5.0 MODEL RESULTS

5.1 Predicted Pollutant Concentrations and Comparison to Observed Concentrations

The CALPUFF model was used as described in preceding sections to calculate daily 24-hour and annual average concentrations at BNP of sulfate (SO_4), nitrate (NO_3), organic carbon (OC) and elemental carbon (EC) particles, and total PM10. One model run used the 1990 emission inventories as described in Section 4.2; a second run simulated impacts from 1997 emissions. Both runs utilized the CALMET meteorological fields for 1990, as described in section 4.3. As explained in section 4.3, 1990 is the only year for which suitable meteorological input data are available. It is assumed that the range and frequency of various meteorological conditions are generally similar from year-to-year. Thus, the average pollutant concentrations and their frequency distributions for the two years should differ only because of changed pollutant emissions.

Model-predicted concentrations were compared to measured concentrations at the BNP IMPROVE monitoring site. To provide the most representative IMPROVE results and utilize all available measurements, monitoring data from 1989 – 1993 were used for comparison to 1990 model predictions, and IMPROVE data for 1994 – 1998 were taken as representative of 1997.

5.1.1 Modeled/Observed Concentrations for 1990

Table 5-1 compares predicted concentrations for each pollutant for 1990 to measured concentrations at BNP from 1989 through 1993. It is clear that predicted concentrations are significantly lower than observed concentrations at BNP. This result was expected, since the modeled Wyoming/South Dakota sources represent only a portion of the many pollutant sources, both natural and manmade, that can potentially affect air quality in Badlands National Park.

TABLE 5-1

PREDICTED AND OBSERVED CONCENTRATION STATISTICS FOR 1990 (µg/m^3)

Pollutant	Model Predictions		IMPROVE Measurements (1989 – 93)	
	Annual Average	95th Percentile 24-hour	Annual Average	95th Percentile 24-hour
Nitrate (NO_3)	0.228	0.90	0.362	1.58
Sulfate (SO_4)	0.044	0.17	1.199	3.12
PM10	1.83	4.21	10.16	22.98
Organic Carbon (OC)	0.033	0.07	0.853	1.80
Elemental Carbon (EC)	0.039	0.08	0.177	0.34

It will be noted that the fraction of observed concentrations that are accounted for by the model results varies with pollutant. Over 50% of observed NO_3 is predicted by the CALPUFF simulation; about 20% of measured PM10 and EC concentrations are predicted from modeled sources, and much smaller fractions of sulfate and organic carbon are accounted for by the model results. The difference between NO_3 and SO_4 probably reflects both the more rapid conversion of NO_x to NO_3 in the atmosphere and the fact that most major SO_2 sources that can potentially affect SO_4 concentrations at BNP are outside of the modeling source inventory region (further west and southwest, and in other directions). Thus, the modeled NO_x sources in the PRB and western South Dakota have a relatively high impact in BNP, while observed SO_4 is overwhelmingly produced by sources outside of the modeling region.

The significant fraction of observed PM10 that can be attributed to modeled sources is reasonable since PM10 has a relatively short residence time in the atmosphere. Modeled sources within a few hundred kilometers of BNP apparently account for around 20% of the observed concentrations. But it should be recognized that local sources (roadways, fires, and wind erosion) likely have the highest impacts, and may not be included in the emission inventory. The difference between the comparisons for organic and elemental carbon is likely due at least in part to the predominant sources of the two types of particulate matter. Elemental carbon is generated primarily from diesel exhaust, while organic carbon originates from natural and anthropogenic organic emissions, and combustion of wood and organic materials. The elemental carbon sources were generally included in the modeled inventory, while forest and range fires and natural organic emission sources were not included.

An attempt was made to correlate 24-hour pollutant concentrations measured at BNP to model predictions for the same days in 1990 when IMPROVE measurements were obtained. For

NO_3, there were several periods during which model results were in reasonable agreement with measured values, suggesting that the impacts of modeled sources were reproduced realistically. In other cases, there was little correspondence between predicted and observed NO_3 concentrations; usually observed concentrations were higher than predicted. For the other pollutants, observed concentrations were nearly always much higher than predictions, and there was no significant correlation between predicted and observed values. It therefore proved impossible to draw any quantitative conclusions on the accuracy of the model predictions. The most that can be concluded is that the predicted NO_3 impacts appear to be realistic in magnitude, and that there is no evidence of major overprediction of impacts for any pollutant.

5.1.2 Modeled/Observed Concentrations for 1997

A comparison between predicted and observed concentrations for 1997 is shown in Table 5-2. The same features as discussed above are evident; the 1997 model results indicate slightly increased impacts over 1990 for NO_3 and SO_4, and slightly lower impacts for PM10, OC, and EC.

It is more instructive to compare predicted and observed changes in concentration from 1990 to 1997, as shown in Table 5-3. For both predicted and observed concentrations, most of the indicated trends are very small and of questionable significance. However for NO_3, the increase in measured concentration represents a more than 20% increase; the CALPUFF model results suggest that about one-third of the observed increase can be ascribed to the modeled emission sources. As discussed in a subsequent section, the predicted and observed changes in nitrate concentration are sufficient to imply a significant visibility impact.

TABLE 5-2

PREDICTED AND OBSERVED CONCENTRATION STATISTICS FOR 1997 ($\mu g/m^3$)

Pollutant	Model Predictions		IMPROVE Measurements (1994 - 98)	
	Annual Average	95th Percentile 24-hour	Annual Average	95th Percentile 24-hour
Nitrate (NO_3)	0.258	1.01	0.449	1.90
Sulfate (SO_4)	0.054	0.21	1.206	2.86
PM10	1.82	4.19	9.87	21.12
Organic Carbon (OC)	0.024	0.06	0.880	2.27
Elemental Carbon (EC)	0.033	0.07	0.173	0.34

TABLE 5-3

PREDICTED AND OBSERVED CONCENTRATION CHANGES, 1990 to 1997 ($\mu g/m^3$)

Pollutant	Model Predictions		IMPROVE Measurements	
	Annual Average	95th Percentile 24-hour	Annual Average	95th Percentile 24-hour
Nitrate (NO_3)	+0.03	+0.12	+0.09	+0.33
Sulfate (SO_4)	+0.01	+0.04	+0.01	-0.26
PM10	-0.01	-0.03	-0.29	-1.86
Organic Carbon (OC)	-0.01	-0.02	+0.03	+0.47
Elemental Carbon (EC)	-0.01	-0.01	0.0	-0.01

5.2 Source Culpability

The relative contributions of the different types of modeled sources to average predicted concentrations for the 1990 CALPUFF simulation is shown in Table 5-4. The results were obtained by executing complete CALPUFF model runs with individual source groups.

Table 5-4 indicates that point sources were the major contributor to NO_3 and SO_4 concentrations, with the county area sources also making large contributions. For PM10, OC, and EC, the county area sources were the overwhelming contributor. Coal mines and coal trains contributed very little to SO_4, OC, and PM10 concentrations, eight percent of EC concentrations, and 13 percent of predicted NO_3 concentrations. Coal trains had approximately twice the impact of PRB mining operations.

Table 5-5 shows the contribution of coal mines and trains to the predicted change in BNP concentrations from 1990 to 1997. The contribution was negligible except for nitrate. For NO_3, 78% of the predicted increase was due to increased coal mining activity; the predicted increase from coal mines and trains accounts for 26% of the increase in average NO_3 concentration actually observed at the BNP IMPROVE monitoring station.

5.3 Model Sensitivity to Input Parameters

Model runs were carried out to determine the sensitivity of model results to several input parameters. The parameters evaluated were background ammonia and ozone concentrations, and particle size parameters for PM10, EC, and OC. Background pollutant concentrations affect the chemical transformation rates of NO_x to NO_3 and SO_2 to SO_4. Particle sizes have a strong influence on the rate at which particles are removed from the atmosphere through surface deposition.

TABLE 5-4

CONTRIBUTION TO PREDICTED 1990 ANNUAL AVERAGE CONCENTRATIONS BY SOURCE TYPE

Pollutant	Point Sources		County Sources		Coal Mines		Coal Trains		Total
	Conc. ($\mu g/m^3$)	% of Total	Conc. ($\mu g/m^3$)	% of Total	Conc. ($\mu g/m^3$)	% of Total	Conc. ($\mu g/m^3$)	% of Total	($\mu g/m^3$)
Nitrate (NO_3)	.099	43	.100	44	.008	4	.021	9	.228
Sulfate (SO_4)	.034	76	.010	22	.001	1	.001	1	.044
PM10	.026	1	1.801	98	.005	1	<.001	0	1.832
Organic Carbon (OC)	0	0	.032	97	.001	1	.001	2	.033
Elemental Carbon (EC)	0	0	.036	92	.001	3	.002	5	.039

TABLE 5-5

CONTRIBUTION TO PREDICTED CHANGE IN ANNUAL CONCENTRATION 1990 – 1997 BY COAL MINES AND TRAINS

Pollutant	Predicted Change ($\mu g/m^3$)	Mines & Trains ($\mu g/m^3$)	% of Total Predicted	Observed Change ($\mu g/m^3$)
Nitrate (NO_3)	+.030	+.023	78	+.087
Sulfate (SO_4)	+.010	+.001	8	+.007
PM10	-.014	+.003	---	-.292
Organic Carbon (OC)	-.008	+.001	---	+.027
Elemental Carbon (EC)	-.006	+.002	---	-.004

Table 5-6 shows the effect of changes in background ammonia and ozone concentrations on predicted NO_3 and SO_4 concentrations for 1990. Higher background ammonia produces slightly higher predicted concentrations; higher background ozone levels lead to significantly higher predicted sulfate concentrations, and to slightly higher predicted nitrate concentrations. Results presented elsewhere in this report are based on 5 ppb ammonia and 40 ppb ozone.

Effects of changed particle size parameters are illustrated in Table 5-7. Case 1 represents the "base case" that was used for all results presented in this report. The mean particle diameters and standard deviations are the default values recommended for general use in the absence of source-specific data (Earth Tech, 1998). In Case 2, the mean sizes of all particles were increased. The result was a decrease in predicted PM10 concentration (due to more rapid deposition of PM10 particles), and a very minor increase in EC and OC concentrations. In Case 3, EC and OC particles were the same as the base case, but PM10 particles were assumed to be smaller with a mean diameter of 2.5 microns. As would be expected, model-predicted PM10 impacts increased significantly because of reduced fallout of particles during transport.

One other modeling parameter was varied in modeling tests. Prior PRB CALPUFF analyses (and the present study) represented railroad emission sources by individual volume sources spaced at ten kilometer intervals along the rail route. The individual sources were characterized by vertical and horizontal standard deviations of 3.0 and 1000 meters, respectively. This representation has been criticized as an oversimplification, since it represents an actual line of emissions by widely spaced discrete emission sources.

The current versions of the CALPUFF model permit railroad sources to be represented as a series of long, narrow area sources with moderate computation time penalty. Therefore, the railroad emissions for the present study were modeled as more realistic area sources to

TABLE 5-6

EFFECT OF BACKGROUND CONCENTRATIONS ON PREDICTED SULFATE AND NITRATE CONCENTRATIONS

	NO_3 ($\mu g/m^3$)		SO_4 ($\mu g/m^3$)	
	Annual Average	Maximum 24-hour	Annual Average	Maximum 24-hour
Background Ammonia				
1 ppb	.177	2.84	.044	.623
5 ppb	.228	2.93	.044	.650
Background Ozone				
20 ppb	.201	2.81	.037	.546
40 ppb	.228	2.93	.044	.650
80 ppb	.262	3.17	.055	.745

TABLE 5-7

EFFECT OF PARTICLE SIZE PARAMETERS ON PREDICTED CONCENTRATIONS

	EC ($\mu g/m^3$)		OC ($\mu g/m^3$)		PM10 ($\mu g/m^3$)	
	Annual Average	Maximum 24-hour	Annual Average	Maximum 24-hour	Annual Average	Maximum 24-hour
Case 1						
EC, OC: D = 0.48 SD = 2.0	.039	.131	.033	.108	1.83	8.66
PM10: D = 5.2 SD = 2.3						
Case 2						
EC, OC: D = 1.0 SD = 1.0	.039	.132	.033	.109	.86	7.66
PM10: D = 8.0 SD = 3.0						
Case 3						
EC, OC: D = 0.48 SD = 2.0	.039	.131	.033	.108	3.20	11.66
PM10: D = 2.5 SD = 2.0						

D = geometric mass mean diameter (microns)
SD = geometric standard deviation (microns)

compare with the discrete volume source approach. Results showed no significant difference in predicted impacts at BNP.

The reason for the comparable results using volume and area sources for rail lines in the present case is undoubtedly the large distance between the railroad sources and the model receptors in BNP (greater than 200 km). Where railroad sources must be modeled within 100 km or less of receptor points, model results could be much different, and the use of a more realistic area source representation is recommended.

5.4 Visibility Results

To determine the implied impact of the model results on visibility in BNP, the methods described in Section 4.3 were applied. The reference conditions of the December 2000 FLAG report (representing natural background) were used to calculate percent change in light extinction. Reference light extinction for BNP is

$$b_{ext} = 0.6\ f(RH)+14.5\ \ Mm^{-1}$$

where 0.6 represents the contribution of hygroscopic particles and 14.5 Mm^{-1} is the contribution of dry particles and Rayleigh scattering. For the results to be presented here, f(RH) was calculated for each day as the average of hourly f(RH) from measured relative humidity at the BNP monitoring station. The applicable daily f(RH) value was used to calculate both reference extinction and the incremental extinction from model-predicted pollutant concentrations.

5.4.1 Model Results and Observed Extinction

The mean value (average over all days of the year) of extinction due to model-predicted concentrations was 5.08 Mm^{-1} for 1990 and 5.42 Mm^{-1} for 1997. These total modeled impacts represent approximately 33 percent of reference (natural) light extinction. The difference

between results for the two years indicates an increase in extinction of 0.34 Mm^{-1} from 1990 to 1997 (about 2 percent of the clean reference condition).

Measured extinction at the BNP IMPROVE monitoring station was analyzed for the two periods 1989 – 93 and 1994 – 98. All measured extinction coefficients not classified as "invalid" were included in the analysis; i.e. "valid" measurements as well as those possibly including interference or otherwise classified as suspect. The median measured light extinction at BNP for 1989 through 1993 was 52 Mm^{-1}, and for 1994 through 1998 was 61 Mm^{-1}. The "20% cleanest" extinction values for the two periods were 33.9 Mm^{-1} (1989-93) and 36.4 Mm^{-1} (1994-98). These data suggest an increase in extinction between 1989-93 and 1994-98 of approximately 7 to 15 %.

Visual range corresponding to the measured extinction values for 1989-93 is 75 km for the median and 115 km for 20% cleanest conditions. For 1994-98 the measured visual ranges are 64 km and 107 km, respectively. These ranges are lower than those shown in Figure 4-7, which is based on only the highest quality data, generally excluding days of high relative humidity or other measurement interferences.

The measured frequency distributions of b_{ext} at BNP were examined in detail, and the two data periods were compared. The major change between 1989 – 93 and 1994 – 98 appears as an increase in the frequency of b_{ext} values in the range of 40 to 50 Mm^{-1}, and fewer days of $b_{ext} < 40$ Mm^{-1}. The change is consistent with an increase in days of significant visibility degradation, and appears to be a real trend in BNP light extinction. However, whether this trend is a result of local pollution sources, an increase in long-range impacts from distant sources, a change in meteorological conditions, or some combination of the three cannot be determined. The

modeled increase in extinction from sources in the modeling area can account for only a small fraction of the observed change.

5.4.2 Impacts of Mining and Coal Trains

The incremental pollutant contributions from modeled PRB coal mines and coal trains were used to calculate potential visibility impacts using the recommended FLAG procedures. Results are shown in Table 5-8. The mean daily extinction due to coal-related sources at BNP was calculated to be 0.39 Mm^{-1} in 1990 and 0.66 Mm^{-1} in 1997. The increase in model-predicted extinction over this time period was therefore 0.27 Mm^{-1}, or 1.7% of the FLAG reference extinction for BNP. The total coal activity contribution in 1997 was still less than 5% of the reference level, at 4.1%. The coal mine/train fraction of total model-predicted extinction averaged 4.9% in 1990 and 7.7% in 1997. Thus, coal-related visibility impacts were, on the average, a small fraction of total predicted impacts for both years, and were, again on an average basis, lower than the FLAG level of concern.

However, the FLAG criteria for significant visibility degradation are not based upon average impacts, but rather upon the potential for given incremental impacts on any specific days of the year. A five percent impact is considered a level of concern. Though no specific number of days has been identified as a threshold, the implication of FLM guidance is that the 5% level should be exceeded very rarely if at all. The second line of Table 5-8 shows the number of days per year that modeling indicated greater than 5% increase in extinction (relative to FLAG reference) due to coal mine/train emissions. Despite the small average contribution of these sources, use of the FLAG methodology indicates that increased coal production from 1990 to 1997 caused an impact "of concern" at BNP on 34 additional days per year.

TABLE 5-8

MODEL-PREDICTED VISIBILITY IMPACTS OF COAL MINES AND COAL TRAINS

	1990	1997	Change 1997 – 1990
Mean Extinction (Mm^{-1})	0.39	0.66	+0.27
Days per Year of 5% Impact (Relative to FLAG Reference)	49	83	+34
Days per Year of 5% Impact (Relative to Actual BNP Conditions)	5	19	+14

The above results illustrate the stringent criteria imposed by the FLM guidance on visibility impacts. For comparison, the last line of Table 5-8 shows the annual number of days of 5 percent impact by coal mines/trains if the incremental increase in light extinction is compared to the actual measured extinction at BNP in 1990 and 1997 on a day by day basis. Clearly there were few days when actual visibility was reduced by 5 percent or more. It should be emphasized that FLAG guidance does not allow for use of actual extinction as a reference level, nor is that procedure advocated here. The intent of the visibility assessment procedures is to estimate potential degradation with respect to natural, clean conditions. The results in Table 5-8 are intended simply to illustrate the conservative nature of the FLAG criteria. It is apparent that very low pollutant concentrations from distant sources have the potential to create visibility impacts that exceed the stringent FLAG criteria, especially if they are projected to occur on days with high humidity.

5.4.3 Alternative Procedures for Use of Relative Humidity in Visibility Impact Determination

The FLAG procedures for determination of visibility impact from modeling results allow use of two alternative procedures to account for relative humidity effects:

1. Use a constant seasonal or annual value for f(RH), based on historical relative humidity data for the area of concern. For BNP, the annual f(RH) value is 2.6, corresponding to a relative humidity of 79%. The annual f(RH) value is the average f(RH), not the f(RH) value corresponding to average humidity. Because f(RH) is a non-linear function of relative humidity (see Appendix A), the two averages are not the same. In general, the average f(RH) corresponds to a relative humidity higher than the mean relative humidity for a season or year.

2. Determine f(RH) for each hour of the model simulation using observed or model-predicted relative humidity at the receptor location; and then calculate the mean f(RH) for each day from the hourly values. These daily f(RH) data should then be used to calculate <u>both</u> the modeled contribution to light extinction and the reference light extinction for that day.

Note that the reference condition (background) is specified as a combination of hygroscopic and dry particle extinction; i.e., for BNP annual conditions

$$b_{back} = 0.6\ f(RH) + 14.5\ Mm^{-1}$$

When the average f(RH) of 2.6 is applied, this reference extinction is 16.1 Mm^{-1}. But a daily value of f(RH) can be used, in which case the reference extinction varies with humidity, being less on dry days and greater on humid days.

For the visibility results presented in the preceding subsections, the second alternative was used. Since measured relative humidity was available for BNP as part of the meteorological data set, application of those data was viewed as more realistic than use of a constant relative humidity factor. But it is of interest to know whether one alternative tends to predict higher impacts (more days with significant impacts) than the other.

The question was investigated by numerical calculations, and also by mathematical analysis of the equations for calculating percent extinction change. It was found that which alternative predicts lower impacts depends upon the relative contributions of hygroscopic and dry particles.

Results from the two alternatives will in general be different because of the nonlinearity of the f(RH) function. Thus, there will normally be more days in the year when the actual mean f(RH) is below the FLAG reference f(RH), compared to days with mean f(RH) above the

reference value. As a consequence of this fact, alternative (2) results in fewer days of high percent extinction increase when the incremental pollutants are mostly hygroscopic, and alternative (1) gives fewer days of high impact for mainly dry particles.

It can be shown that the combination of hygroscopic and dry particle concentrations for which the two alternatives give identical results is given by

(a) x (d) = (b) x (c)

where

a = 4.125 (SO_4) + 3.870 (NO_3)

b = 4 (OC) + 0.6 (PM10) + 10 (EC) + 10

c = reference hygroscopic extinction coefficient (0.6 for Badlands National Park)

d = reference dry extinction (14.5 for Badlands National Park)

(all units Mm^{-1})

If (a) x (d) is greater than (b) x (c), alternative (2) will predict fewer days of high impact; if (a) x (d) is less than (b) x (c), alternative (1) will predict fewer days of impact exceeding a given level.

The above analysis assumed that relative humidity at the receptor site is statistically independent of predicted pollutant concentrations. The conclusion may not hold if there is a correlation between predicted impacts and relative humidity on the days of those impacts. Thus, results from the two alternatives will depend in general upon both the ratio of hygroscopic to dry particles, and the relationship, if any, between predicted concentrations and relative humidity.