Chapter 5. Investigation of heterogeneity in the coal.

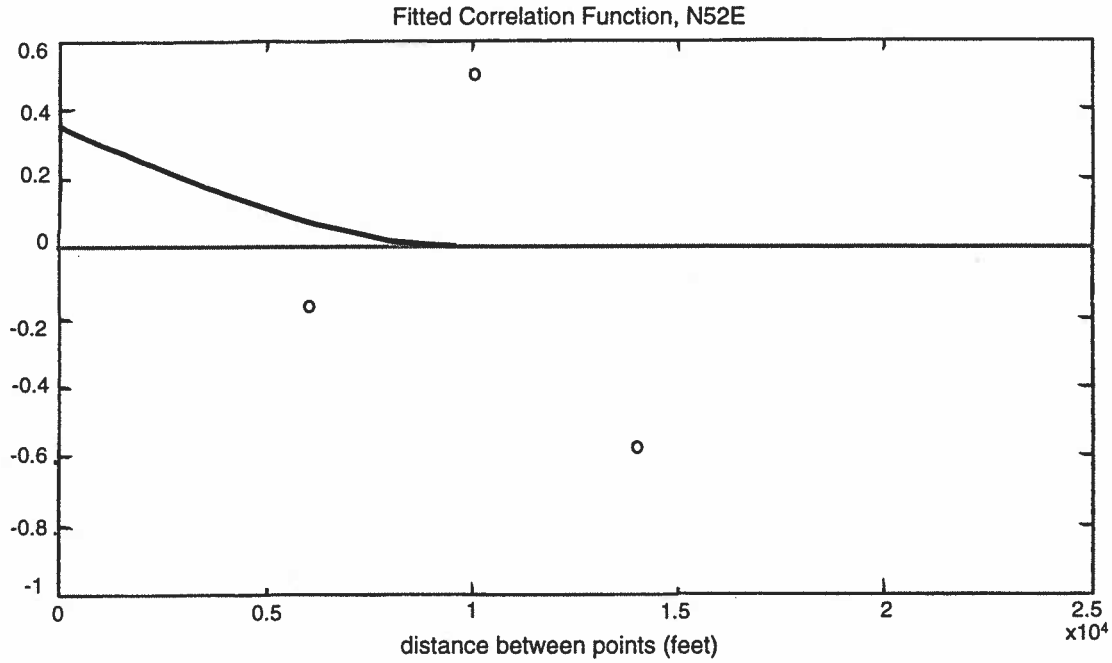
I. Introduction

Throughout the investigations to this point, a coal layer with homogeneous hydraulic conductivity (K) has been used. However, the pump-test data indicate that the coal is heterogeneous. In addition, the poor fit of the models from chapters 3 and 4 indicate that the use of homogeneous coal results in inadequate calibration. The amount of K data which has been collected is limiting, but it can be shown that the introduction of heterogeneity into the coal will improve the calibration of the model. First to be demonstrated is that the introduction of heterogeneity in the coal improves calibration and second is that manipulation of the heterogeneity further improves calibration.

II. Method

Log transformed hydraulic conductivity, estimated from 38 aquifer tests, was used to investigate the directional range of correlation for hydraulic conductivity in the coal aquifer. Figure 5-1 shows the directional correlation functions in the directions N52E and S38E respectively. Although 38 data points is only marginally sufficient to deduce anisotropy, it can be seen that the range of influence is substantially longer in the S38E direction than in the N52E direction. An approximate ratio of anisotropy ranging from 2:1 to 3:1 can be seen, with a dominant wavelength in the northwest-southeast direction of approximately 20000 feet, and 10000 feet in the northeast-southwest direction. When a physical process exhibits nearly periodic behavior in space, the dominant wavelength is approximately 4 times the range of influence in the covariance function (Kern, 1995).

Modflowp was run with a kriged K array (Figure 5-2), which was constructed utilizing all of the available data of adequate quality (Kern, 1997b). Six conditioning points were then chosen from the kriged array, and an heterogeneous K array was conditionally simulated (Borgman, 1994) and run through Modflowp (Figure 5-3). Finally, using the result of the previous run, ten additional conditioning points were chosen by observing where there were large magnitude residuals resulting from calibration (Figure 5-4). A K array was conditionally simulated using these sixteen points and run through Modflowp in an attempt to further improve



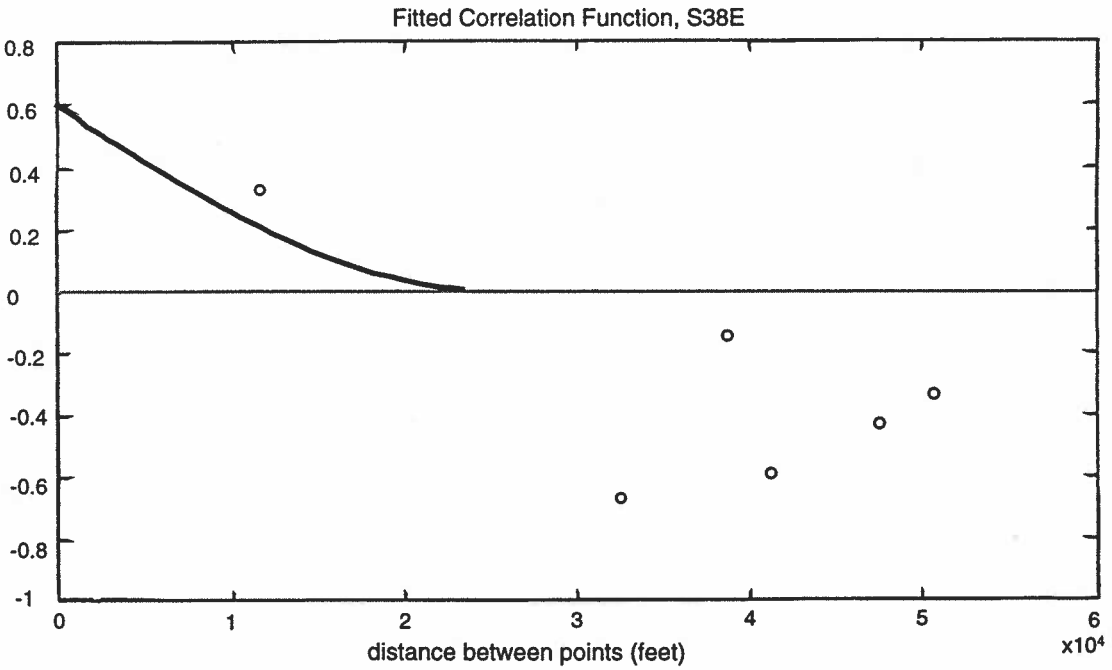


Figure 5-1. Fitted correlation functions for kriging of coal K data.

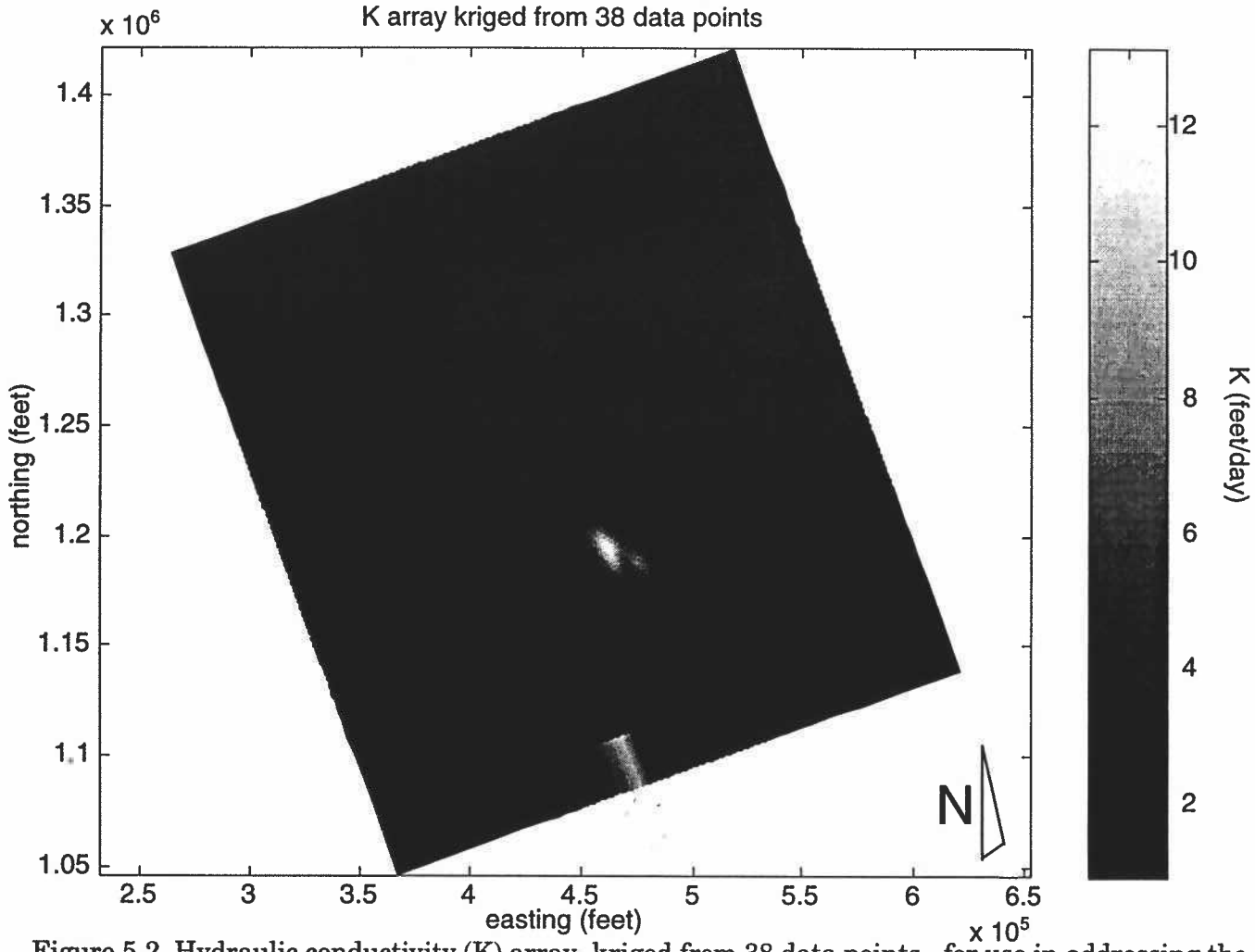


Figure 5-2 Hydraulic conductivity (K) array, kriged from 38 data points, for use in addressing the issue of heterogeneity in the coal.

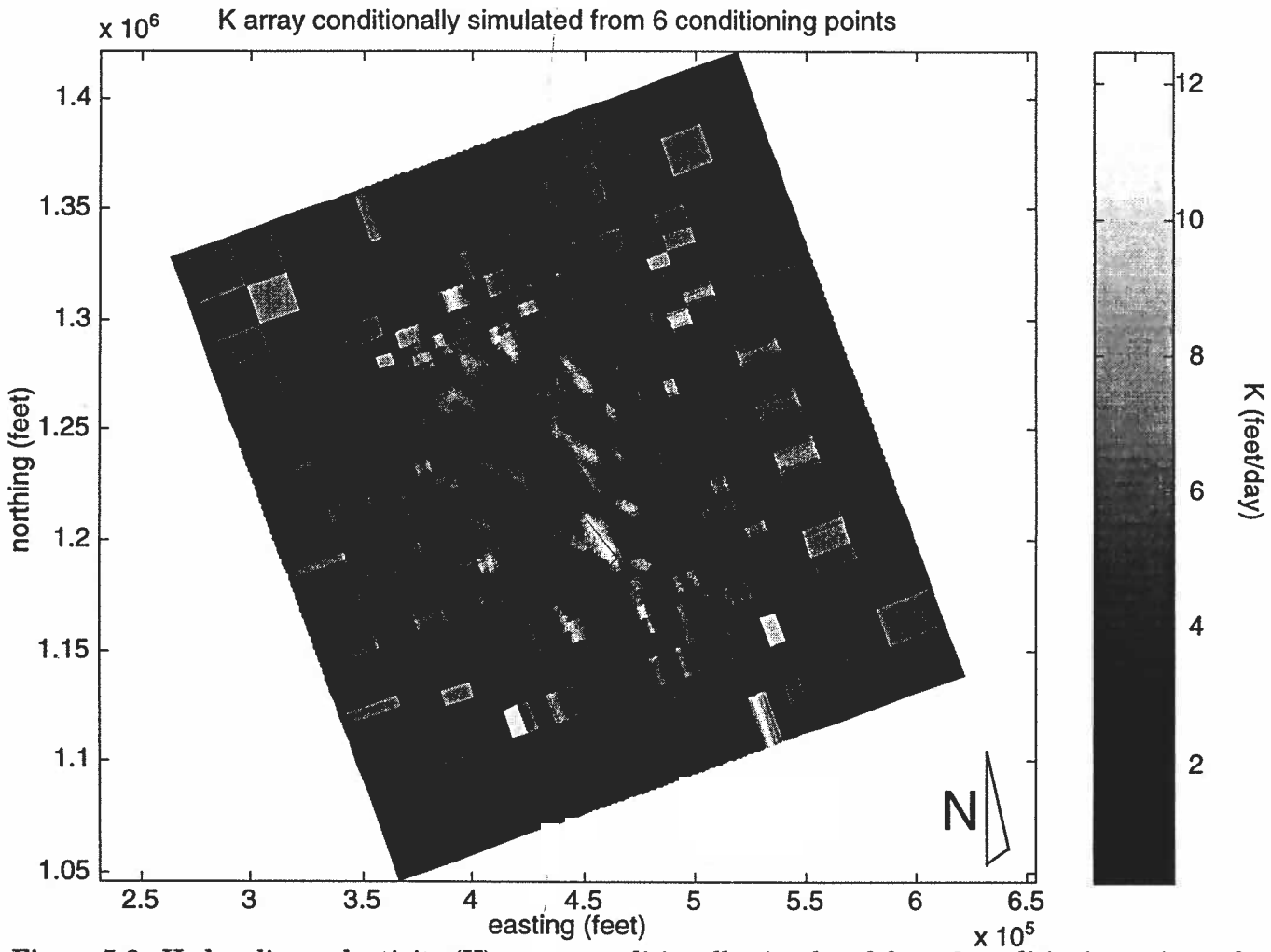


Figure 5-3. Hydraulic conductivity (K) array, conditionally simulated from 6 conditioning points, for use in addressing the issue of heterogeneity in the coal.

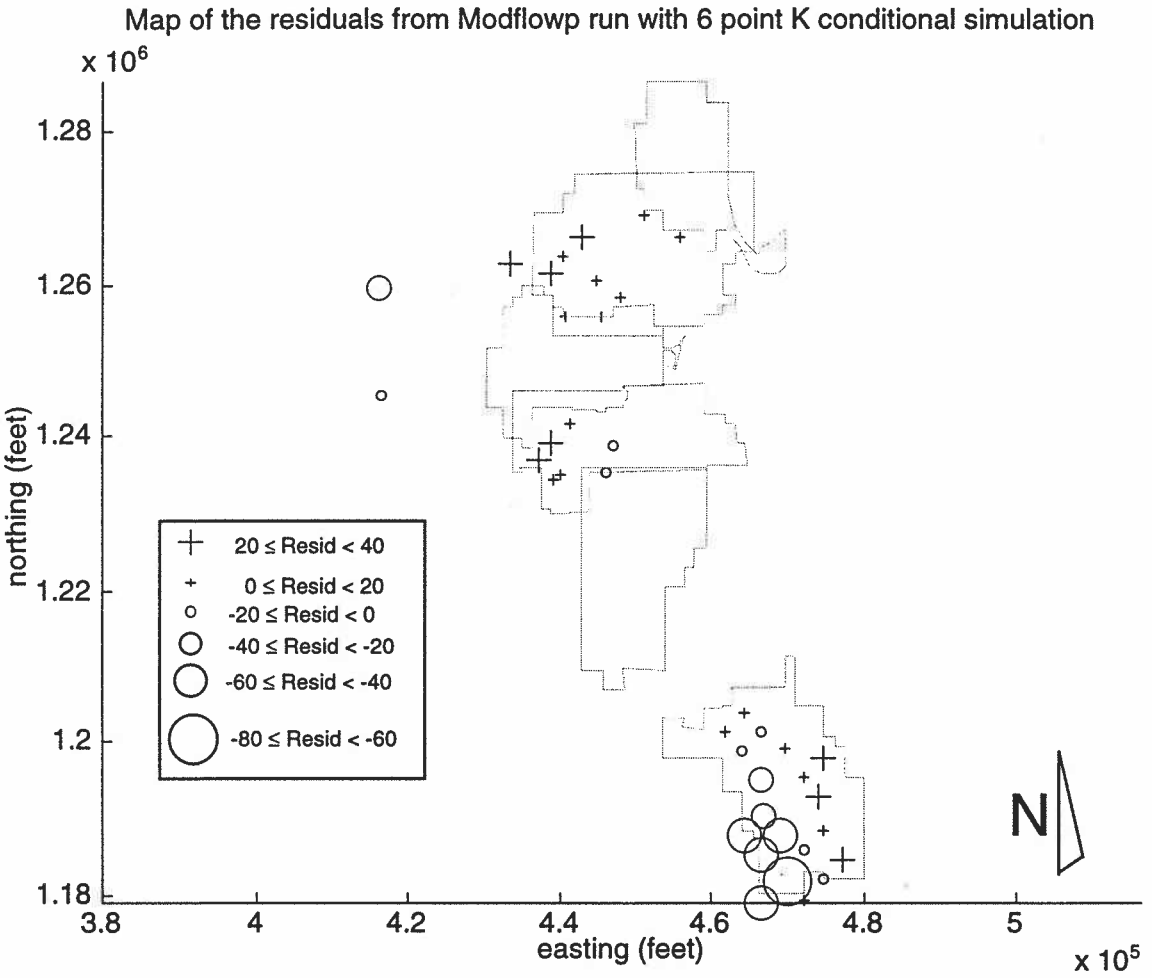


Figure 5-4. Residuals resulting from Modflowp run with coal K array conditionally simulated from 6 conditioning points.

calibration (Figure 5-5). The residuals from this run are shown in figure 5-6. The magnitudes of the conditioning points used in the conditional simulations were somewhat arbitrary. Where a high positive residual was observed, it was replaced with a conditioning point of 10 feet/day, where a low negative residual was observed, it was replaced with a conditioning point of 1 foot/day.

The conditional simulation technique allowed simulation of arrays of heterogeneous hydraulic conductivity with the same mean, variance, statistical distribution and spatial correlation structure as that observed in the aquifer test data. In addition, the simulated conductivity surfaces also interpolated the known aquifer test values.

In these simulations CH was fixed at 4160 feet. Models were run using the best-fit results of chapter 4. A one zone KV equal to 4.5E-6 feet/day was used first, a two zone KV equal to 1E-6 and 5E-6 feet/day was used second, and a three zone KV equal to 5E-6, 5E-6 and 5E-7 feet/day was used third.

In order to draw a more reasonable picture of the system, the calibration wells for this portion of the study were limited to the forty wells found within the fully refined area of the model grid. Seventeen wells were discounted because they were located in unrefined grid cells. As a test of how this would affect the root mean squared (rms) error for subsequent models, the best fit scenario from chapter 4 with three zone KV was run with the forty calibration wells. The root mean squared error for this run improved by 17.67 feet, from 42.13 feet to 24.46 feet.

III. Results

Complete results of these simulations are presented in table 5-1. The results were similar no matter which configuration of the confining layer was used. The kriged K array yielded rms errors of approximately 29 feet. The K array conditionally simulated with six points yielded rms errors of approximately 28 feet. The K array conditionally simulated with 16 points yielded rms errors in the neighborhood of 22 feet. Mean residuals ranged from 7.79 to –2.00 feet. The budget discrepancies ranged from –1.26 to –0.85%. The sand lens residuals were in the vicinity of –35 to –50 feet. The heads calculated with the 16 point conditionally simulated K array for layers 1 and 2 are shown in figures 5-7 and 5-8.

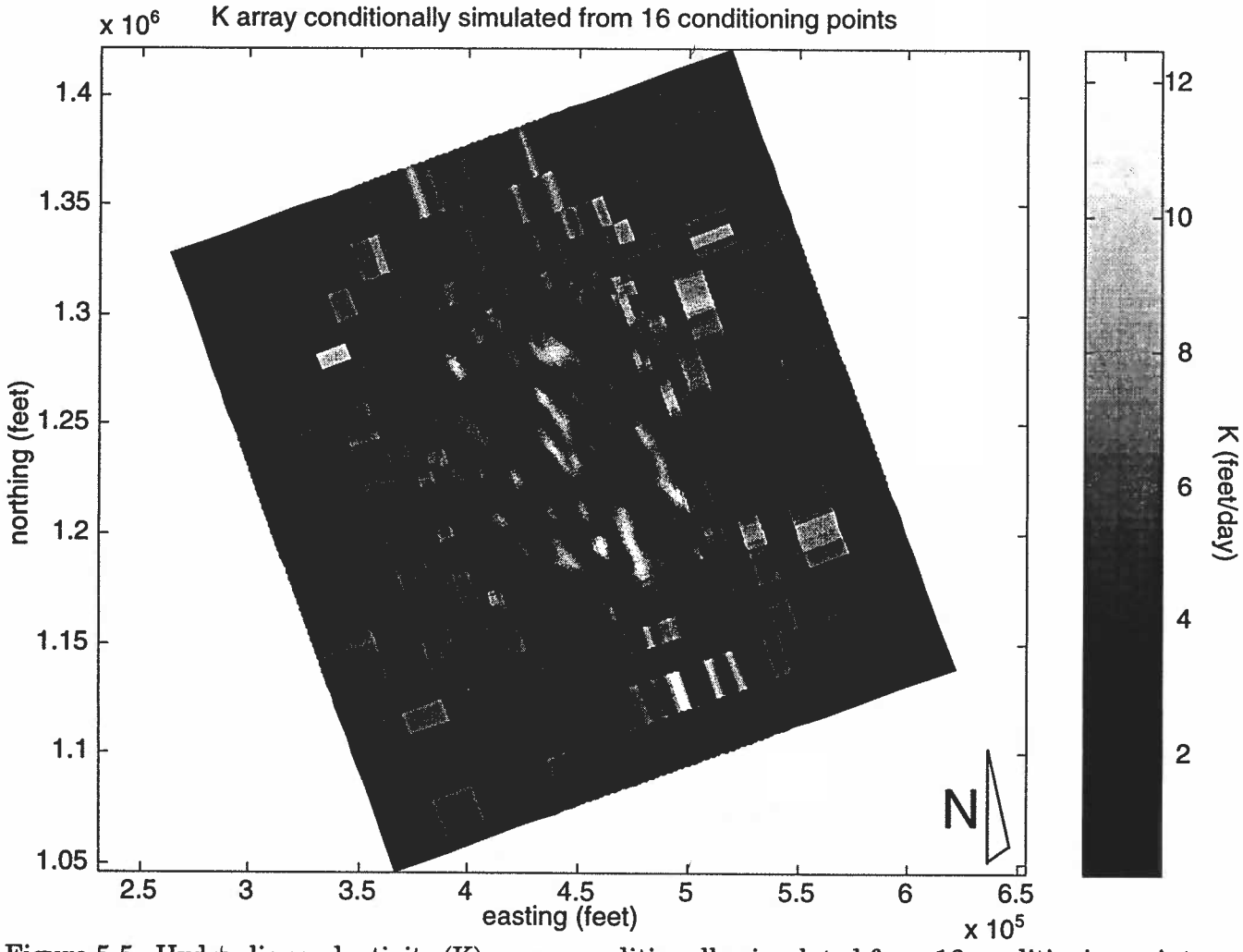


Figure 5-5. Hydraulic conductivity (K) array, conditionally simulated from 16 conditioning points, for use in addressing the issue of heterogeneity in the coal.

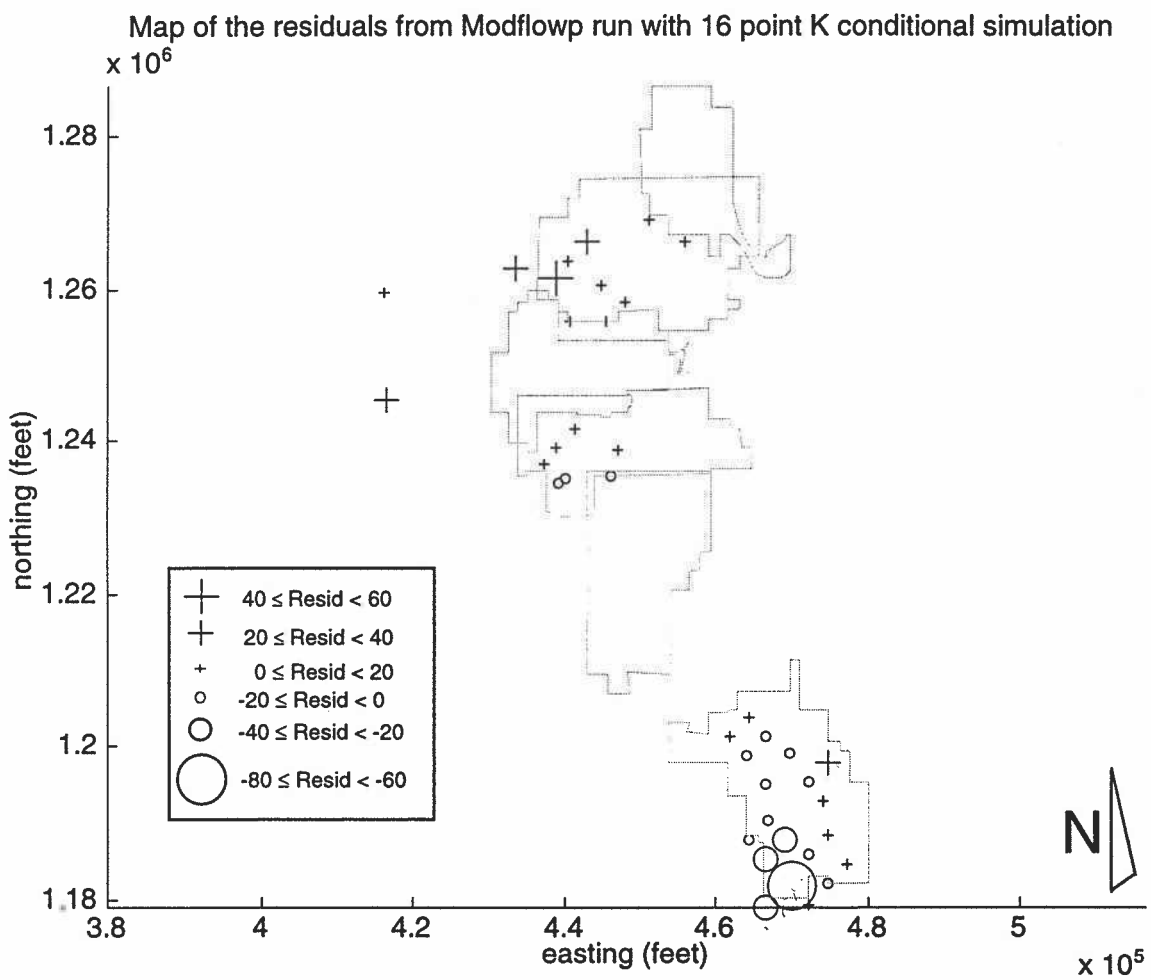


Figure 5-6. Residuals resulting from Modflowp run with coal K array conditionally simulated from 16 conditioning points.

Table 5-1. Results from investigations of heterogeneous coal

CH=4160

simulation no.	coal K array	KV zone 1 (feet/day)	KV zone 2 (feet/day)	KV zone 3 (feet/day)	sum of the squared residuals	mean residual (feet)	budget discrepancy (%)	sand lens resid. #1	sand lens resid. #2	rmse (feet)
1	kriged	4.50E-06	NA	NA	33494	7.79	-0.86	-33.0	-49.1	28.9
2	kriged	1.00E-06	5.00E-06	NA	33658	7.52	-0.88	-34.6	-51.3	29.0
3	kriged	5.00E-06	5.00E-06	5.00E-07	33119	7.61	-0.85	-34.0	-48.2	28.8
4	6pt. cond. sim.	4.50E-06	NA	NA	30598	-1.82	-1.26	-33.9	-50.8	27.7
5	6pt. cond. sim.	1.00E-06	5.00E-06	NA	31100	-2.08	-1.24	-35.3	-52.9	27.9
6	6pt. cond. sim.	5.00E-06	5.00E-06	5.00E-07	30430	-2.00	-1.25	-34.8	-50.0	27.6
7	16pt. cond. sim.	4.50E-06	NA	NA	20014	0.05	-1.04	-34.3	-50.6	22.4
8	16pt. cond. sim.	1.00E-06	5.00E-06	NA	20403	-0.23	-1.04	-35.8	-52.7	22.6
9	16pt. cond. sim.	5.00E-06	5.00E-06	5.00E-07	19798	-0.14	-1.03	-35.2	-49.8	22.2

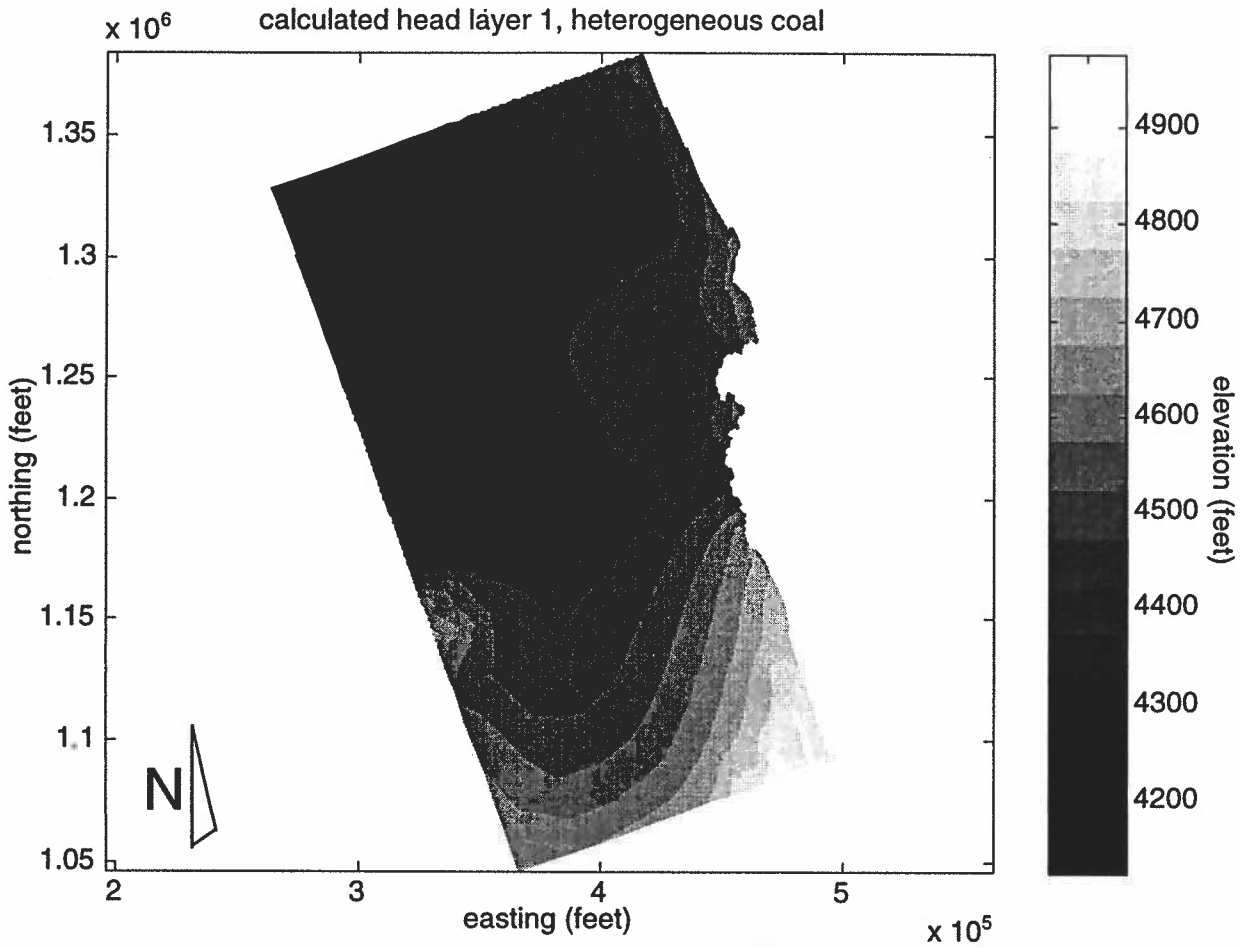


Figure 5-7. Head calculated with heterogeneous coal, layer 1; heterogeneous coal, heterogeneous transition zone, non-clinker cropline cells inactive, KV = 4.5E-06 feet/day. Coal K array conditionally simulated with 16 conditioning points.

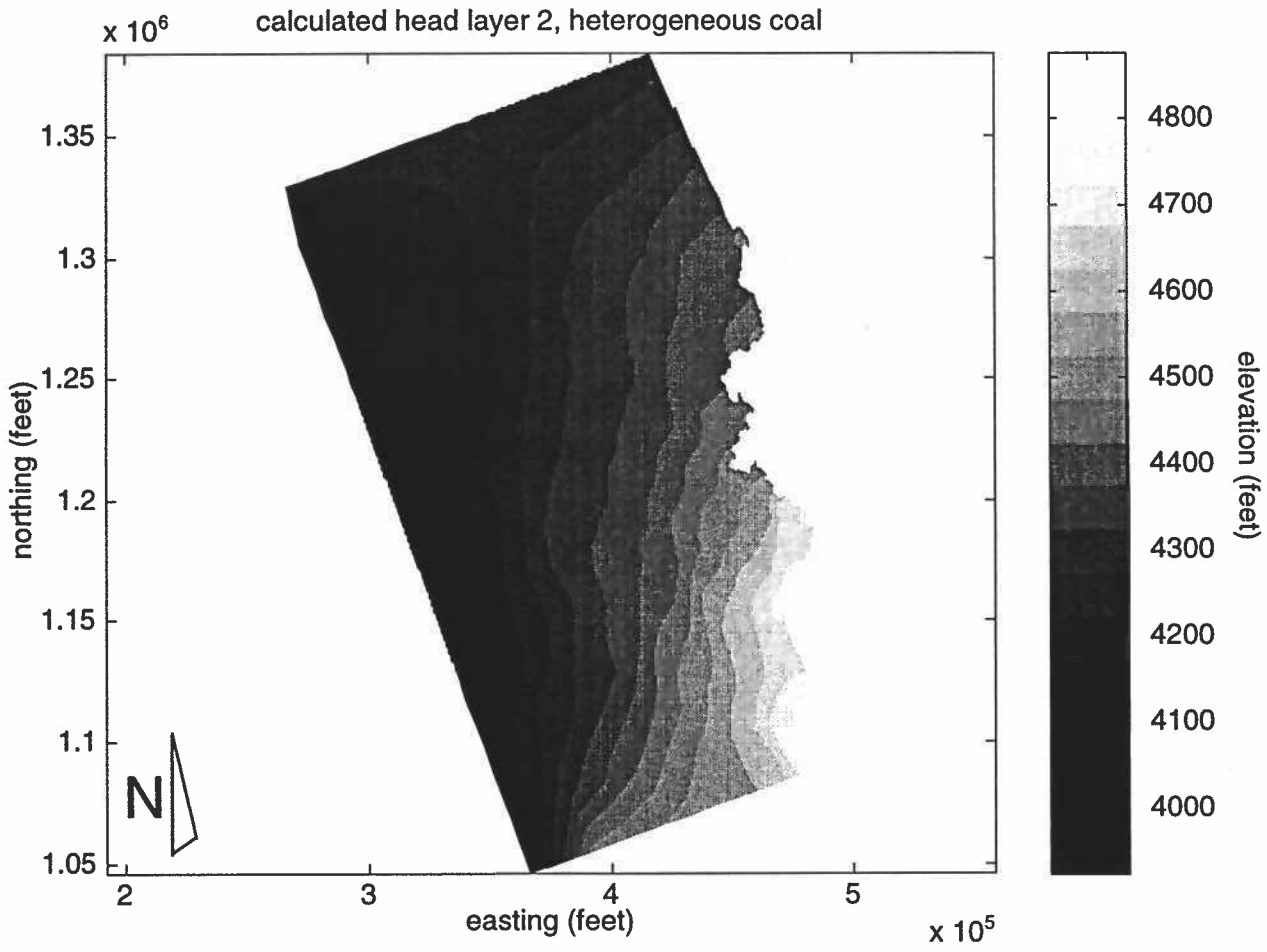


Figure 5-8. Head in layer 2 calculated with heterogeneous coal; heterogeneous coal, heterogeneous transition zone, non-clinker cropline cells inactive, KV = 4.5E-06 feet/day. Coal K array conditionally simulated with 16 conditioning points.

IV. Conclusions

It is fair to say that a heterogeneous coal layer improves calibration. The method used to show this was somewhat arbitrary, being based loosely on a kriged K array. The conditioning points were located at points where high magnitude residuals were found. The magnitude of the conditioning points was also arbitrary. It is intuitive that a coal heterogeneity based on more complete observation of the aquifer parameters and including some knowledge of the structure of the layer would result in an even better fit.