Chapter 3 Calibration of the conceptual model.

I. Introduction

In an attempt to improve the calibration of the steady-state flow model with the set of 55 coal monitoring wells, four progressively more complex scenarios or conceptual models were tested. The four scenarios were: 1) homogeneous coal with no transition zone between the coal and the crop line; 2) homogeneous coal with a homogeneous transition zone all along the cropline; 3a) homogeneous coal with a heterogeneous transition zone; 3b) homogeneous coal with a heterogeneous transition zone and only clinker cells active east of the cropline. The attempt was to alter the concept of how the parts of the natural system, about which the least is known, behave, in a logical, step-by-step manner, until the model agreed with the data that was collected.

As constructed, the partial differential equation (PDE) being solved in the steady-state flow model is the Poisson elliptical PDE with Dirichlet boundary conditions,

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = -\frac{R(x,y)}{T} \qquad \text{(Wang and Anderson, 1982)}$$

where

h = hydraulic head (feet)
T = transmissivity (square feet/day)
R = recharge (cubic feet/day).

The hydraulic head at all points on the boundary has been specified. In relation to this PDE, it can be said that the solutions of this equation can not achieve a strong relative maximum or minimum in the interior of the domain, given that vertical recharge is a constant over the entire domain (Garabedian, 1964). Hence, the maximum and minimum of the solution are dictated by the choice of heads on the boundary and occur on the boundary. This is highly significant since in many flow models of this type and size, boundary heads are one of the least known parameters. In this case the heads are fairly well established on the eastern boundary but known only poorly on the western boundary. The heads on the western boundary have been set up to

conform to the conceptual model, i.e. hydraulic heads somewhere between the top of the coal and the elevation of the land surface, with a gradient to the northwest.

II. Method

A discussion of Modflowp input is necessary at this point. Modflowp utilizes zone arrays to control the distribution of given parameters. These arrays consist of zones, each of which is made up of repetitions of a unique positive number. Each unique number is assigned a parameter value. The zone array for case one is represented graphically in figure 3-1. In addition, Modflowp allows for manipulation of the following parameters of interest in this model: 1) head on the boundary (CH); 2) hydraulic conductivity (K); and 3) vertical hydraulic conductivity of a confining bed (KV). CH consists of a single elevation value, which can be estimated, and a gradient along a row, which is fixed. At this stage CH and K will be manipulated in layer 2, the coal layer.

Case 1

Case 1 consists of homogeneous coal and no transition zone along the cropline (Figure 3-1). Models were run with coal K varying from 2 to 92 feet/day and CH varying from 4000 to 4160 feet (Figure 3-2). In measuring the quality of the fit between the predicted head and the observed head, two properties were observed: the budget discrepancy, reported in percent; and the mean residual, measured in feet. The budget discrepancy is calculated by taking water in minus water out, dividing by total quantity of water involved and multiplying by 100%. The mean residual is a measure of the bias in the model. A positive mean residual indicates that the calculated head is below the observed head. A negative mean residual indicates that the calculated head is above the observed head.

Case 2

Case 2 consists of homogeneous coal and an homogeneous transition zone (Figure 3-3). The transition zone is continuous along the entire length of the cropline and separates the coal from the clinker and non-clinker material east of the cropline. As described in chapter two, clinker has an elevated K value. Clinker formation does not cease cleanly along a line in space. There undoubtedly exists a zone between clinker, formed from fully combusted coal, and unaltered coal, in which the effects of combustion are only partial. It would be logical to assume

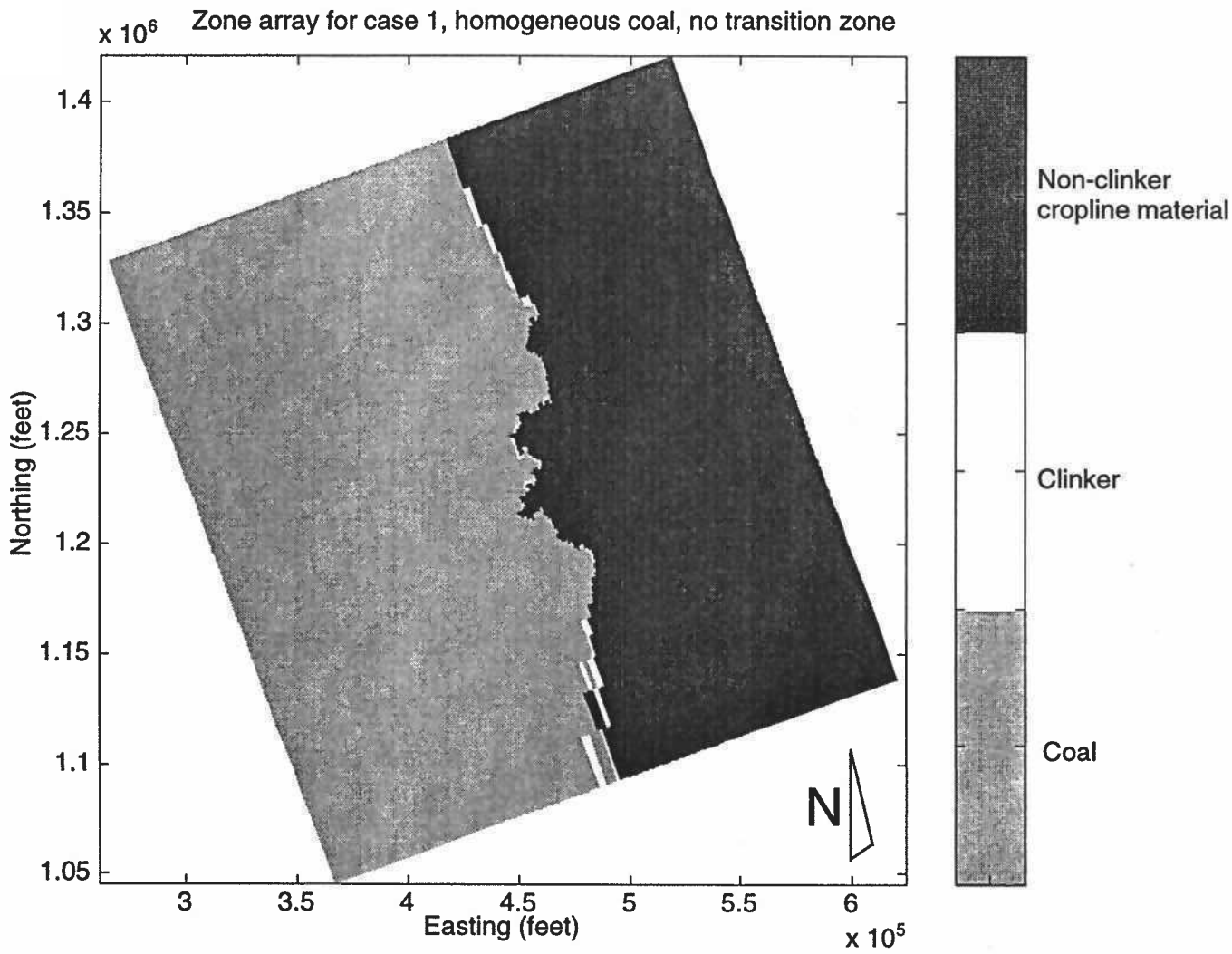
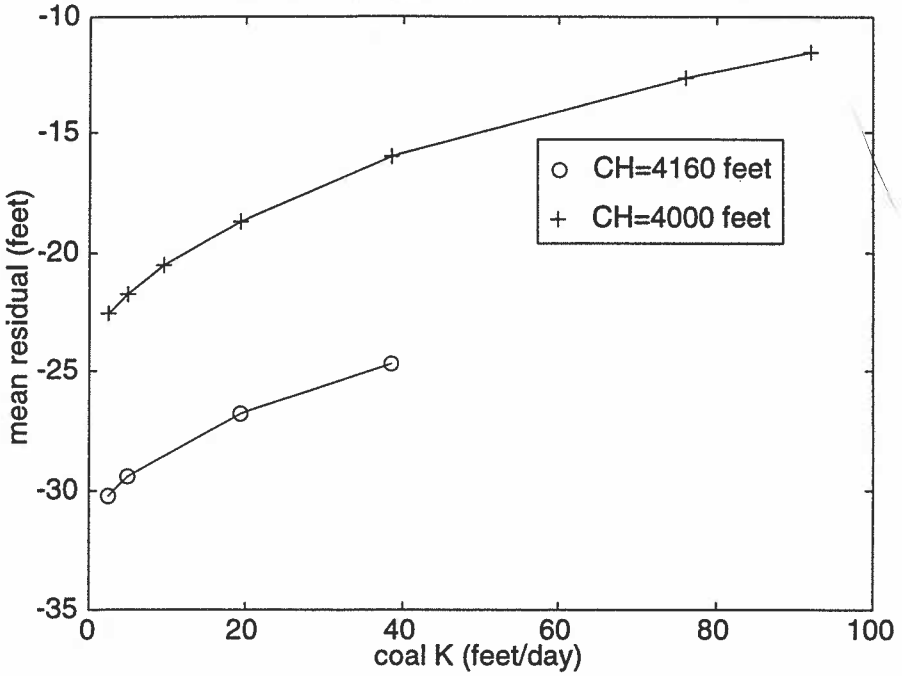


Figure 3-1. Zone array for case1, homogeneous coal, no transition zone.

coal K vs. mean residual, homogeneous coal, no transition zone, CH=4160 and 4000



coal K vs. budget discrepancy, homogeneous coal, no transition zone, CH=4160. and 4000.

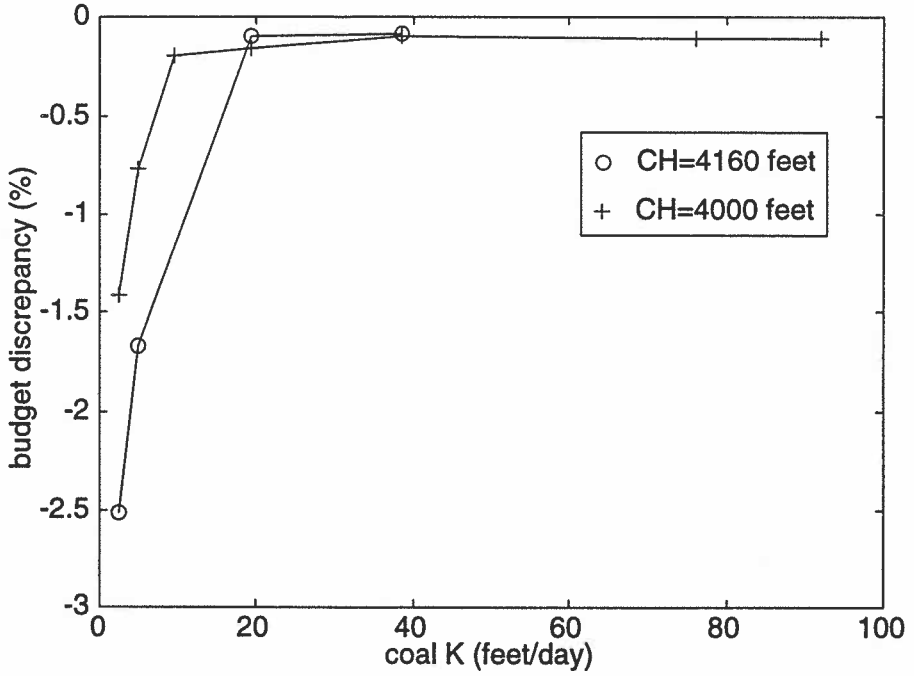


Figure 3-2. Case 1, homogeneous coal with no transition zone. Budget discrepancy and mean residual as a function of coal K. CH held constant at 4000 and 4160 feet.

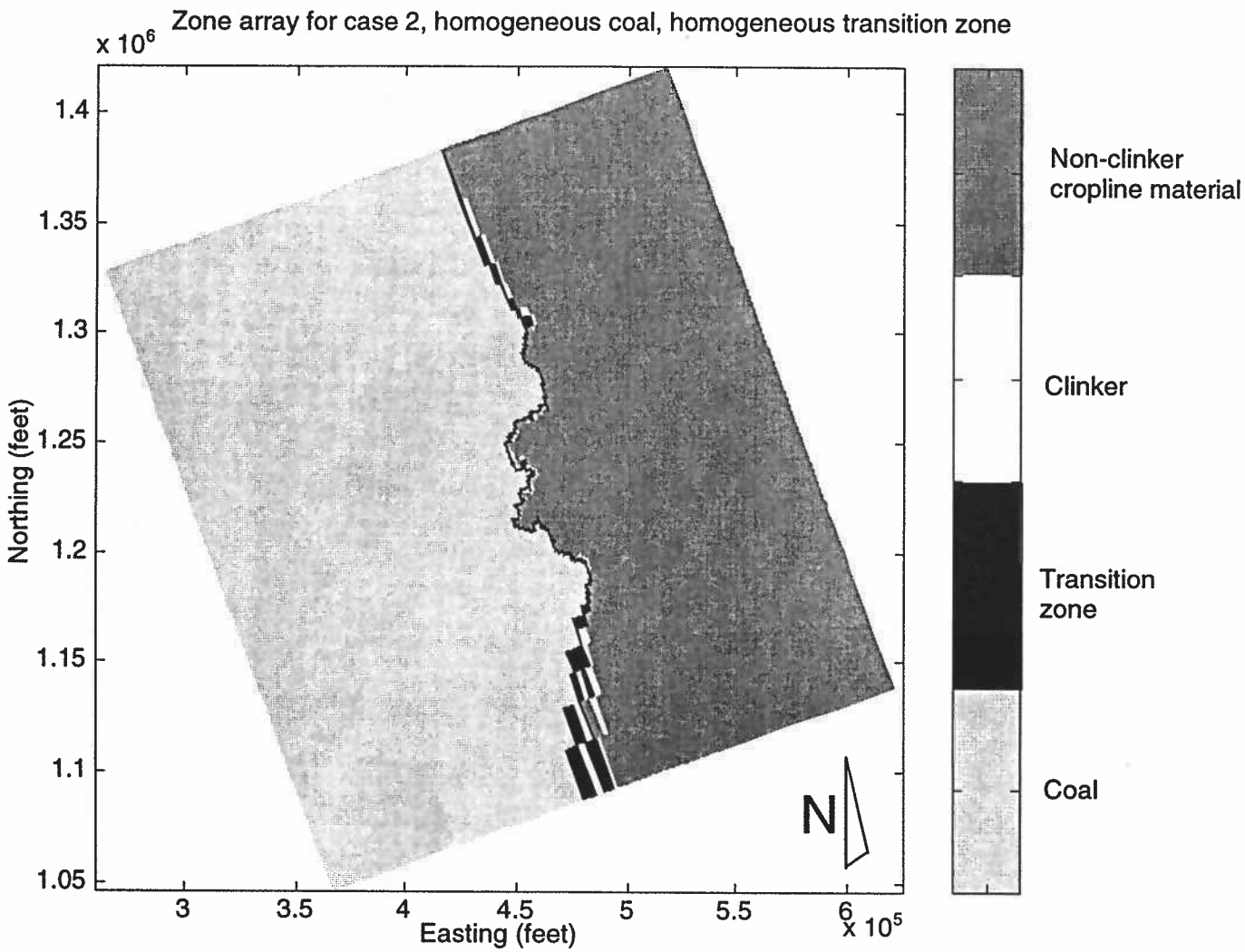


Figure 3-3. Zone array for case 2, homogeneous coal, homogeneous transition zone.

that this zone has K values between those of clinker and those of coal. Never the less, models were run with a full range of values for the transition zone, from lower than coal to somewhere between clinker and coal. CH was held fixed at 4160 feet.

Case 3a

Case 3a consists of homogeneous coal with a heterogeneous transition zone along the cropline. The transition zone was separated into five pods, each of which is adjacent to clinker cells on the cropline. All transition zone cells that were adjacent to non-clinker crop-line material were reverted to coal cells (Figure 3-4). CH was held fixed at 4160 feet.

Case3b

In an attempt to reduce the inflow of water from the east, the non-clinker cropline cells were inactivated (Figure 3-4). This model consists of homogeneous coal, heterogeneous transition zone, and inactive non-clinker cropline cells. Inactive cells are no-flow cells, and do not draw water into or out of the model. CH was held fixed at 4160 feet.

III. Results

Case 1

The results of case one are shown in figure 3-2 and table 3-1. The best fit at CH=4000 was with coal K = 92, resulting in budget discrepancy of -0.11% and mean residual of -11.5 feet, which indicates an overestimation of the potentiometric surface in the domain (Figure 3-2). The best fit at CH=4160 was with coal K=38.4, resulting in a budget discrepancy of -0.14% and a mean residual of -24.7 (Figure 3-2). This was sufficient for conclusions to be drawn; no further models were run for this case.

Case 2

The best fit scenario in case 2 occurred with coal K=63 feet/day and transition zone K=16 feet/day, resulting in a budget discrepancy of -0.10% and a mean residual of -5.39. Complete results are shown in figures 3-5 and 3-6 and table 3-2.

Case 3a

The lowest mean residual and budget discrepancy for this scenario occurred with a coal K=63 and a transition zone K=2.4, resulting in a budget discrepancy of -0.07%, and a mean residual of 0.776 feet. Complete results are shown in figures 3-7 and 3-8 and table 3-3.

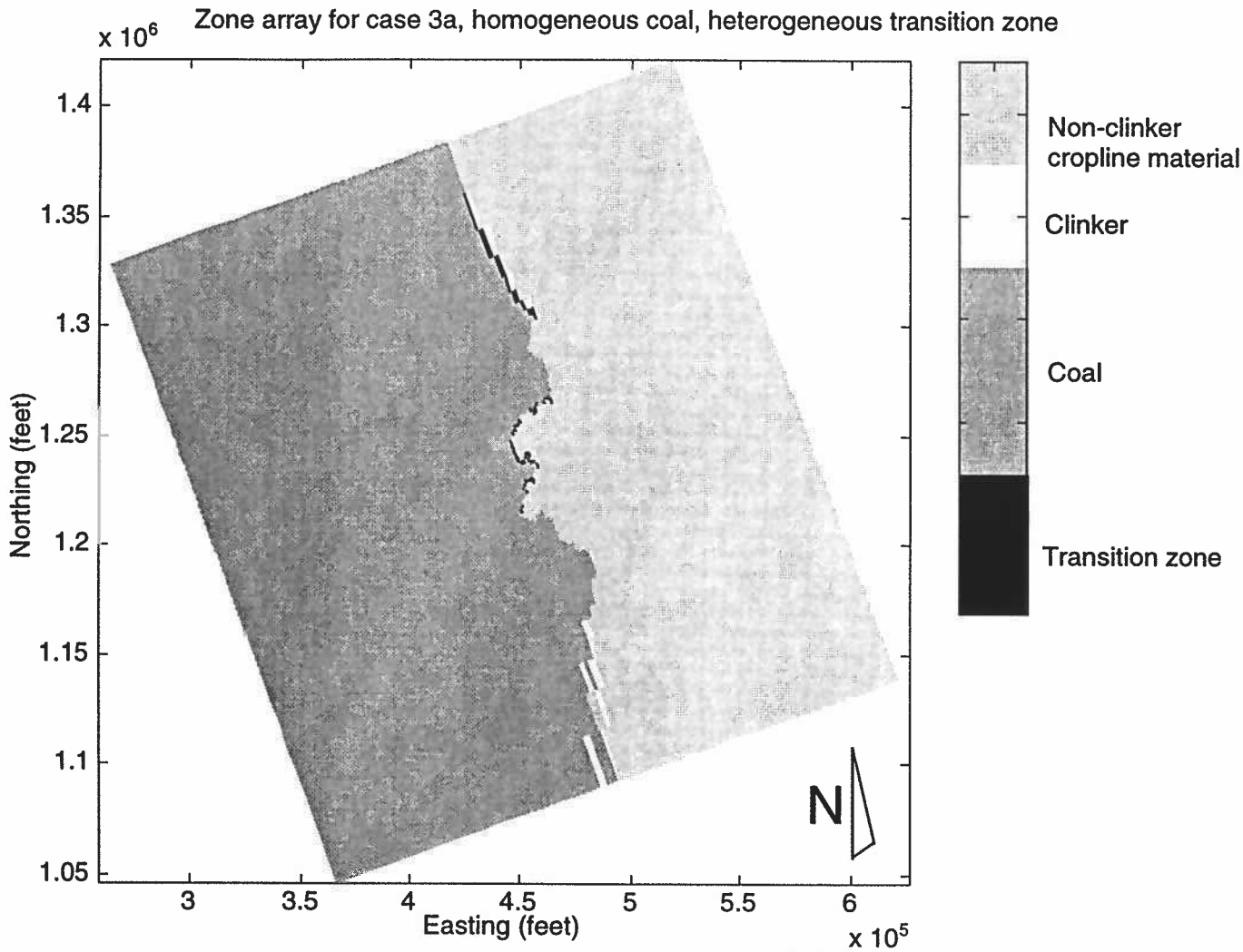


Figure 3-4. Zone array for cases 3a and 3b. In case 3b the zone labeled non-clinker cropline material is inactive.

Table 3-1. Results from chapter 3 case 1

simulation no.	CH (feet)	coal K (feet/day)	KV (feet/day)	sum of the squared residuals	mean residual (feet)	budget discrepancy %	rmse (feet)
1	4160	2.4	1.00E-11	145550	-30.2	-2.51	51.4
2	4477	2.4	1.00E-11	192330	-42.8	2.48	59.1
3	4160	4.8	1.00E-11	142210	-29.4	-1.67	50.8
4	4160	19.2	1.00E-11	132610	-26.8	-0.10	49.1
5	4160	38.4	1.00E-11	125390	-24.7	-0.09	47.7
6	4100	19.2	1.00E-11	127530	-23.8	-0.14	48.2
7	4050	19.2	1.00E-11	124210	-21.3	-0.15	47.5
8	4000	19.2	1.00E-11	121810	-18.7	-0.16	47.1
9	4000	38.4	1.00E-11	116000	-16.0	-0.10	45.9
10	4000	76.2	1.00E-11	111150	-12.6	-0.11	45.0
11	4000	92	1.00E-11	110270	-11.5	-0.11	44.8
12	3950	100	1.00E-11	110840	-8.0	-0.04	44.9
13	3950	150	1.00E-11	110930	-5.7	-0.01	44.9
14	4000	2.4	1.00E-11	131410	-22.6	-1.42	48.9
15	4000	9.6	1.00E-11	126590	-20.5	-0.20	48.0
16	4000	4.8	1.00E-11	129490	-21.7	-0.77	48.5

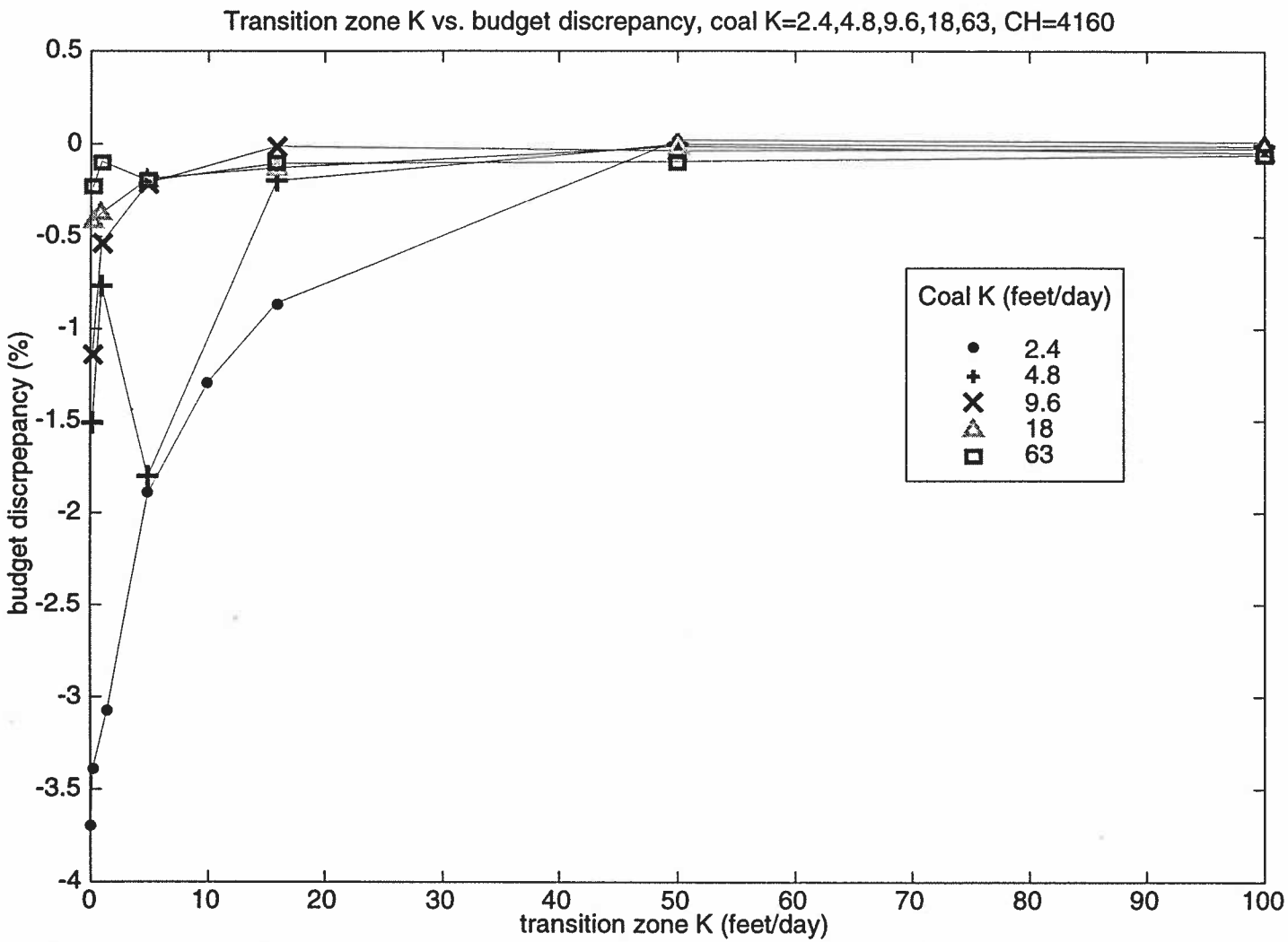


Figure 3-5. Case 2, homogeneous coal, homogeneous transition zone. Budget discrepancy as a function of transition zone K at given values of coal K. CH=4160.

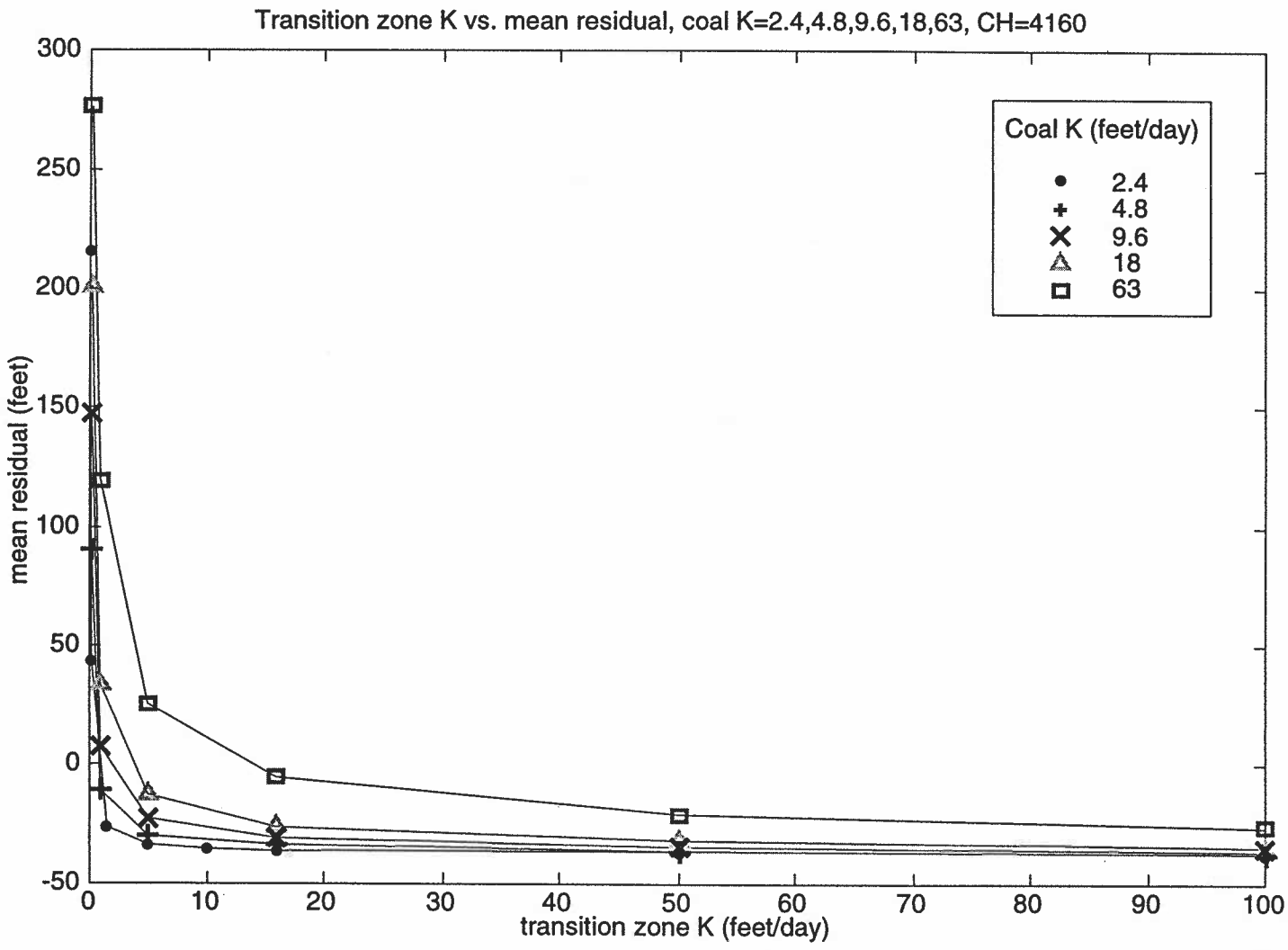


Figure 3-6. Case 2, homogeneous coal, homogeneous transition zone. Mean residual as a function of transition zone K at given values of coal K. CH=4160.

Table 3-2. Results from chapter 3 case 2

CH = 4160 feet, KV = 0.10E-10 feet/day

simulation no.	coal K (feet/day)	transition zone K (feet/day)	sum of the squared residuals	mean residual (feet)	budget discrepancy (%)	rmse (feet)
1	2.4	1.4	125060	-26.2	-3.06	47.7
2	2.4	0.1	220580	43.1	-3.39	63.3
3	2.4	0.01	3335700	216.0	-3.72	246.3
4	2.4	10	178400	-35.3	-1.29	57.0
5	18	1	164480	33.5	-0.37	54.7
6	18	0.1	2.89E+07	201.0	-0.42	724.9
7	41	1	614320	85.6	-0.31	105.7
8	2.4	5	166170	-33.5	-1.89	55.0
9	0.63	0.16	95588	-20.1	-8.41	41.7
10	6.3	1.6	87593	-13.9	-0.51	39.9
11	63	16	81847	-5.4	-0.10	38.6
12	630	160	108750	11.8	-0.01	44.5
13	2.4	16	183780	-36.3	-0.86	57.8
14	2.4	50	188570	-36.8	0.02	58.6
15	2.4	100	190500	-37.4	0.01	58.9
16	9.6	0.1	164164	148.0	-1.14	54.6
17	9.6	1	80320	7.4	-0.53	38.2
18	9.6	5	113870	-22.7	-0.21	45.5
19	9.6	16	152900	-30.9	-0.01	52.7
20	9.6	50	173980	-34.6	-0.03	56.2
21	9.6	100	181140	-36.0	-0.02	57.4
22	18	5	87204	-13.0	-0.19	39.8
23	18	16	128970	-26.1	-0.13	48.4
24	18	50	159390	-32.1	-0.01	53.8
25	18	10	171050	-34.3	-0.05	55.8
26	63	0.1	530170	276.0	-0.23	98.2
27	63	1	1111200	120.0	-0.09	142.1
28	63	5	132260	25.7	-0.20	49.0
29	63	50	112600	-20.6	-0.09	45.2
30	63	100	133810	-26.3	-0.06	49.3
31	4.8	1	81707	-10.8	-0.77	38.5
32	4.8	5	143340	-29.6	-1.80	51.1
33	4.8	16	171120	-34.0	-0.20	55.8
34	4.8	50	183510	-36.1	0.00	57.8
35	4.8	0.1	680220	90.9	-1.51	111.2
36	4.8	100	187530	-37.0	-0.01	58.4

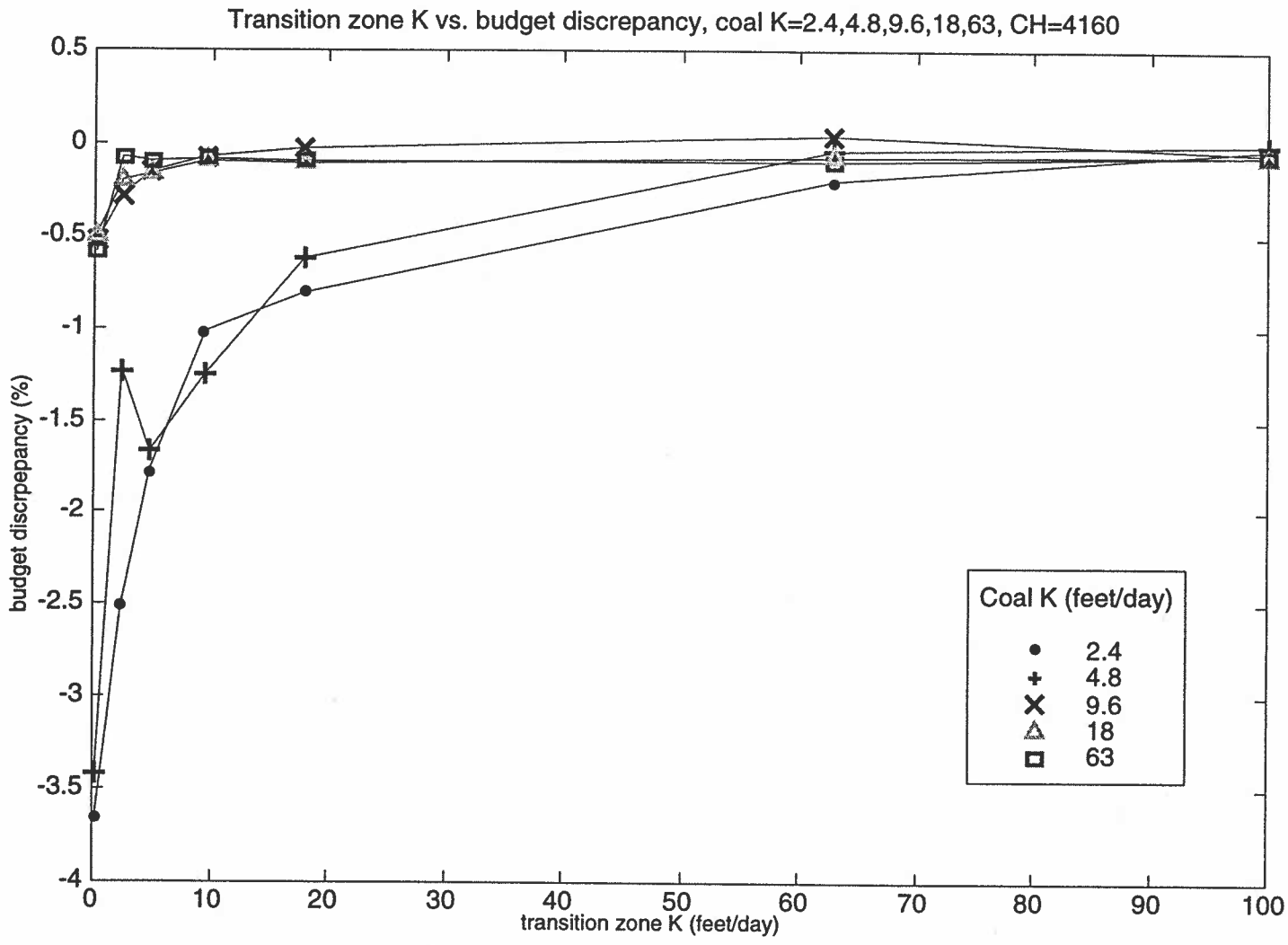


Figure 3-7. Case 3a, homogeneous coal, heterogeneous transition zone. Budget discrepancy as a function of transition zone K at given values of coal K, CH=4160.

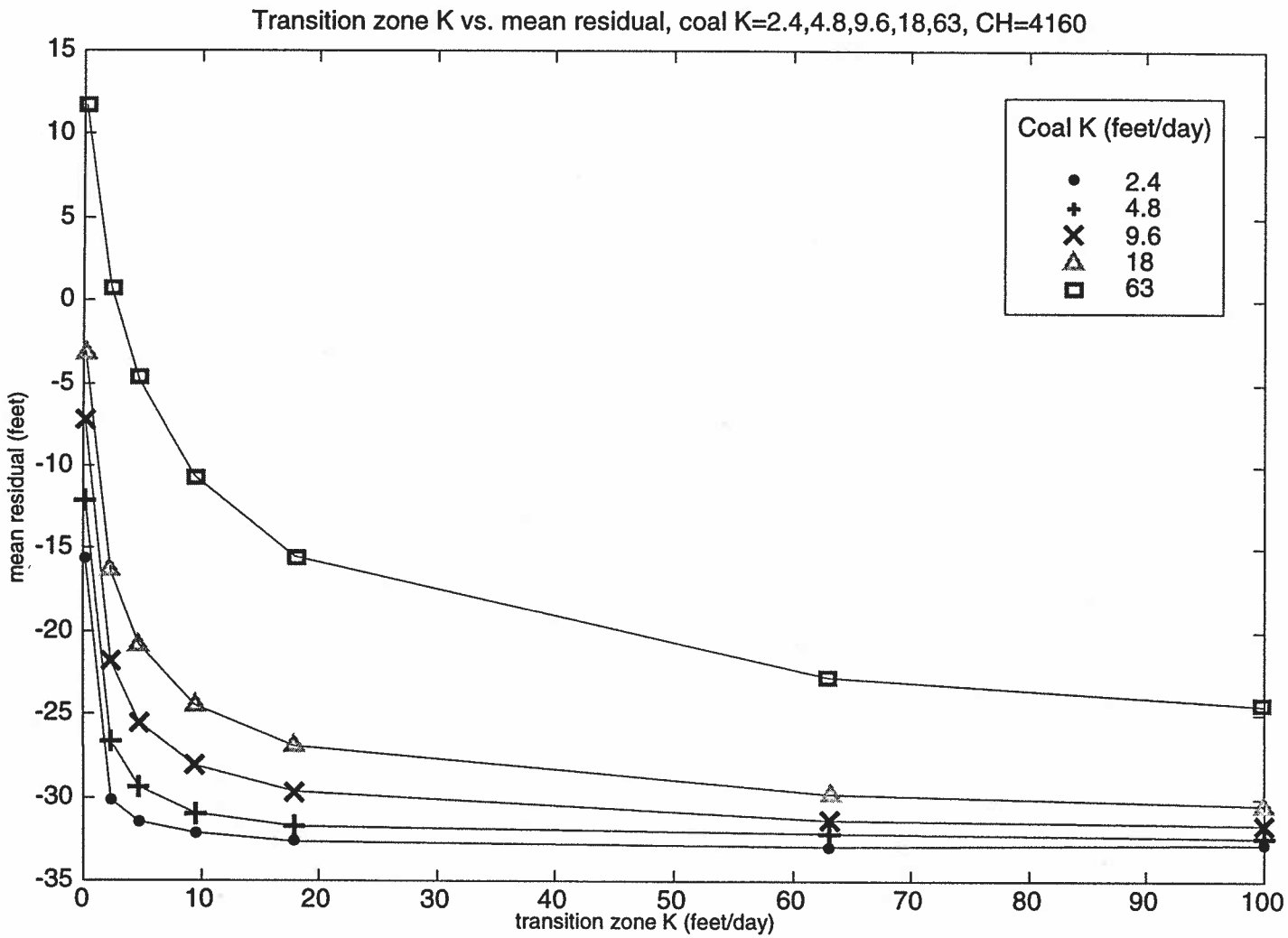


Figure 3-8. Case 3a, homogeneous coal, heterogeneous transition zone. Mean residual as a function of transition zone K at given values of coal K, CH=4160.

Table 3-3. Results from chapter 3 case 3a

CH = 4160 feet, KV = 0.10E-10 feet/day

simulation no.	coal K (feet/day) zone 1	transition zone K (feet/day) zone 2,3,4,6	transition zone K (feet/day) zone 5	sum of the squared residuals	mean residual (feet)	budget discrepancy (%)	rmse (feet)
1	2.4	0.1	2.4	87678	-15.6	-3.66	39.9
2	2.4	2.4	2.4	145550	-30.2	-2.51	51.4
3	2.4	4.8	2.4	155560	-31.5	-1.77	53.2
4	2.4	9.6	2.4	161920	-32.2	-1.02	54.3
5	2.4	18	2.4	165880	-32.7	-0.80	54.9
6	2.4	63	2.4	169290	-32.9	-0.20	55.5
7	2.4	100	2.4	169860	-32.8	-0.30	55.6
8	4.8	0.1	4.8	82546	-12.1	-3.42	38.7
9	4.8	2.4	4.8	127230	-26.7	-1.22	48.1
10	4.8	4.8	4.8	142210	-29.4	-1.67	50.8
11	4.8	9.6	4.8	152840	-31.0	-1.25	52.7
12	4.8	18	4.8	159360	-31.7	-0.62	53.8
13	4.8	63	4.8	166170	-32.2	-0.04	55.0
14	4.8	100	4.8	167410	-32.4	0.00	55.2
15	9.6	0.1	9.6	81951	-7.3	-0.53	38.6
16	9.6	2.4	9.6	107660	-21.9	-0.28	44.2
17	9.6	4.8	9.6	123210	-25.5	-0.15	47.3
18	9.6	9.6	9.6	137860	-28.1	-0.07	50.1
19	9.6	18	9.6	148200	-29.7	-0.02	51.9
20	9.6	63	9.6	160200	-31.3	0.04	54.0
21	9.6	100	9.6	162890	-31.6	-0.05	54.4
22	18	0.1	18	83246	-3.0	-0.49	38.9
23	18	2.4	18	91699	-16.4	-0.20	40.8
24	18	4.8	18	104340	-20.8	-0.16	43.6
25	18	9.6	18	119980	-24.4	-0.10	46.7
26	18	18	18	132860	-26.9	-0.11	49.1
27	18	63	18	151210	-29.8	-0.07	52.4
28	18	100	18	155450	-30.4	-0.06	53.2
29	63	0.1	63	113090	11.8	-0.59	45.3
30	63	2.4	63	85229	0.8	-0.07	39.4
31	63	4.8	63	80820	-4.8	-0.10	38.3
32	63	9.6	63	84035	-10.6	-0.08	39.1
33	63	18	63	93433	-15.5	-0.09	41.2
34	63	63	63	119910	-22.7	-0.10	46.7
35	63	100	63	128770	-24.5	-0.06	48.4

Case3b

The best fit for this scenario occurred with a coal K=2.4 feet/day and a transition zone K=63 feet/day, resulting in a budget discrepancy 0f -0.12% and a mean residual of 0.0126 feet. Complete results are shown in figures 3-9 and 3-10 and table 3-4. Head calculated for layer 2 in case 3b is shown in figure 3-11.

IV. Conclusions

Case 1

Increasing the coal K returns a smaller residual and a smaller budget discrepancy. However, the high values of coal K are unreasonable and indicate that this conceptual model is inadequate. Too much water is entering the model from the east, and, since CH has been fixed, coal K must be elevated to dissipate the water.

According to Darcy's law,

$$q = -K\frac{dh}{dl} \qquad \text{(Anderson, 1992),}$$

where q = discharge rate (cubic feet/day)
K = hydraulic conductivity (feet/day)
h = hydraulic head (feet)
l = flow-path length (feet)

if all variables are held constant, with the exception of dh and K, it is clear that these two variables are related inversely. In the case of the model, CH could be elevated to decrease the coal K. However, doing so increases both the mean residual and budget discrepancy (Figure 3-12). Therefore a plausible CH which allows for good calibration must be found and kept fixed. As shown in figure 3-12, this value is CH=4160 feet. Therefore, subsequent results are reported at CH=4160 feet.

Case 2

A high value of 63 feet/day for coal K runs counter to what is expected and indicates that this conceptual model is not adequate to describe the system. The coal K has, however, been reduced slightly.

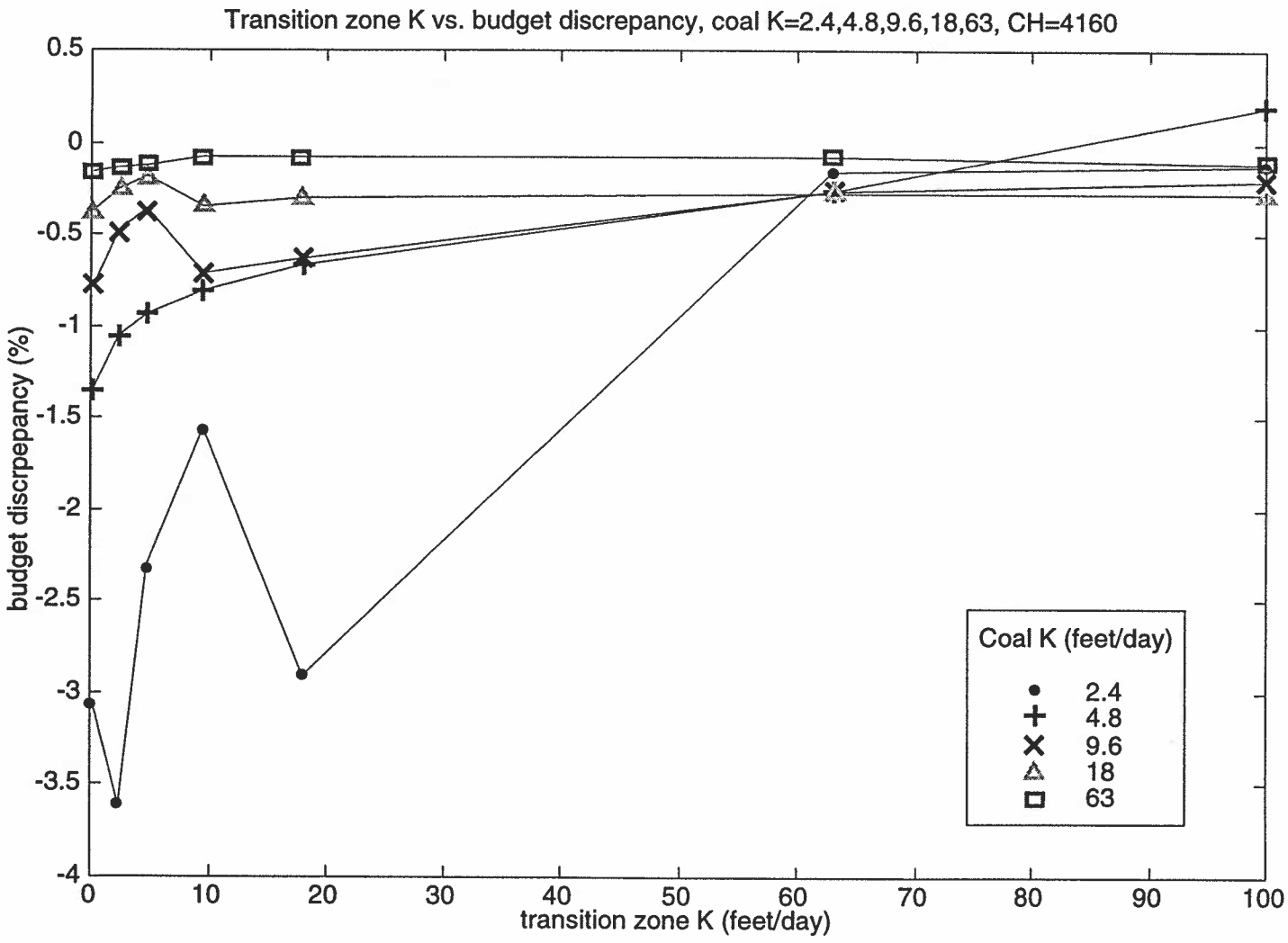


Figure 3-9. Case3b, homogeneous coal, heterogeneous transition zone. Non-clinker cropline cells inactive. Budget discrepancy as a function of transition zone K at given values of coal K, CH=4160.

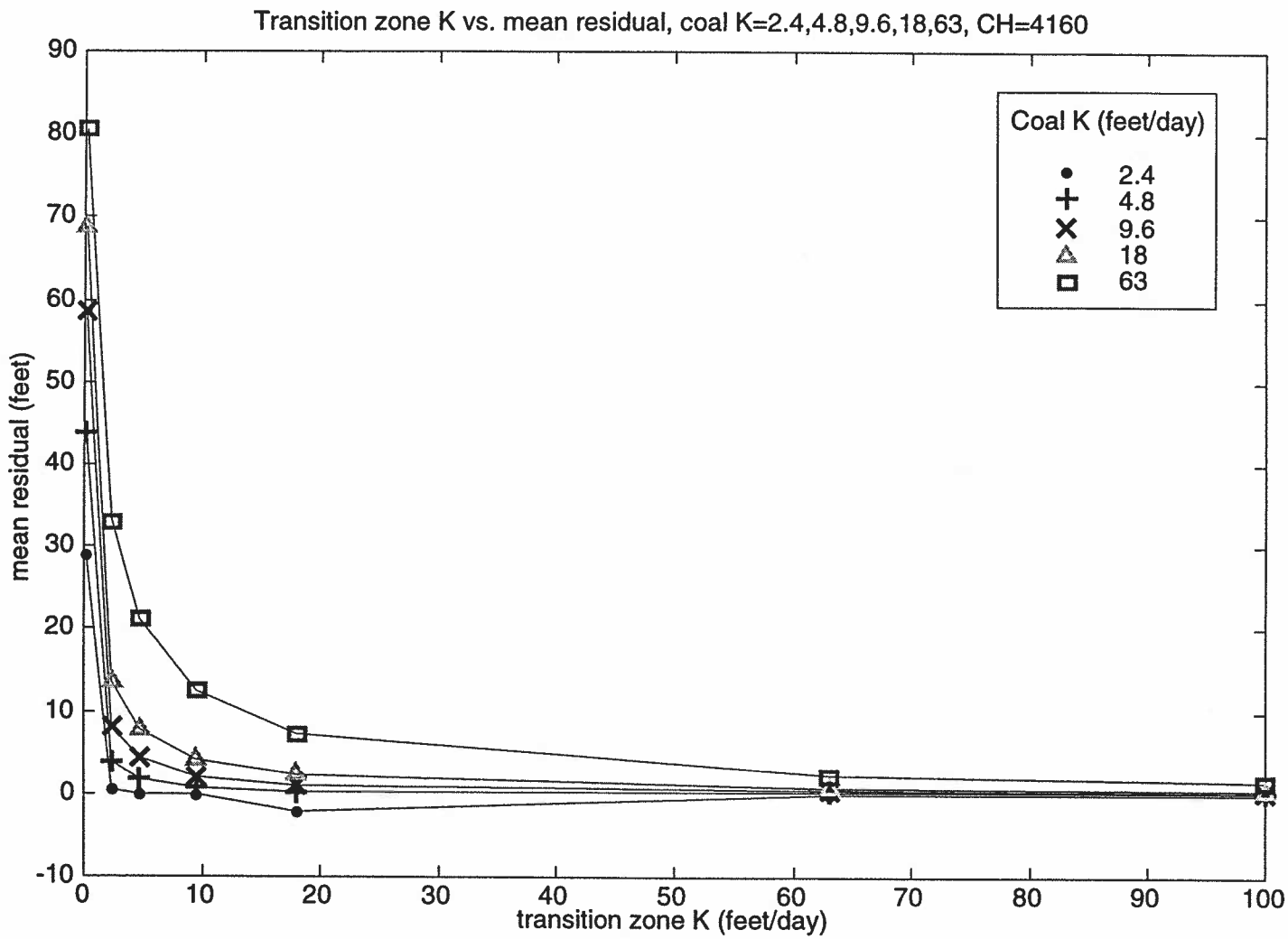


Figure 3-10. Case3b, homogeneous coal, heterogeneous transition zone. Non-clinker cropline cells inactive. Mean residual as a function of transition zone K at given values of coal K, CH=4160.

Table 3-4. Results from chapter 3 case 3b

CH = 4160 feet, KV = 0.10E-10 feet/day, non-clinker cropline cells inactive

simulation no.	coal K (feet/day)	transition zone K (feet/day)	transition zone K (feet/day)	sum of the squared residuals	mean residual (feet)	budget discrepancy (%)	rmse (feet)
	zone 1	zone 2,3,4	zone 5,6				
1	2.4	0.1	2.4	281700	28.90	-3.06	71.6
2	2.4	2.4	2.4	108190	0.49	-3.61	44.4
3	2.4	4.8	2.4	107270	-0.01	-2.31	44.2
4	2.4	9.6	2.4	107060	-0.17	-1.56	44.1
5	2.4	18	2.4	104160	-2.02	-2.91	43.5
6	2.4	63	2.4	107660	0.01	-0.16	44.2
7	2.4	100	2.4	107700	0.04	-0.12	44.3
8	4.8	0.1	4.8	449250	43.70	-1.35	90.4
9	4.8	2.4	4.8	117780	3.91	-1.05	46.3
10	4.8	4.8	4.8	111990	1.87	-0.93	45.1
11	4.8	9.6	4.8	109410	0.82	-0.80	44.6
12	4.8	18	4.8	108330	0.32	-0.66	44.4
13	4.8	63	4.8	107960	0.20	-0.26	44.3
14	4.8	100	4.8	107840	0.14	-0.19	44.3
15	9.6	0.1	9.6	677380	58.70	-0.78	111.0
16	9.6	2.4	9.6	132150	8.00	-0.47	49.0
17	9.6	4.8	9.6	118630	4.29	-0.36	46.4
18	9.6	9.6	9.6	112190	2.00	-0.71	45.2
19	9.6	18	9.6	109760	1.01	-0.63	44.7
20	9.6	63	9.6	108280	0.38	-0.26	44.4
21	9.6	100	9.6	108090	0.29	-0.21	44.3
22	18	0.1	18	861610	68.80	-0.04	125.2
23	18	2.4	18	160420	13.60	-0.25	54.0
24	18	4.8	18	131310	7.69	-0.18	48.9
25	18	9.6	18	117970	4.08	-0.35	46.3
26	18	18	18	112790	2.27	-0.30	45.3
27	18	63	18	108930	0.69	-0.27	44.5
28	18	100	18	108410	0.45	-0.28	44.4
29	63	0.1	63	1110300	80.50	-0.16	142.1
30	63	2.4	63	320170	33.30	-0.14	76.3
31	63	4.8	63	209560	21.20	-0.12	61.7
32	63	9.6	63	153520	12.50	-0.07	52.8
33	63	18	63	129730	7.37	-0.08	48.6
34	63	63	63	113230	2.41	-0.08	45.4
35	63	100	63	111200	1.58	-0.11	45.0

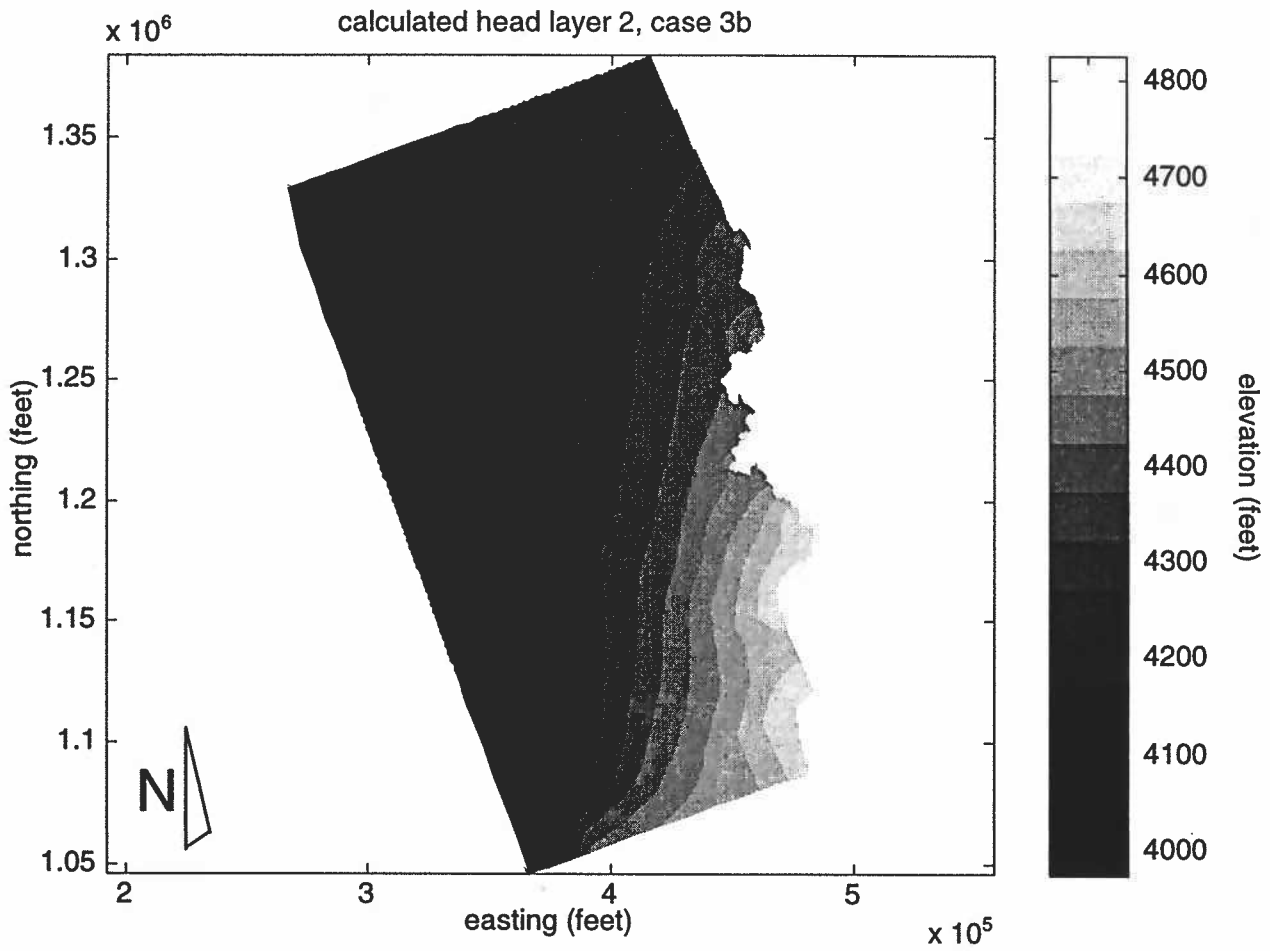
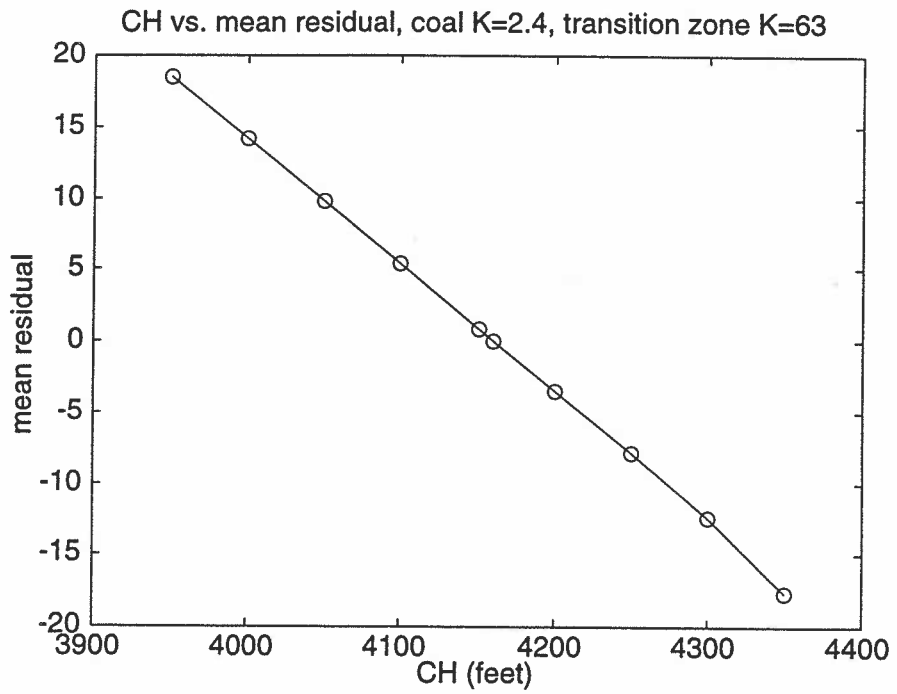


Figure 3-11. Head calculated in case 3b, layer 2; homogeneous coal, heterogeneous transition zone, non-clinker cropline cells inactive.



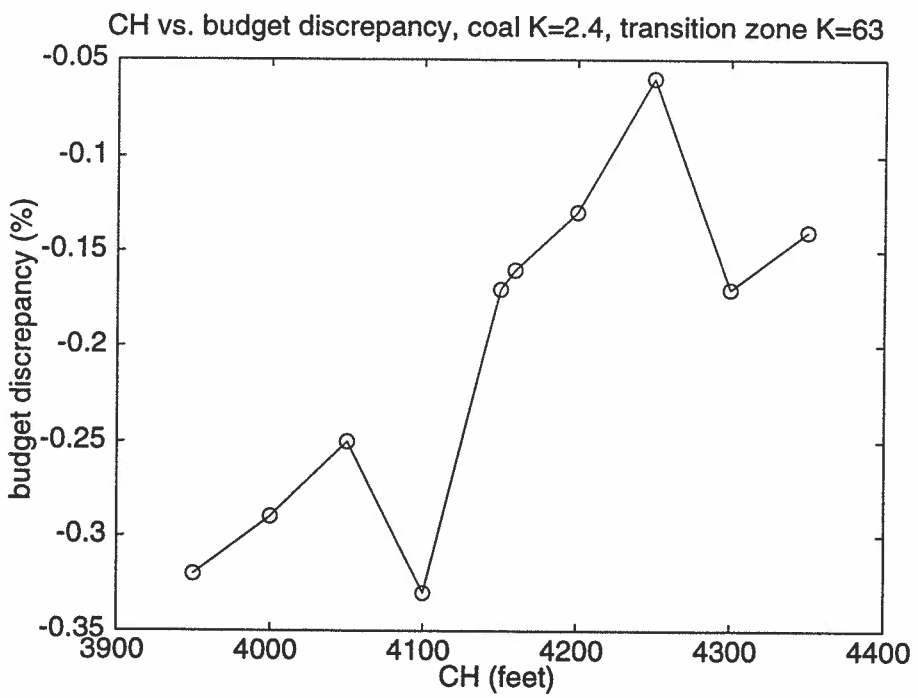


Figure 3-12. CH vs. mean residual and budget discrepancy. Coal K=2.4, transition zone K=63, heterogeneous transition zone, non-clinker cropline cells inactive.

Case3a

The results of case 3a are an exceptional fit. However, the coal and transition zone K's are reversed from what is expected from the data. Sixty-three is far too high for coal K. This may be due to too much water entering the model from the east, encouraging Modflowp to increase the coal K.

An interesting byproduct of this model is the indication by Modflowp that transition zones in the southern half of the model have a nearly 100% correlation with the coal of the rest of the model. This may indicate that either these transition zones have very low K, on the order of coal, that there is no transition zone in this area, or that the clinker in this area is not in connection with the coal due to a structural feature. For this and the following cases, the transition zones which correlated with coal were lumped back in with the coal.

Case3b

This is a model that is both plausible and fits our calibration criteria well. This model will be the starting point for investigations into the vertical hydraulic conductivity of the confining layer between the Wasatch sand lens and the Wyodak coal, and the heterogeneity of the coal.