern, 1997a).

III. Statigraphic Model

III.1. Compilation and Correlation of Stratigraphic Data

Driller's logs were compiled from USGS Open-File Reports, the Montana Bureau of Mines and Geology, Permit to Mine Applications, Martens and Peck Stratigraphic Test Holes, a BLM database courtesy of Jim Bauer, a BLM database courtesy of Ken Peacock, and the Original BLM Public database. The accumulated logs totaled nearly 1800. The logs were entered into the relational database program STRATIFACT (StratiFact Software, 1995).

The study area was broken into manageable portions by correlating 50 cross sections, approximately half of which ran north-south and half of which ran east-west. More cross sections were constructed in areas of greater data density. Smaller cross sections were then constructed perpendicular to the 50 previously correlated, beginning and ending with points that were already correlated.

The stratigraphy was broken into six hydrostratigraphic units: the Wasatch Formation, the Fort Union Formation Wyodak A Member, the Fort Union Formation Wyodak Parting Member, the Fort Union Formation Wyodak B Member, the Fort Union Formation Wyodak Wyo Member (where no parting could be identified), and Fort Union Formation Tongue River Member. Everything above the Wyodak coal was labeled Wasatch, except for one sand lens as discussed. Everything below the Wyodak coal was labeled as Fort Union Formation Tongue River Member. In order to identify the geometry of the monitored sand lens in the Wasatch Formation, the formation was subdivided into Oversand deposits, the Wasatch Sand Lens, and Undersand deposits.

In order to minimize the number of layers to be included in the ground-water-flow model, only partings larger in vertical extent than 15 to 20 feet were correlated. Smaller partings were lumped into coal layers. In addition, only one parting per hole was correlated. In cases where there were multiple thick partings separated by thin coals, the coals were lumped in with the

partings. In cases where the interbedded coals were more substantial, all but the largest parting were lumped in with the coals. In locations with multiple substantial partings, some care was taken to maintain consistent correlation of the selected parting from one log to the next.

III.2. Construction of the Geologic Model

Data sets for the tops and bottoms of the following layers, in order of increasing depth, were generated from the correlated logs: Oversand deposits, the Wasatch Sand lens, Undersand deposits, Generic Wasatch (where no sand lens was located), Wyodak A, Generic Wyodak (where no parting was located), Parting, Wyodak B, and Fort Union Tongue River. These layers were not designed to correspond with accepted stratigraphic nomenclature. Rather, they were designed as a convention to facilitate the development of the conceptual geologic model.

As a matter of quality control the following data sets were generated: bottom of Oversand deposits, top of sand lens, bottom of sand lens, top of Undersand deposits, bottom of generic Wasatch, top of Wyodak A and top of generic Wyodak, bottom of Wyodak A, top of parting, bottom of parting, top of Wyodak B, bottom of Wyodak B and bottom of generic Wyodak, and top of the Fort Union Tongue River. The designation of Wasatch and Tongue River were conventions to describe the material above and below the coal respectively. To insure that only legitimate tops and bottoms were to be used in the geologic model, only those tops that were coincident with bottoms of overlying layers, and bottoms coincident with tops of underlying layers, were used. Logs, in which the bottom of a layer is registered without the top of the underlying layer, end in the layer being registered and do not indicate the actual bottom of the layer. Logs in which the top of a layer is registered without the bottom of the overlying layer end in the layer being registered and do not indicate the actual top of the layer. Such data points were not used in further development of the geologic model. Logs in which the top of the uppermost layer coincides with the ground surface elevation were used with ground surface elevation determining the top of the uppermost layer.

Some additional data, which was correlated by other workers, was made available and incorporated into the regional data set.

The resulting data set was manually investigated to identify errors. This resulted in the removal of two data points where the overall thickness of coal was anomalously high, 419 and 170 feet respectively, and may have been the result of correlations erroneously labeling coal

seems overlying the Wyodak seam as top of the Wyodak seam. The final data set contained 1766 logs which could be divided into four categories: Logs with two coal seams separated by a parting, logs with one coal seam and no parting, logs with a B seam only, and logs with no coal (Figure 2-3). The logs used in the development of the sand lens were a subset of these logs and are not presented on figure 2-3. Table 2-1 presents an analysis of the data sets ultimately used in the development of the geologic model.

GEOMAT (Kern, 1996), a geostatistical computer code written for MATLAB (Mathworks, 1996), was used to universally krig the individual data sets. Covariance functions were modeled for each data set (Figure 2-4) and anisotropy ellipses were determined (Table 2-2). The thickness of the parting was kriged first to determine where it dropped below 20 feet, or did not exist according to the correlation convention. The overall thickness of the coal seam, consisting of both coal and parting thickness data, where appropriate, summed, was then kriged. The top of the A seam off of which the other thickness' are to be hung was then kriged (Figure 2-5). This was followed by the A seam thickness, the B seam thickness', and the parting thickness (Figures 2-6, 2-7, 2-8, 2-9 and 2-10). The thickness' of the A seam, B seam, and parting are only defined where these layers exist. The tops of these layers were determined by arithmetic manipulation of the thickness'. In locations where the kriged parting thickness was less than 20 feet, the parting thickness was set to zero. Table 2-2 presents the results of geostatistical analyses of the data sets as well as inputs into the kriging routine.

For use in the ground water flow model, the bottom and thickness of one monitored sand lens in the Wasatch Formation was modeled using the same methods as outlined above (Figures 2-11 and 2-12).

IV. Discretization

IV.1. Model Domain - Grid

The grid consists of a rectangle with 100 cells on each side with its long axis rotated to N27W. The grid is centered on an 80 by 80 block of fully refined cells. Bordering the refined area is a layer of 10 unrefined grid cells arrived at by sequentially multiplying the refined column width by 1.34 and the row height by 1.4. The model domain is nearly square with sides of 57.4 miles in the northeast-southwest direction and 62.3 miles in the northwest-southeast direction

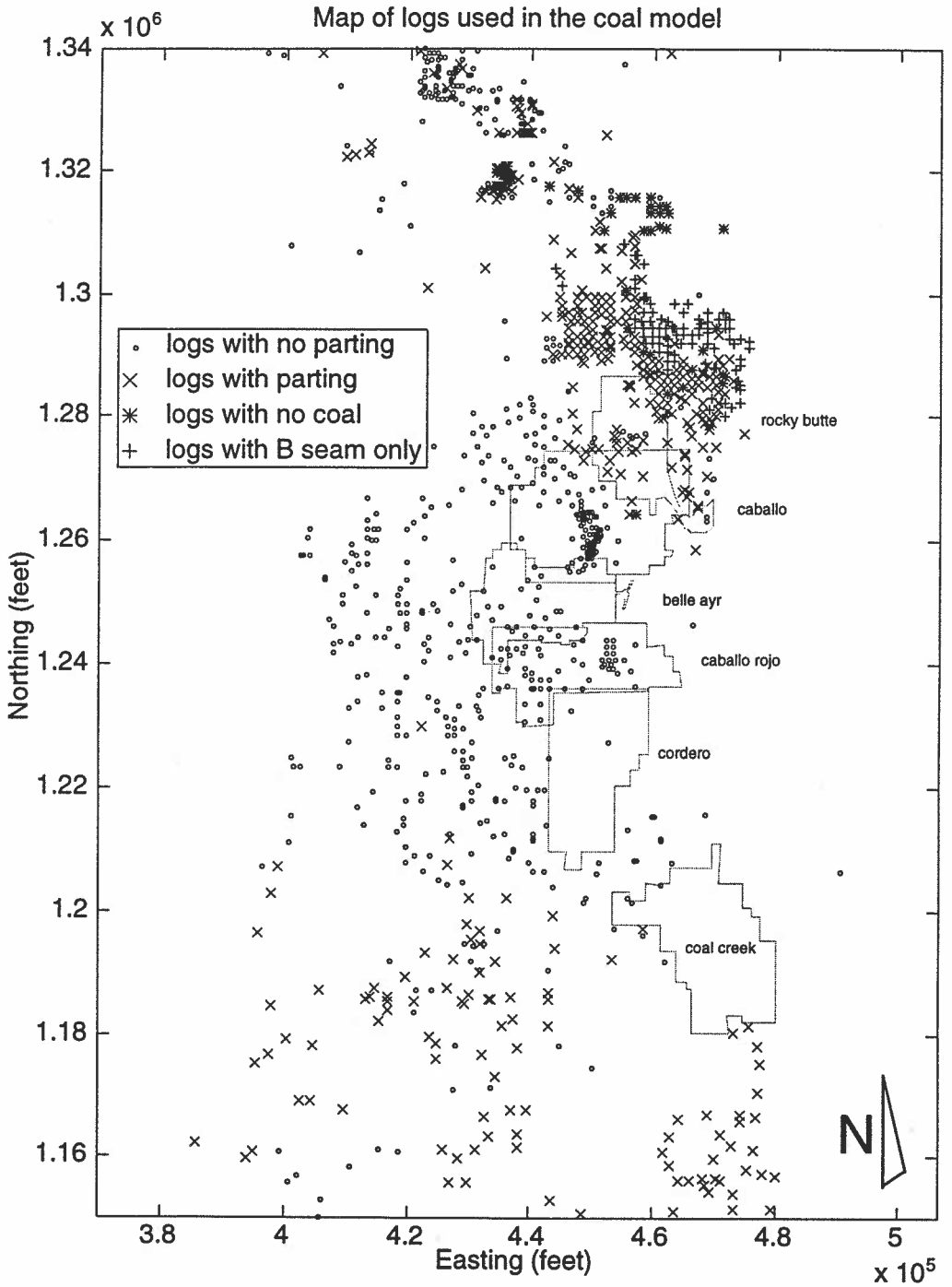

Figure 2-3. Map of the four different species of coal geometry observed in driller's logs within the study area. Mine permit boundarys shown for orientation.

Table 2-1. Descriptive Statistics of Geologic Model Input Files.

Data Set	number of points	range	mean	standard deviation
sand lens bottom	110	4292 / 4650	4494.8	52.8116
sand lens thickness	106 / 822*	2 / 264	66.88	40.8474
Wyodak A seam top	1325	3834 / 4882	4389.3	181.0438
Wyodak A seam thickness	460	0 /170.5	43.07	27.9955
parting thickness	395 / 1766*	1 / 217	56.7	47.3667
Wyodak Bseam thickness	502	0 / 111	29.94	21.3808
overall thickness of coal	1033	0 / 293	92.96	48.7769

* indicates the number of points including points where quantity is not present.
Listed statistics are for points where quantity is present.

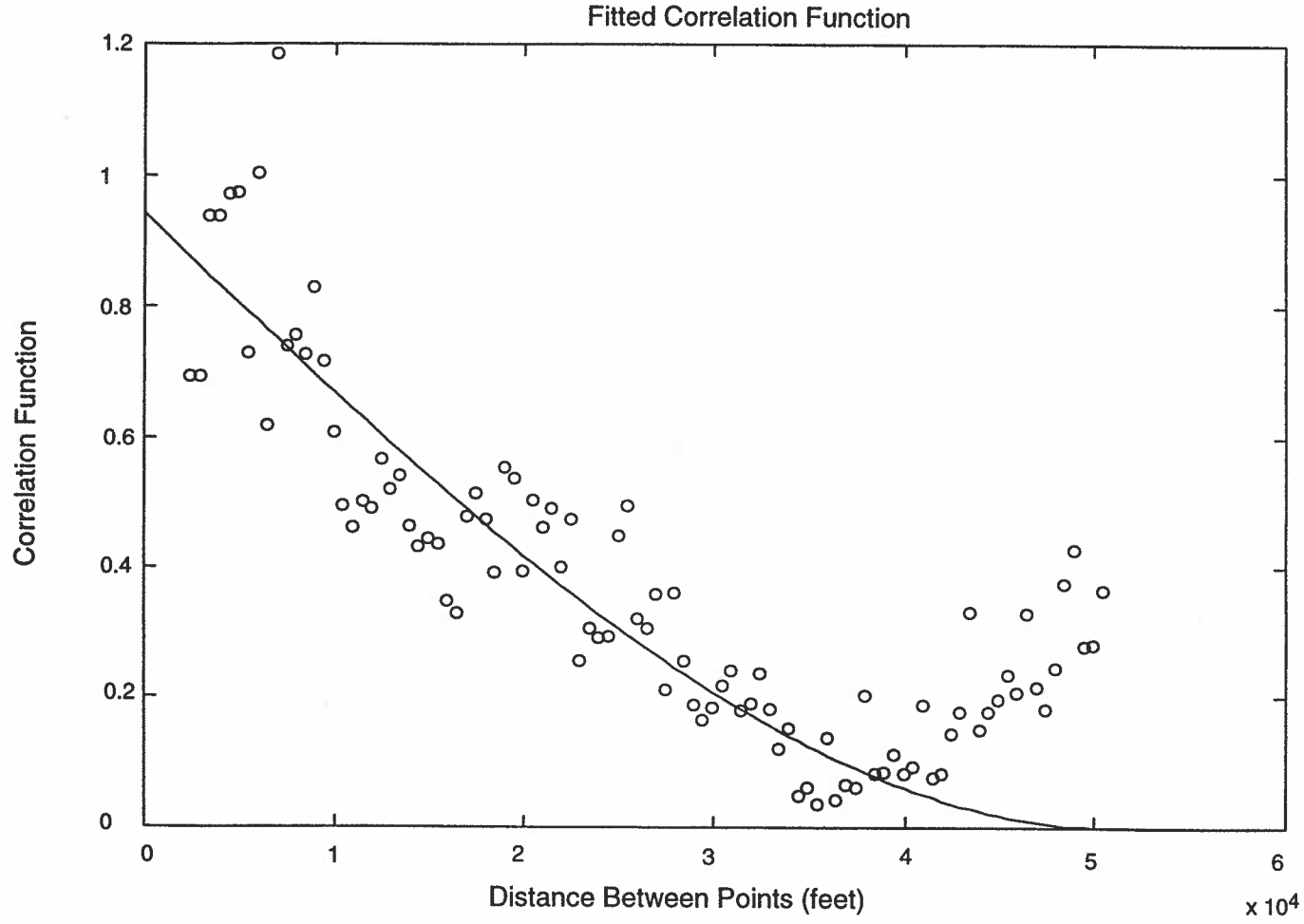

Figure 2-4. Covariance function for the overall thickness of the coal seam, oriented N60W, the direction of the major axis of anisotropy. The estimates were kernal smoothed with an effective band width of 500 feet and a maximum distance of 50000 feet. The major axis was 50773 feet in length in this case.

Table 2-2. Results of Covariance Modeling and Kriging Parameters

			Anisotropy				Trend surface					search radius
			major axis		minor axis							for major axis
Data set	model	nugget	angle (degrees)	length (feet)	angle	length	equation	slope	intercept	R^2	variance	(feet)
overall coal thickness	spherical	0.1949	N60W	50773	N30E	17285	NA	NA	NA	NA	2380.4	60000
sand lens bottom	spherical	0.328	N50E	8152.5	N40W	2682.9	NA	NA	NA	NA	2788.6	80000
sand lens thickness	spherical	0.3774	N30W	13485	N60E	2609.9	NA	NA	NA	NA	716.5	60000
Wyodak A seam top	spherical	0.1632	N20W	90533	N70E	33003	linear in x	9.36E-03	4389.27	0.8861	32781.4	60000
Wyodak A seam thickness	spherical	0.3826	N30W	25387	N60E	10249	NA	NA	NA	NA	783.4	80000
parting thickness	spherical	0.2186	N70W	20001	N20E	7125.3	NA	NA	NA	NA	1059.3	60000
Wyodak Bseam thickness	spherical	0.2948	N70W	15180	N20E	5179.5	NA	NA	NA	NA	457.2	80000
bottom of coal	spherical	0.4235	N45W	56740	N45E	25640	linear in x	9.20E-03	4337.1	0.9506	30881.9	60000

Universal Kriging Parameters

1. Maximum system size = 16
2. grid of 100 x 100 cells
3. State Plane Coordinates of Grid

	min	max
x	3.50E+05	5.00E+05
y	1.15E+06	1.34E+06

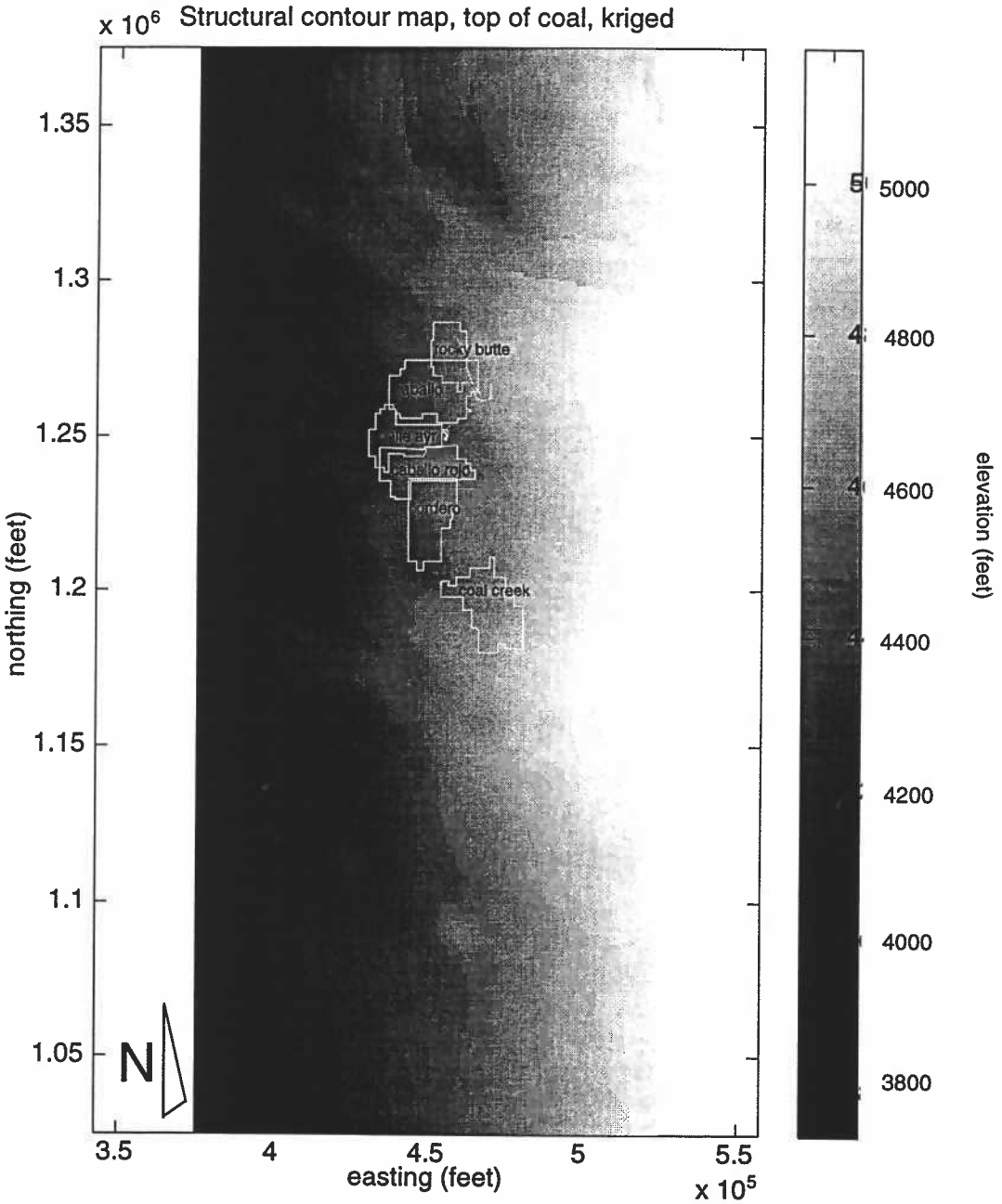

Figure 2-5. Kriged top of coal. Mine permit boundaries shown for orientation.

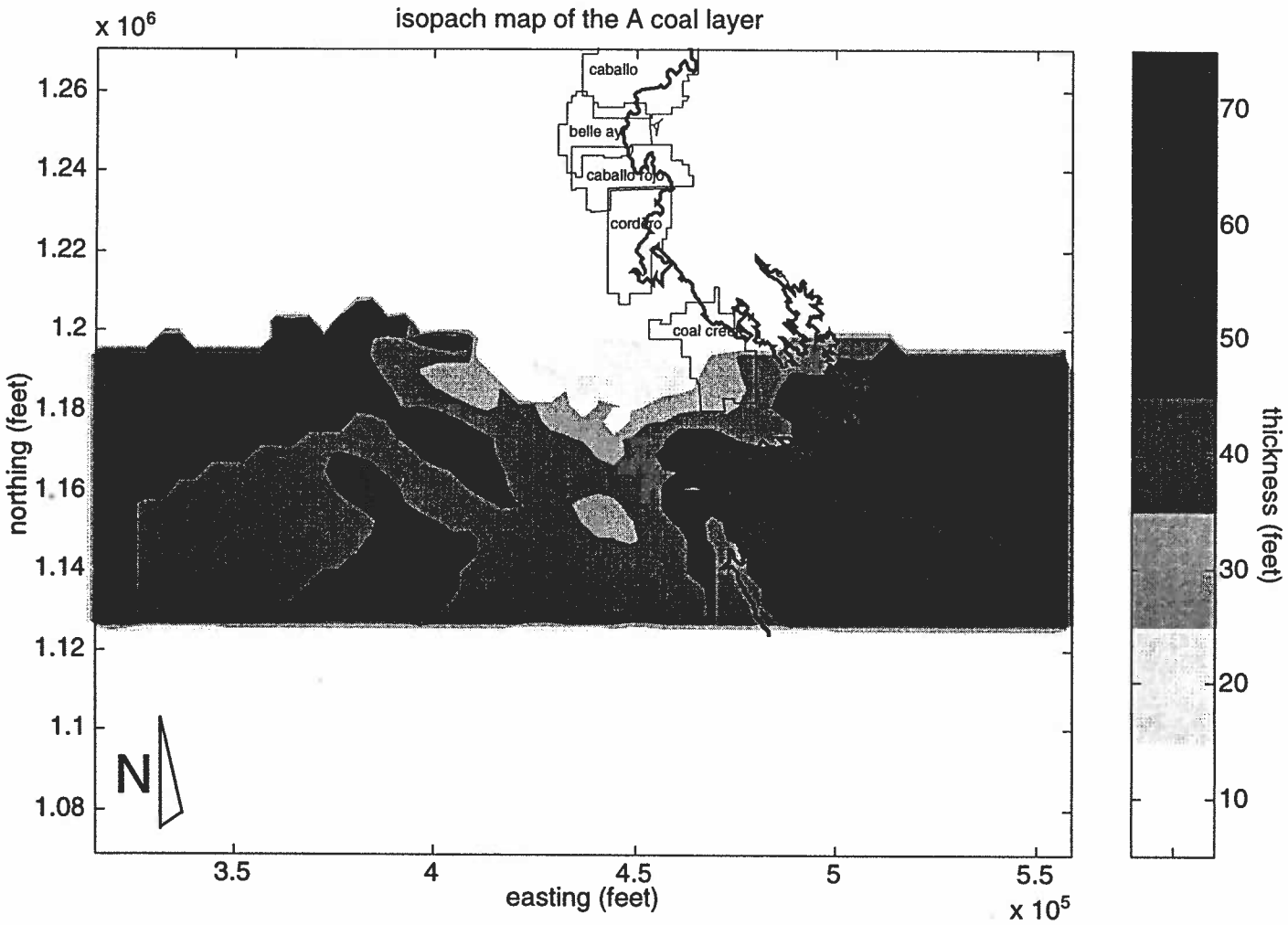

Figure 2-6. Isopach map of the A coal layer. Cropline and mine permits shown for orientation.

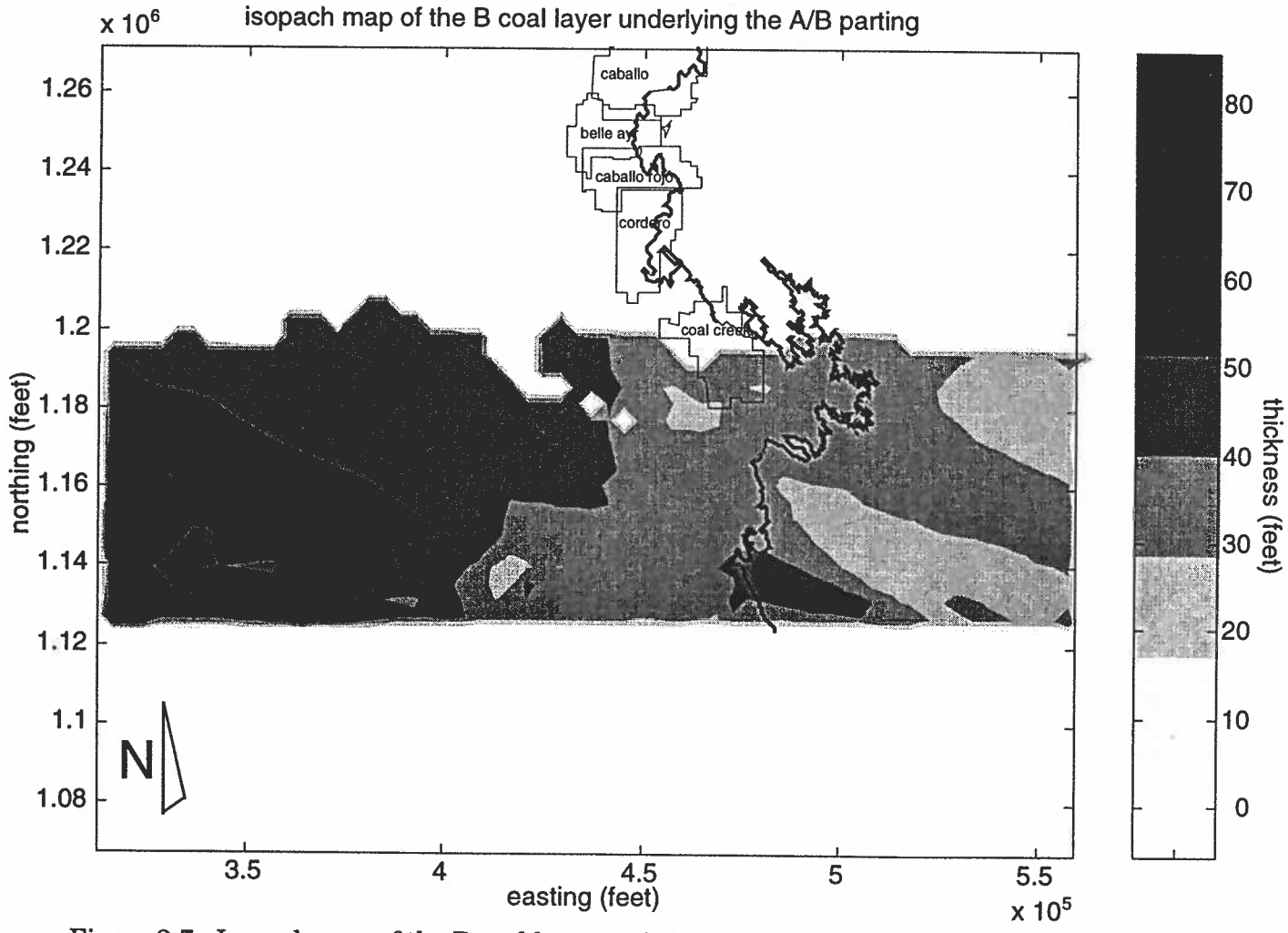

Figure 2-7. Isopach map of the B coal layer underlying the A/B parting. Cropline and mine permits shown for orientation.

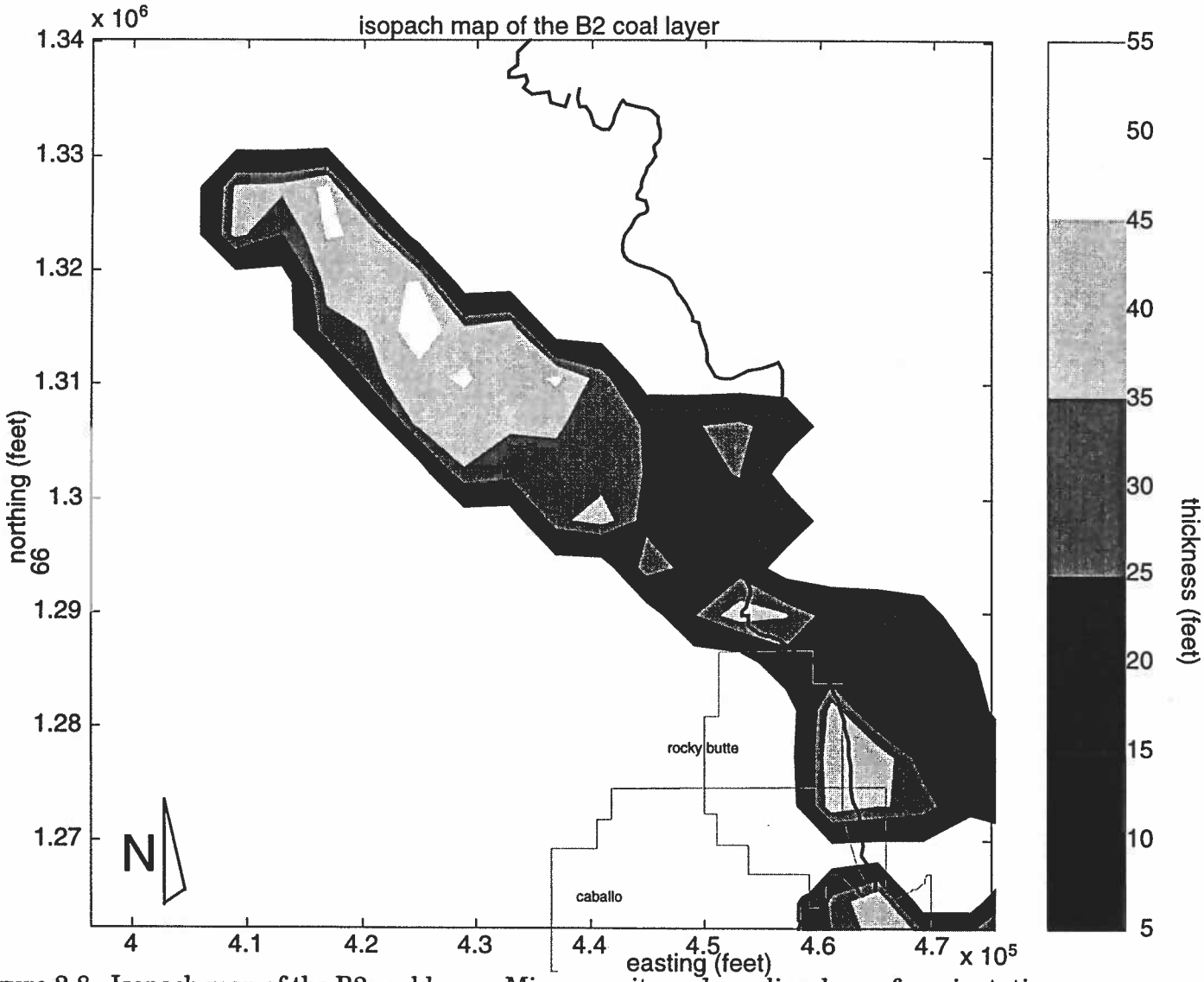

Figure 2-8. Isopach map of the B2 coal layer. Mine permits and croplineshown for orientation.

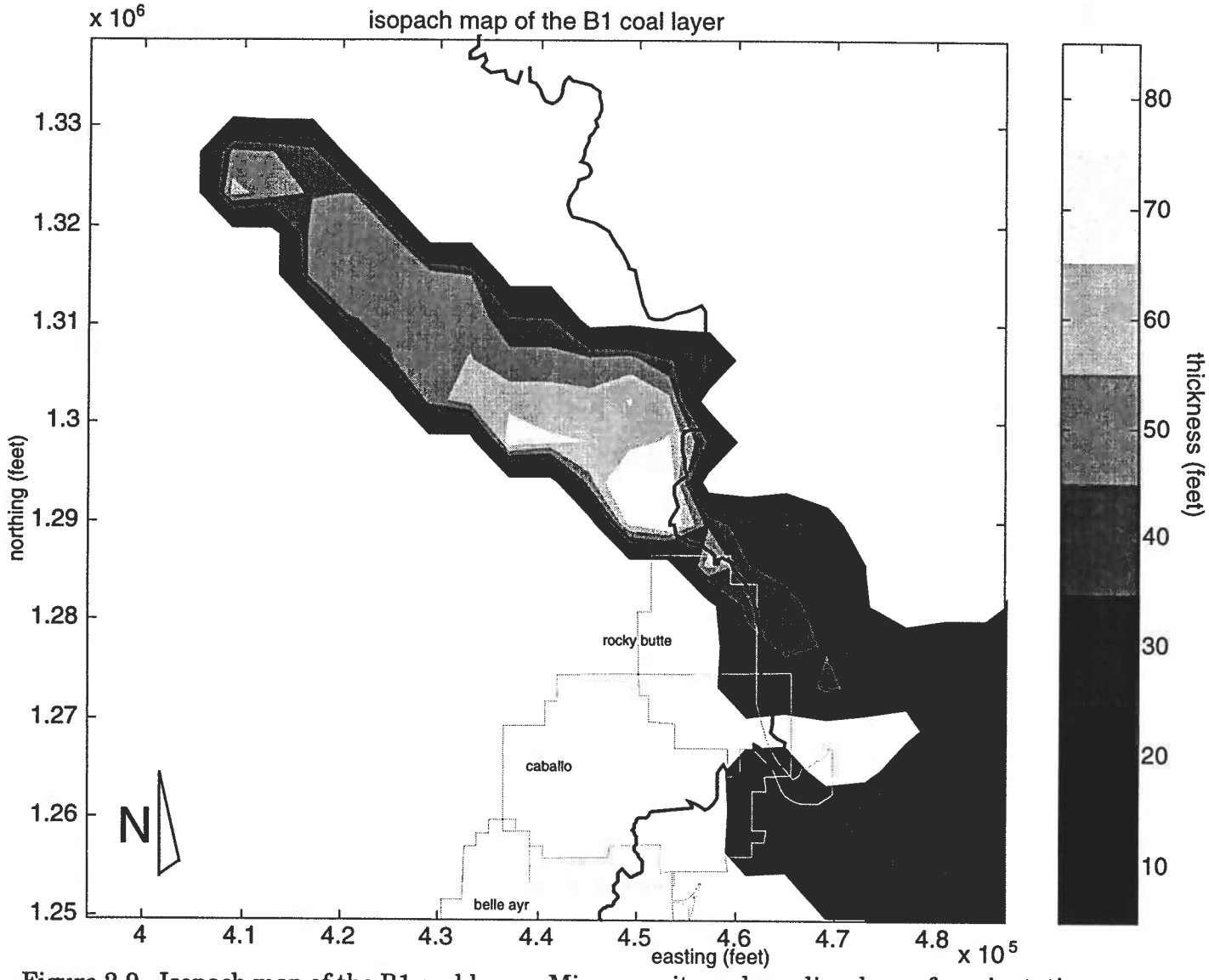

Figure 2-9. Isopach map of the B1 coal layer. Mine permits and croplineshown for orientation.

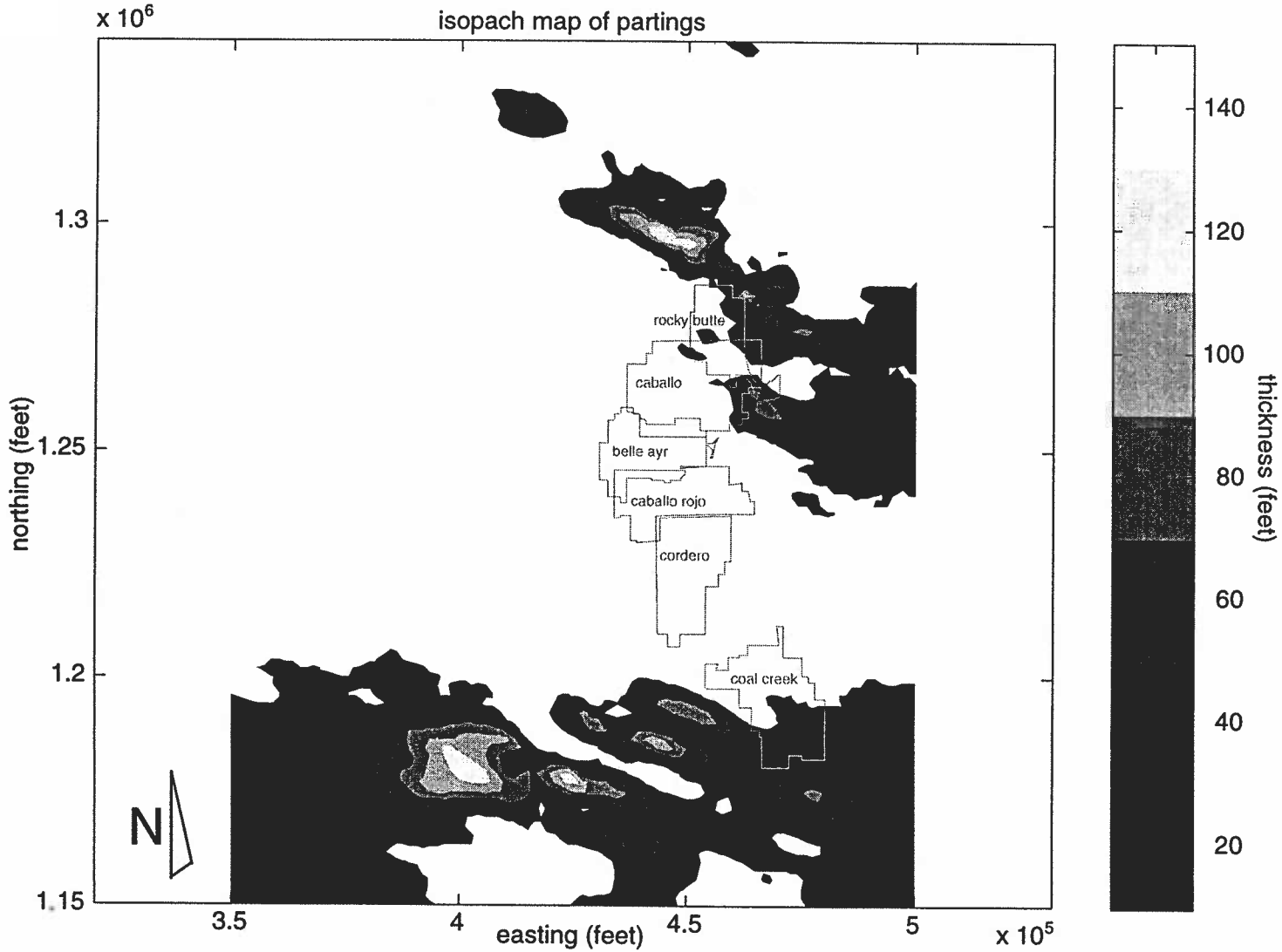

Figure 2-10. Isopach map of the partings in the coal. Mine permits shown for orientation.

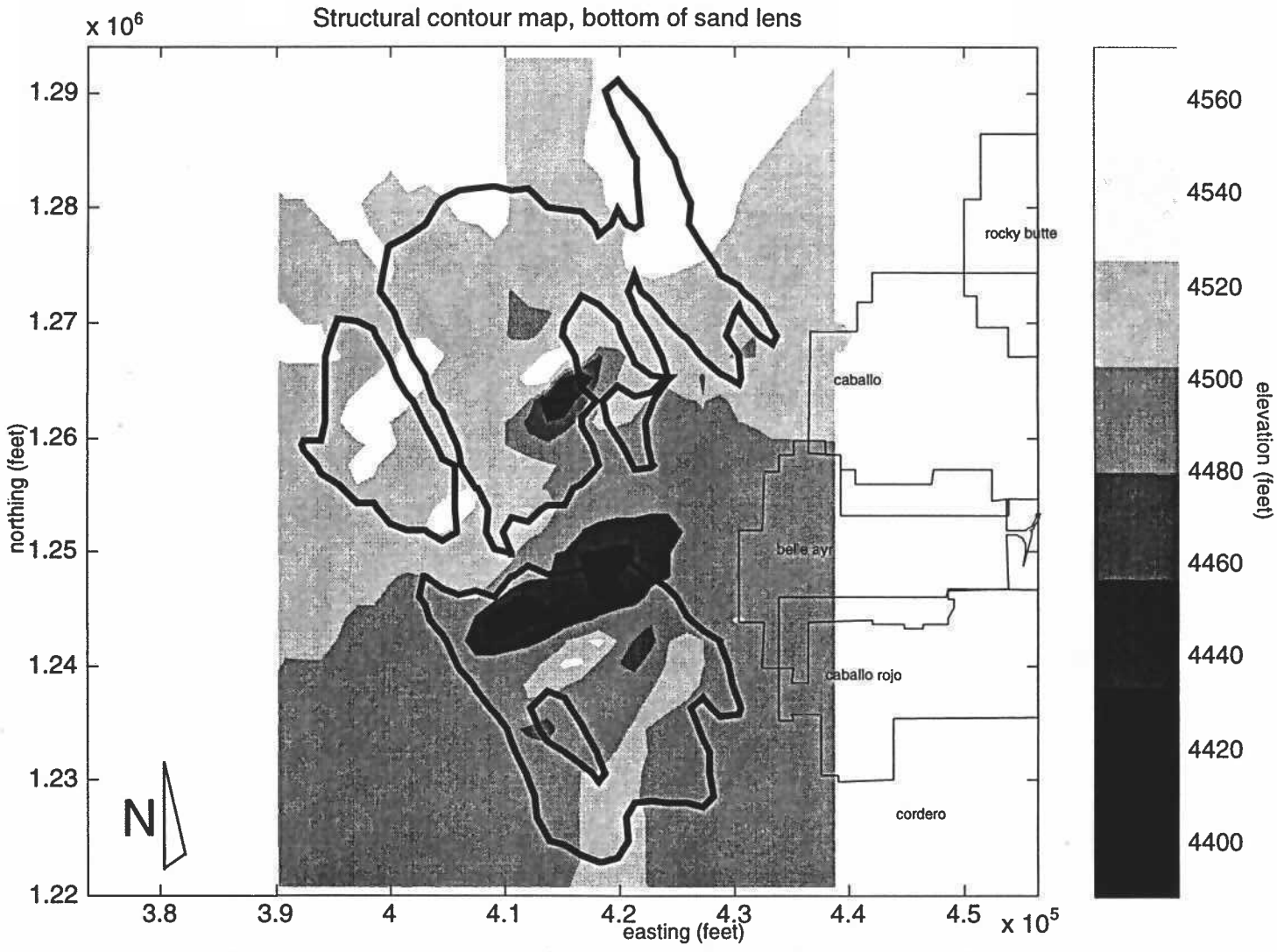

Figure 2-11. Structural contour map, bottom of the Wasatch sand lens. Mine permits shown for orientation. Surface is only defined within 20 foot isopach, shown in black.

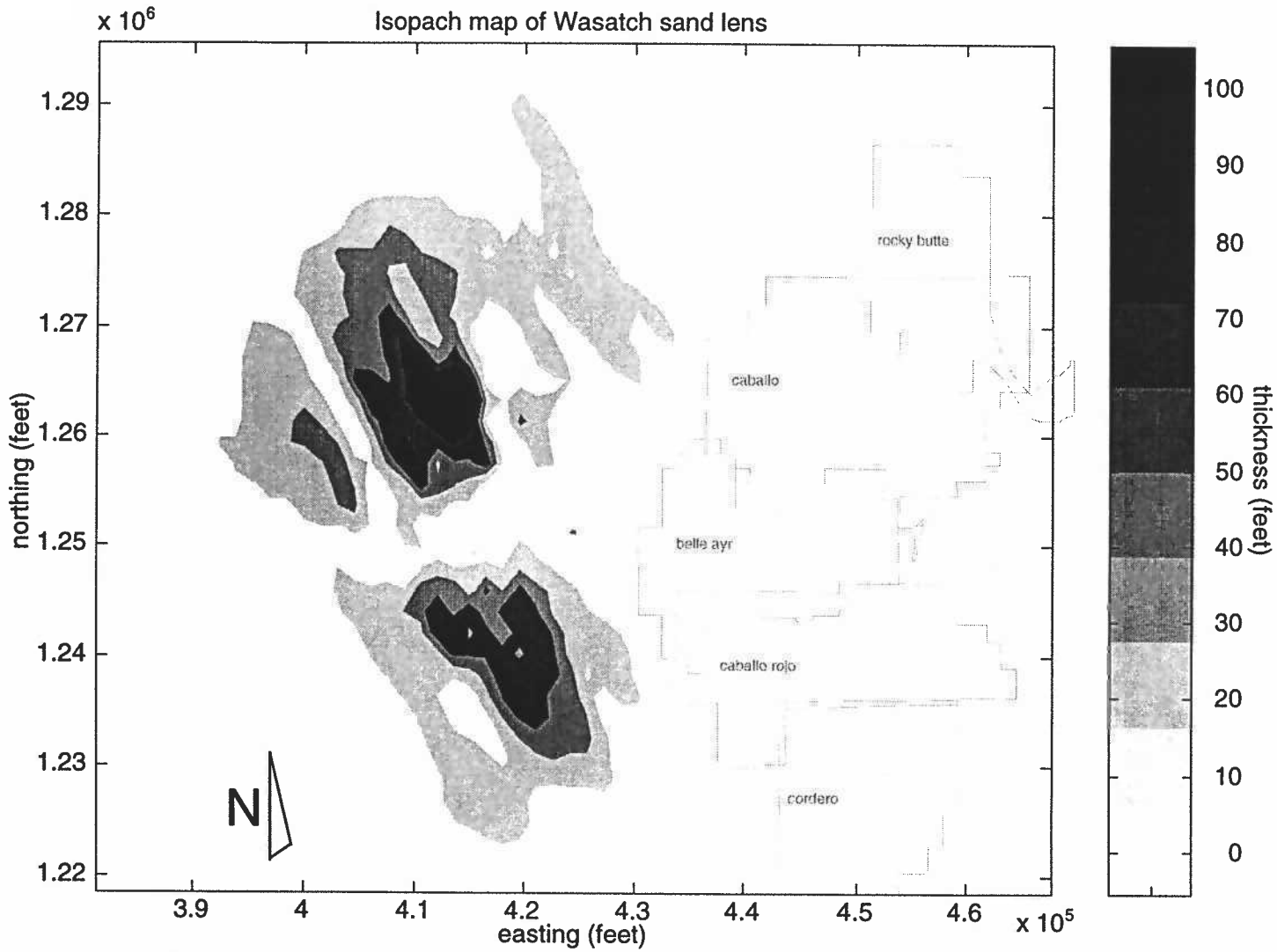

Figure 2-12. Isopach map of the Wasatch sand lens. Mine permits shown for orientation.

(Figure 2-13). The entire model grid covers an area of 3576 square miles. The row spacing varies from 1100 to 31818 feet. The column spacing varies from 1500 to 27998 feet. The most refined grid cells are 1100 feet by 1500 feet and cover an area of 1.65e6 square feet, 37.88 acres. The lest refined grid cells are 31818 by 27998 feet and cover an area of 8.91e8 square feet, 20451 acres, 32 square miles. The refined area of the grid is designed to incorporate all of the stress locations and the extent of the Wasatch Sandstone Lens aquifer. The corners of the grid are, from upper right going clockwise, 528751E 1439641N, 641232E 1130602N, 356481E 1026961N, 244000E 1336000N. The grid covers T45N through T50N and R71E through R77E.

IV.2. Model Layers

The model consists of two explicit layers and one implicit layer as previously described. The thickness' of the layers were linearly interpolated from the stratigraphic model to the nodes of the modflow grid. The top of the coal layer was used as a bench-mark for the construction of the layers of the model. Thickness' were manipulated arithmetically to calculate the tops and bottoms of the model layers.

In order to minimize computer processing time and model setup time, the coal was modeled as one layer. To the south, the parted coal is located in unrefined grid cells, in an area of sparse hydraulic conductivity and starting head data. Lumping the parting and coal together was simply a matter of adjusting the hydraulic conductivity of the parting material. Since the partings consist of shale, sandy and silty shale, carboniferous shale, minor interbedded sandstone and some coal, the increase in hydraulic conductivity was less than one order of magnitude. Presently there is only indirect evidence that this adjustment is indeed incorrect. The lumping of the northern parting and coal together may be more troublesome since the parting is contained partially within fully refined cells. However, in a model of this coarseness such a simplification is necessary, and may not affect the outcome unduly.

In addition, were the coal to be modeled as two coal layers separated by parting material, starting heads would be necessary for each layer. This level of data density is simply unattainable at present.

IV.3. Model Modifications

The dip of the Wyodak coal caused some problems in reference to the discretization of the coal into the model grid. The dip of the three western-most rows had to be decreased in order

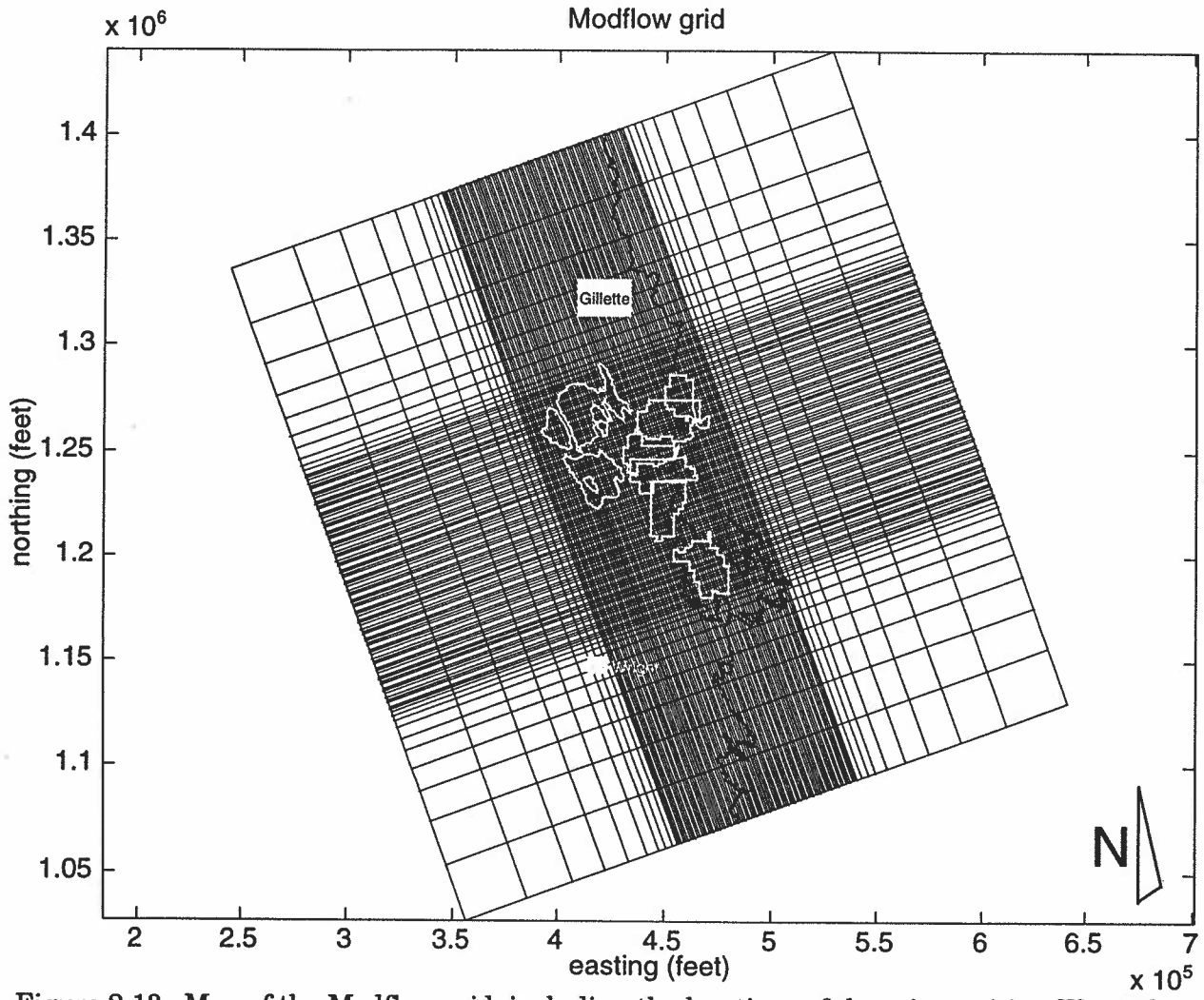

Figure 2-13. Map of the Modflow grid, including the locations of the mines, cities, Wasatch sand lens, and cropline.

to eliminate discontinuities between adjacent cells. Much more of the sand lens layer had to be modified in this fashion. However, the modification of the sand lens layer was confined to unrefined cells and did not affect the sand lens itself. Modification of the coal layer can further be justified by realizing that the axis of the Powder River Basin is in the vicinity of the western edge of the study area. Therefore, the dip of the coal must be reduced and eventually reversed in this area.

V. Setup of specific model inputs

V.1. Top and bottom of coal

The top of the coal was kriged as listed in table 2-2 (Figure 2-14). Since the coal model covered a smaller area than the modflow grid, it was necessary to expand the top of coal surface into a portion of the modflow grid with the trend surface of the top of coal. The same procedure was used to krig the bottom of the coal seam and extend it to fill the study domain(Table 2-2). The thickness of the coal was then calculated arithmetically from the top and bottom surfaces (Figure 2-15).

V.2. Top and bottom of sand lens layer

The bottom of the sand lens layer was kriged (Table 2-2) and retained within a rectangle which encompassed the sand lens 20 foot isopach. The sides of the rectangle were made up of rows 85 and 48 and columns 10 and 51 (Figure 2-16). The mean thickness of the implicit confining layer within this rectangle is 364 feet. Since the top of the coal layer was the bench-mark for all other structural surfaces, the thickness of the confining layer was added to the top of the coal to generate the bottom of the sand lens layer. The thickness of the confining layer was set to the calculated values within the rectangle shown in figure 2-16. The northern boundary of the rectangle was replicated to fill the rest of the columns to the north. The same procedure was applied to the southern boundary. The thickness of the confining layer was set at 500 feet at the western edge of the model grid. A linear interpolation was made between the values in row 85 and row 100; the western edge of the model. The thickness of the confining layer was set to zero along the cropline. Thickness values between row 48 and the crop line were linearly interpolated along columns (Figure 2-17).

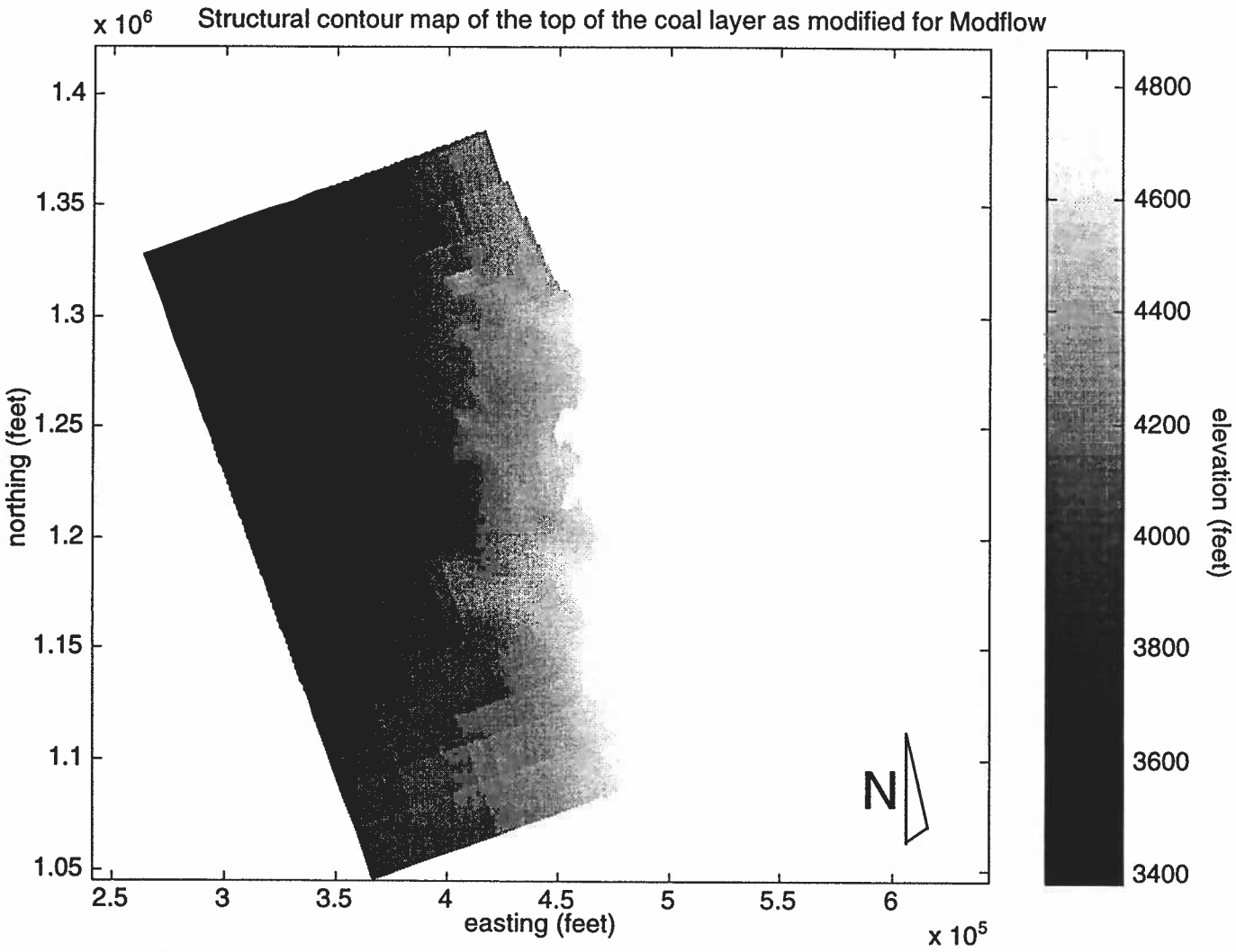

Figure 2-14 . Structural contour map of the top of the coal layer as modified for Modflow.

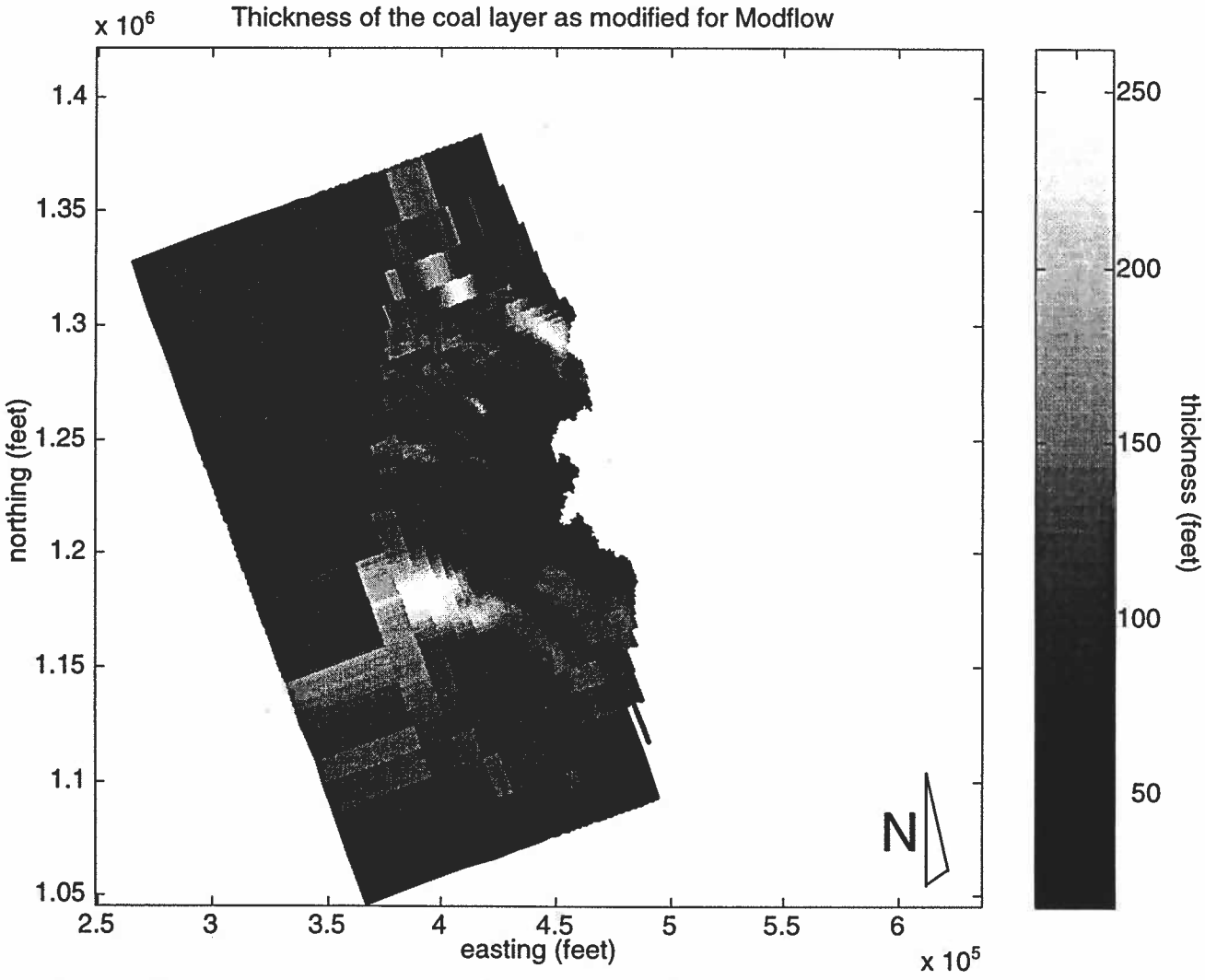

Figure 2-15 . Isopach map of the coal layer as modified for Modflow.

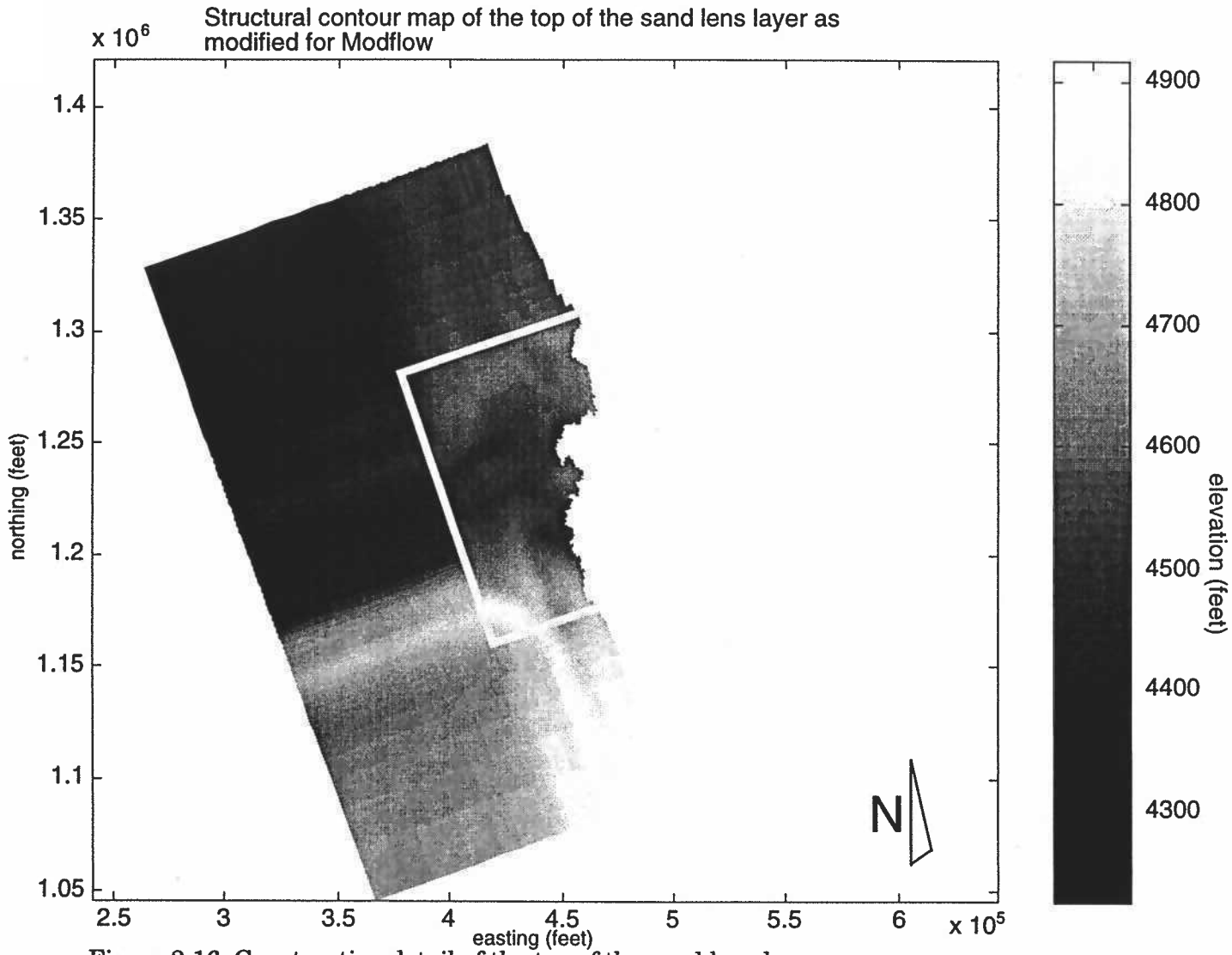

Figure 2-16. Construction detail of the top of the sand lens layer.

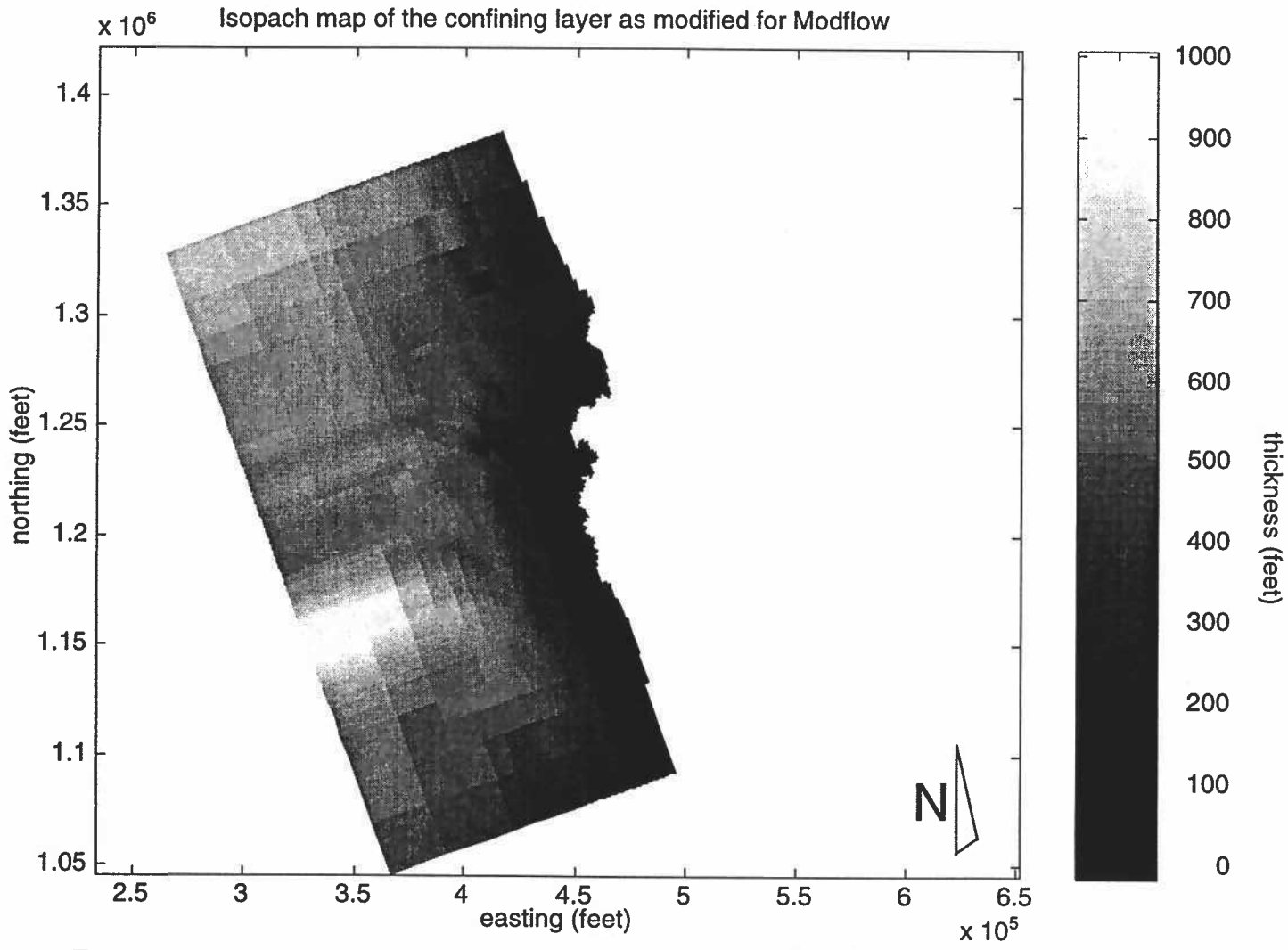

Figure 2-17. Isopach map of the confining layer as modified for Modflow.

The thickness of the sand lens layer was generated in similar fashion (Figure 2-18). The thickness of the entire layer was kriged, but only retained within the 30 foot isopach. The thirty foot isopach was used, in place of the twenty foot isopach, in order to create a thicker layer which would not be as susceptible to discontinuities due to the interaction of dip and discretization. From row 48 through 100, outside of the thirty foot isopach, the thickness of the sand lens layer was set to 30 feet. the thickness of the sand lens layer was set to zero at the crop line. Values between row 48 and the cropline were linearly interpolated.

The bottom of the sand lens layer was then determined by adding the thickness of the confining bed to the top of the coal. The top of the sand lens layer was determined by adding the thickness of the sand lens layer to the calculated bottom of the sand lens layer.

V.3. IBOUND arrays

IBOUND arrays for this model consist of 100 by 100 arrays of positive or negative numbers or zeros which indicate whether the model cells are active, specified head or inactive respectively. Specified head cells maintained the same head value throughout the simulations. An IBOUND array for the coal layer (Figure 2-19) was generated by overlaying the modflow grid onto maps of the cropline and clinker distribution (Hefferin 1997), and qualitatively determining which cells were contained within coal, clinker, or other material east of the cropline. The IBOUND array for the sand lens layer included all of the above in addition to the sand lens itself (Figure 2-20).

V.4. Hydraulic conductivity arrays

The IBOUND arrays were refined beyond what was absolutely necessary in order to be used as tools for the distribution of hydraulic conductivity (K) values in the model. East of the full seam crop line, clinker cells were distinguished from cells of other material, so that their K values could be different. The sand lens itself was distinguished from undifferentiated Wasatch in this fashion. In addition, border cells were distributed around the sand lens and between the crop line and the rest of the model in order to allow the K values to step down more gradually in the interest of numerical stability. The starting K arrays are shown in figures 2-21 and 2-22.

The values used to generate these arrays were calculated as follows. The mean of 46 coal hydraulic conductivity aquifer tests was calculated to be 3.5 feet/day. This value was accepted as the effective K for the coal. Since the anisotropy of the coal is known to be 2:1, the K value was

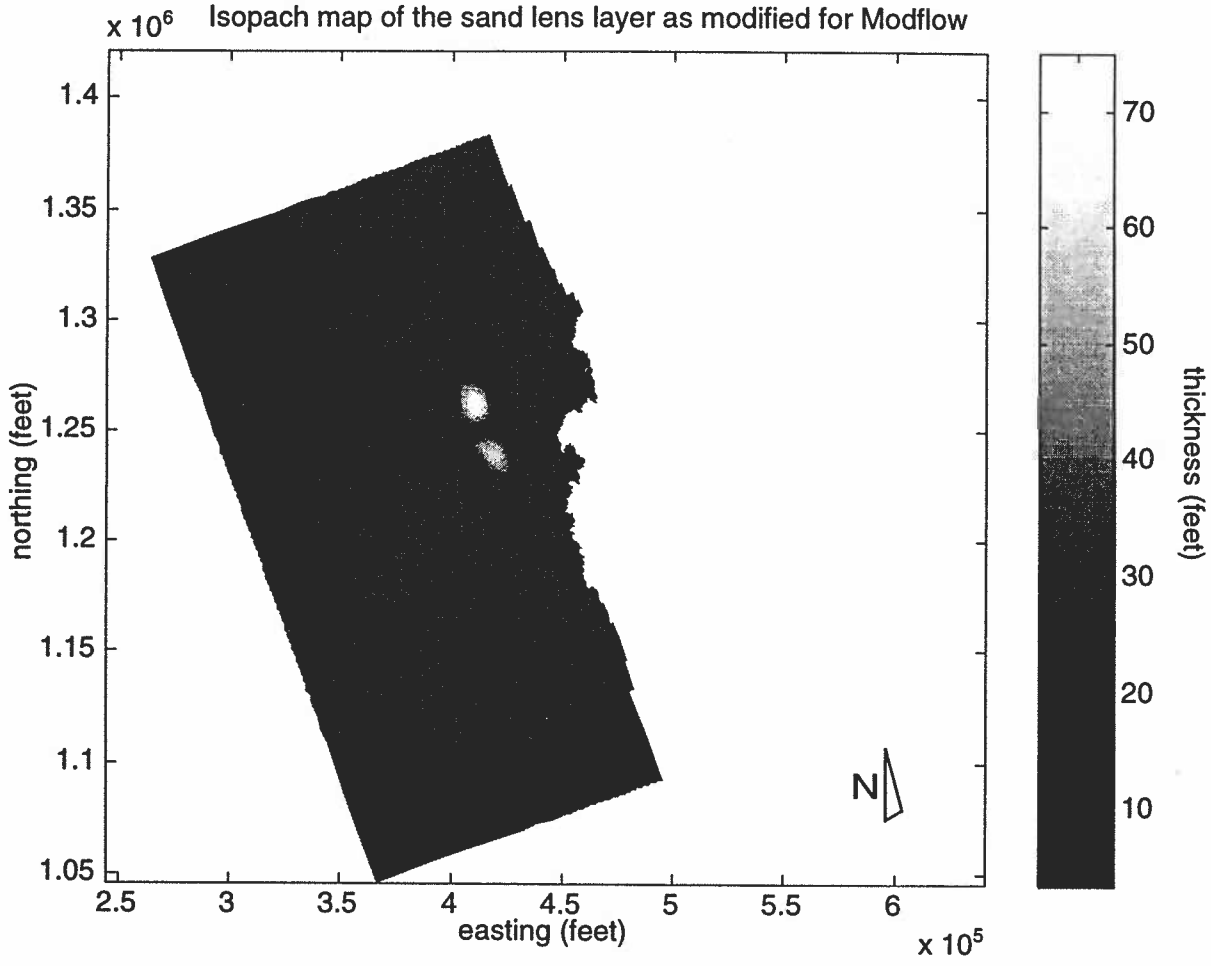

Figure 2-18. Isopach map of the sand lens layer as modified for Modflow.

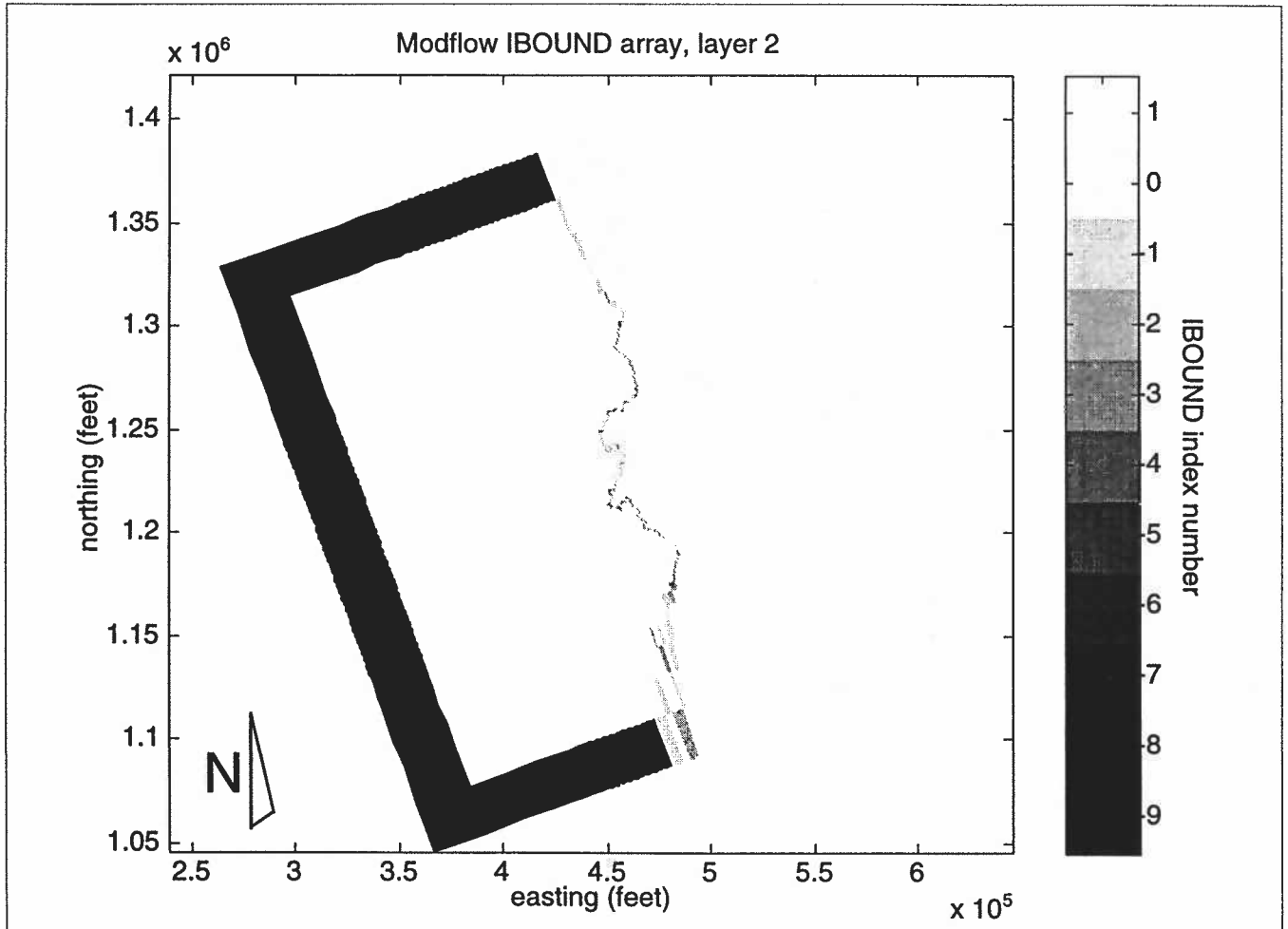

Figure 2-19. Modflow IBOUND array, layer 2. Negative cells are specified head, positive cells are active and zero indicates inactive cells.

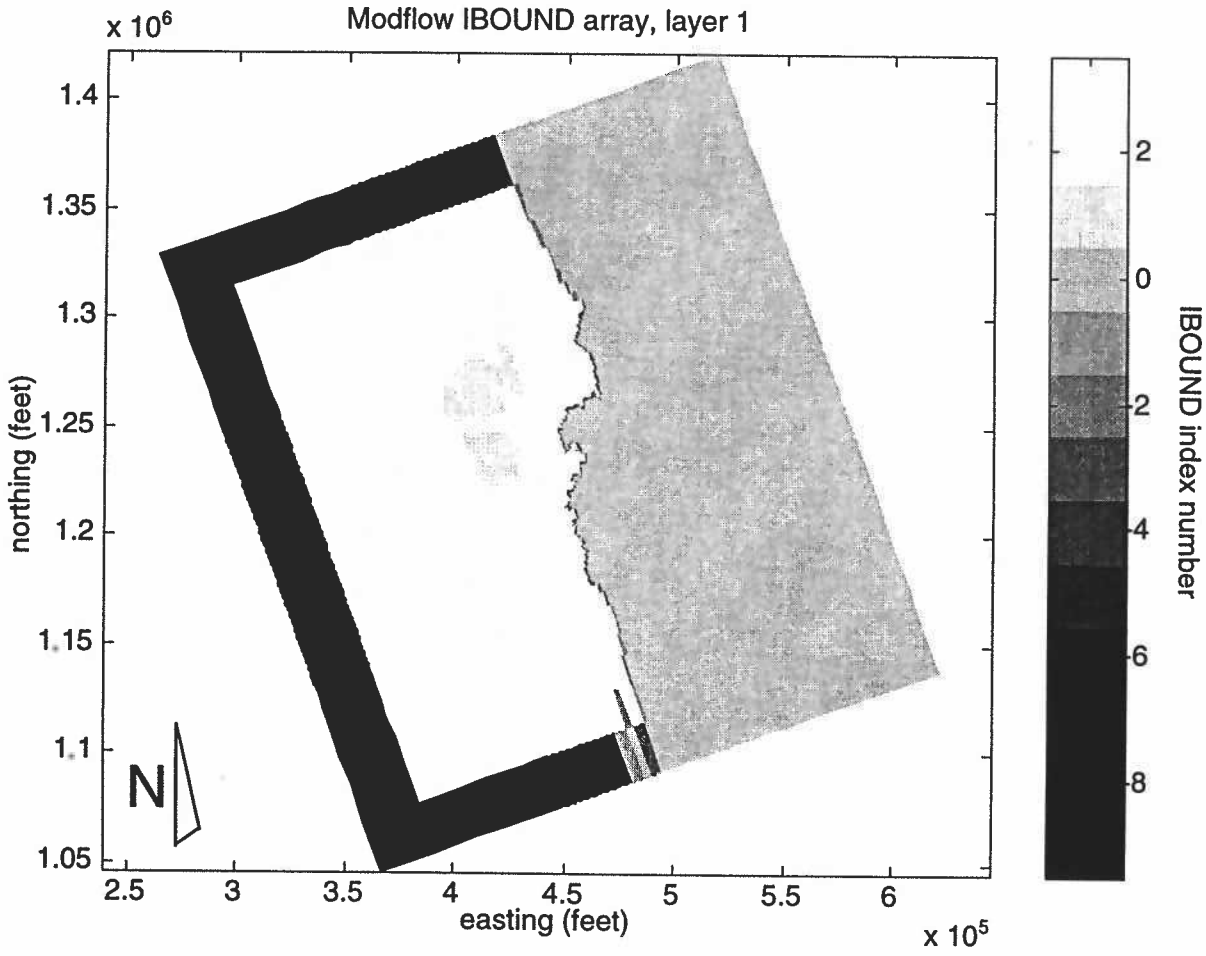

Figure 2-20. Modflow IBOUND array, layer 1. Negative cells are specified head, positive cells are active and zero indicates inactive cells.

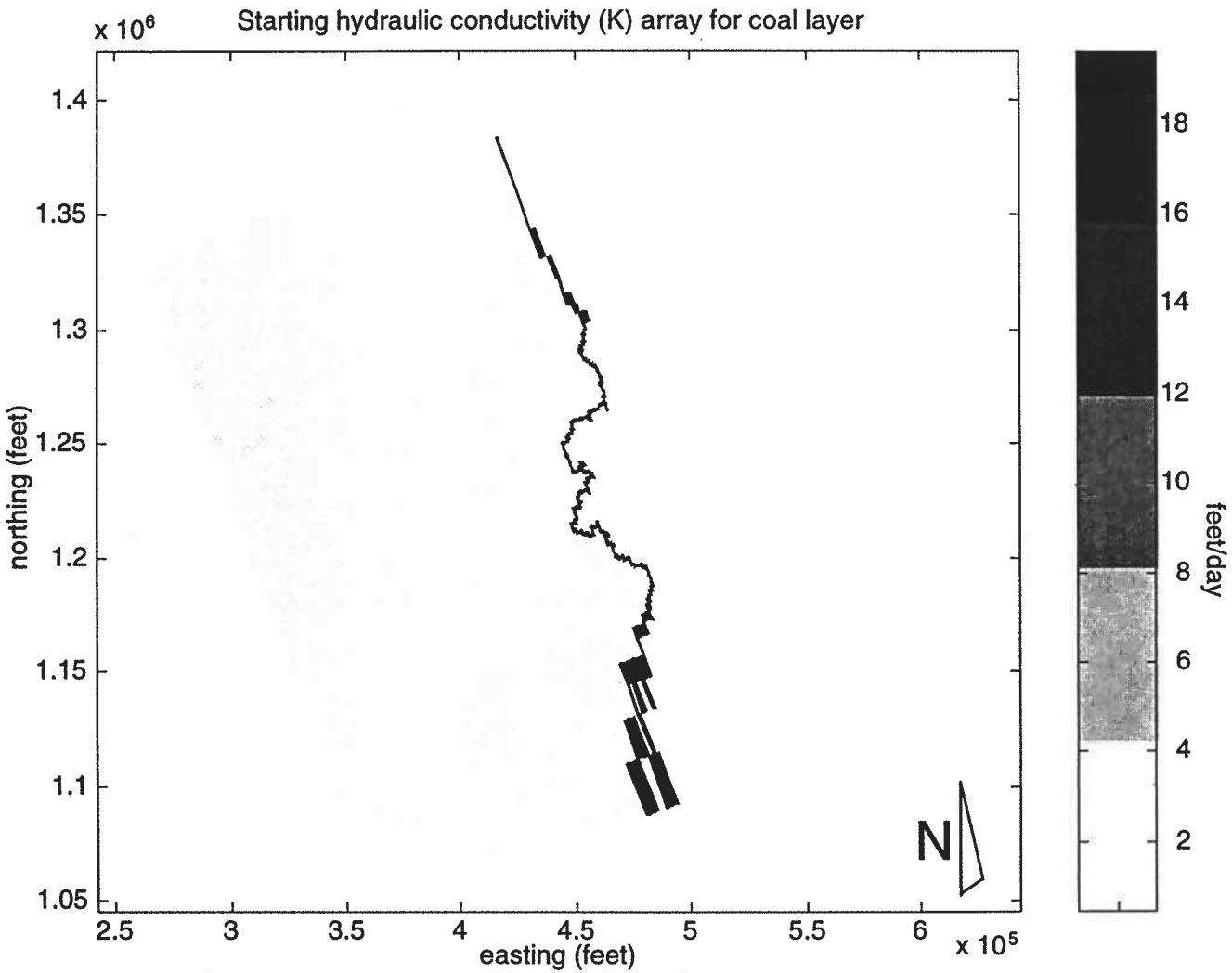

Figure 2-21. Hydraulic conductivity (K) array for coal layer as used in Modflow. Clinker cells, with a K of 12685 feet/day, are not shown on this figure, but can be seen on figure 2-19 represented by -1.

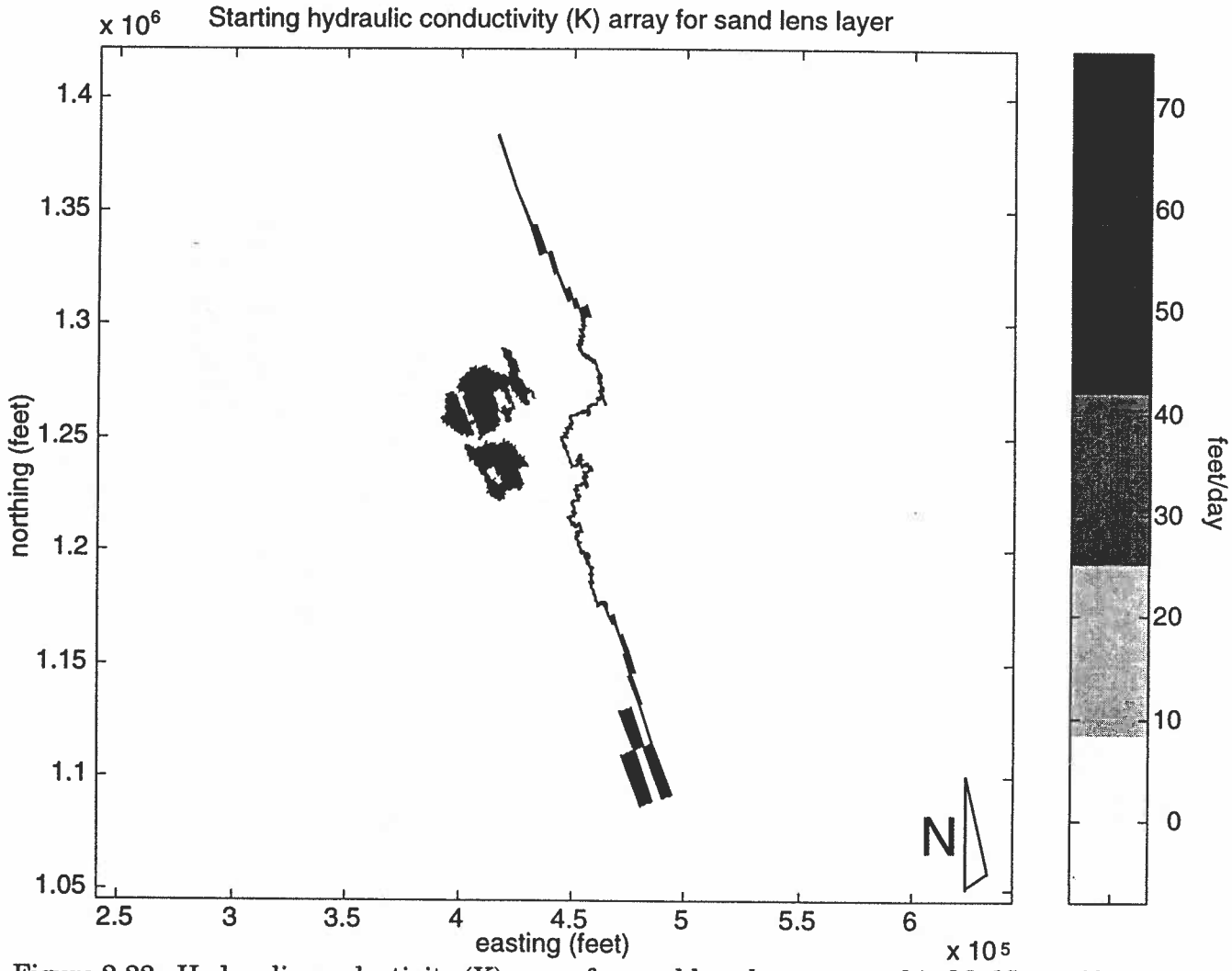

Figure 2-22. Hydraulic conductivity (K) array for sand lens layer as used in Modflow. Clinker cells, with a K of 12685 feet/day, are not shown on this figure, but can be seen on figure 2-20, represented by -1.

resolved into vectors. The resulting K along columns was 2.4 feet/day. The K value for the Wasatch Formation outside of the sand lens was calculated by taking the mean of 46 aquifer tests, resulting in a value of 0.35 feet/day. This value was also used for the confining layer in the calculation of VCONT (section V.5.). The K of the sand lens itself could only be determined qualitatively from lithology information. A value of 50 feet/day, which represents a fine-grained, moderately sorted sand was used. A value of 12685 feet/day, which is the mean of 15 aquifer tests in the clinker, was used as the K value of the clinker.

V.5. VCONT

The VCONT, or vertical hydraulic conductivity divided by thickness, array was generated using the thickness' of the sand lens layer, coal, and confining bed. In addition, vertical hydraulic conductivity was approximated as 0.1 times the horizontal hydraulic conductivity (Anderson 1993). VCONT was calculated by,

$$vcont = \frac{1}{\left(\left(\frac{dzu}{kzu}\right)+\left(\frac{dzl}{kzl}\right)+\left(\frac{dzc}{kzc}\right)\right)}$$ (Mcdonald and Harbaugh, 1988)

where,

dzu=0.5*sand lens layer thickness,
dzl=0.5*coal layer thickness,
dzc=confining layer thickness,
kzu=vertical hydraulic conductivity of the sand lens layer,
kzl=vertical hydraulic conductivity of the coal layer,
kzc=vertical hydraulic conductivity of the confining bed.

V.6. Coal starting head

The starting head in the coal layer was spline contoured through 80 data points using Earth Vision (Dynamic Graphics Inc., 1995). An effort was made to deterministically manipulate the splined coal head surface in the area of the cropline to conform with the conceptual head gradient model. The three other boundaries were modeled as specified head, with head values taken directly from the splined head surface.

V.7. Sand lens layer starting head

The starting heads for the sand lens layer began as a splined surface through 80 data points. Where the bottom of the sand lens layer was above this kriged surface the head was set to saturate the layer. Where the sand lens layer would have started out dry; where the top of the kriged head surface was below the bottom of the sand lens layer, the head was set to the top of the sand lens layer. In essence, much of the sand lens layer was constructed in the pursuit of numerical stability. This is justified given that where the sand lens itself is mapped, all data were honored, and since our interests lie only within the sand lens itself for this layer.

V.8. Recharge

According to Marston (1990), the Powder River Basin receives 0.0029 feet of precipitation per day. It is assumed that 0.02% of this precipitation infiltrates into the groundwater system (Peacock, 1997a). This calculates to 6.00E-7 feet/day of vertical recharge, which is applied as a constant over the entire model domain.

V.9. Calibration points

In order to calibrate the early runs of the model, water level data from 55 monitoring wells was used. These wells were coal mine monitoring wells and were used to monitor drawdown over time in the vicinity of the mines. It was determined that these wells had the best observations of the premining potentiometric surface available. In addition, the two BLM monitoring wells were included to calibrate to the sand lens aquifer.