

PM2.5 Modeling Capabilities of CALINE4

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PM_{2.5} Modeling Capabilities of CALINE4
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ABSTRACT

This paper explores the range of CALINE4's PM_{2.5} modeling capabilities by comparing previously collected PM_{2.5} data with CALINE4 predicted values. The PM_{2.5} data were collected to be representative of three receptors adjacent to an intersection in Sacramento, CA. We looked at the predicted concentrations graphed against the observed concentrations; the percentage of points falling within the factor-of-two prediction envelope was expected to be greater or equal to 75%. Data estimated for the receptor located next to the roadway near the ground were closest to observed values. The other two receptors were located near the road (at a higher position from the ground), and further from the roadway, and produced similar results: both did not fall within the 75% factor-of-two envelope. Although greater discrepancies were observed in the data furthest from the emission source, the three receptors combined produced results that fell within the acceptable factor-of-two percentage envelope. A reverse dispersion test was also conducted using observed and calculated emission factors, and although it showed correlations between the observed values and CALINE4 predicted values, it could not conclusively prove that the model is accurate at predicting PM_{2.5} concentrations. Although this study's results suggest that CALINE4 PM_{2.5} predictions may be reasonably close to observed values, the data set used to verify the model was small; therefore, findings should be considered exploratory and additional testing should be conducted.

INTRODUCTION

Combustion processes in gasoline and diesel engines produce a wide variety of particulate matter (PM), and are a significant source of particles with diameters smaller than $2.5\mu\text{m}$ ($\text{PM}_{2.5}$) in urban areas (1). PM exposure can affect human health in a variety of ways, including lung disease, increased cancer risk, and increased risk of cell mutations (1-6). Many studies have shown that $\text{PM}_{2.5}$ is potentially more dangerous to human health than larger particles; therefore the regulation of combustion emissions is necessary to reduce fine particulate exposure (1,4). One way to quantify the impact of vehicular emissions is with the California Line Source Dispersion Model (CALINE). This model was first published as a response to the National Environmental Policy Act of 1969 and was designed as a modeling tool to predict roadside carbon monoxide concentrations given travel and meteorological parameters (7,8). The dispersion and transport elements of CALINE were initially based on a modified form of a Gaussian point source plume (7); the most recent version of this model, CALINE4, has been extended to incorporate lateral plume spreads in addition to thermal turbulence as a result of hot vehicular emissions (8). An option for modeling PM is included in the updated CALINE4, along with the capability to predict nitrogen oxides and conservative pollutants such as carbon monoxide. Although CALINE4 was developed with the capability of predicting PM_{10} concentrations (8), its ability to accurately predict $\text{PM}_{2.5}$ has not been assessed. This paper uses collected $\text{PM}_{2.5}$ data to assess CALINE4's $\text{PM}_{2.5}$ modeling capabilities.

METHODS

The data set used for the $\text{PM}_{2.5}$ validation was prepared for Caltrans by the University of California at Davis (9). The study was conducted in 1994, and includes $\text{PM}_{2.5}$ and PM_{10} samples from the intersection of Florin Road and Stockton Boulevard in Sacramento, CA. The corresponding meteorological data needed for the CALINE4 analysis were also obtained from this study, which included the ambient air temperature, wind velocities, and atmospheric stability (9). A mixing height of 1000m was used in the model, and all particle settling and deposition velocities were assumed to be zero. A full description of sampling methods and meteorological equipment can be found in the original Caltrans report (9).

The $\text{PM}_{2.5}$ data was collected over a 4 day period in increments of 3 to 5 hours; the receptor locations (from the curb) and heights are given in Table 1 below.

TABLE 1 Receptor locations and heights

Receptor Name	X Coordinate from Reference Corner ^a	Y Coordinate from Reference Corner ^a	Height from Roadway
D1	18.0m	19.4m	3m
D1	18.0m	19.4m	9m
D4	74.5m	75.6m	3m

^a The reference corner is the north-west corner of the intersection

In reviewing the data, we discarded 4 sets of observations (out of 14) due to negative or missing emission factors. The vehicular emission rates were calculated using a box model approach, which is described fully in the Caltrans report (9). In summary, the box model is

used to calculate the mass flux of PM_{2.5} across a fixed downwind plane. This downwind flux is obtained by measuring wind speeds and the vertical PM_{2.5} concentration profile, using upwind PM_{2.5} concentrations as background amounts. The emission rate is then calculated as,

$$EF = \frac{3.6 \times v_n \times h_b \times C_p \times \cos(\theta)}{N_0} \quad (1)$$

where,

EF = Emission factor (g/VKT)

v_n = Wind velocity (m/sec)

h_b = Height of the mixing box (m)

C_p = Pollutant concentration ($\mu\text{g}/\text{m}^3$)

N_0 = Number of vehicles per hour

θ = Angle of the wind to the ideal direction (degrees)

3.6 converts the units to g/VKT

A mixing box height of 3m was used in the model, and was estimated using the vertical profile data collected at downwind site D1 (9). The traffic volumes observed for the intersection with corresponding emission factors are shown in Table 2 below.

TABLE 2 Observed emission rates and traffic volumes

Run	Emission Rate (mg/VKT ^a)	Traffic Volume (Vehicles per hour)
1	43.0	3838
2	72.0	4517
3	-	1536
4	67.0	2417
5	142.0	3897
6	42.0	3973
7	54.0	1064
8	73.0	2221
9	-	4093
10	-	4479
11	30.0	1294
12	34.0	1463
13	-	3694
14	10.0	3699

^a milligrams of PM_{2.5} per vehicular kilometer traveled

- indicates missing or discarded emission factors

Missing or discarded emission factors were the result of either missing PM_{2.5} concentrations, or negative emission factors calculated. In the vehicular emission factor calculation, upwind PM_{2.5} concentrations were averaged and used as ambient air PM_{2.5} concentrations; however, these estimated ambient concentrations were sometimes

indistinguishable from the downwind PM_{2.5} concentrations. If the downwind PM_{2.5} concentrations entered into the model are larger than the ambient PM_{2.5} concentrations, negative PM_{2.5} emission factors are calculated. For many sampling periods, the wind velocity was measured at levels < 1m/sec. At these low wind events, stagnant conditions may occur, resulting in the collection of PM_{2.5} above the roadway. If the PM_{2.5} is caught in stagnant conditions, it is not dispersed thoroughly by the wind, and there will not be a clear distinction between PM_{2.5} emitted by vehicles, and PM_{2.5} already present in the atmosphere. These negative emission factors were most likely the result of small wind velocities during the sampling period, causing upwind and downwind PM_{2.5} concentrations to become indistinguishable. Therefore, these negative points were discarded and not used in the following CALINE4 PM_{2.5} analysis.

The box model emission factors were compared to emission factors calculated according to *The Compilation of Air Pollutant Emission Factors*, AP-42, published by the EPA (9). The AP-42 emission factors are shown below in Table 3.

TABLE 3 AP-42 calculated emission factors

Silt Loading (mg/m ²)	Vehicle Weight (tons)	Emission Rate (mg/VKT ^a)
1.6	2.15	12
15	2.15	53
54	2.15	122

^a milligrams of PM_{2.5} per vehicular kilometer traveled

The emission factors from the box model calculations were in a range of 51± 39 mg/VKT, which is a more narrow range than the factors calculated by AP-42. Because the box model emission factors were contained within this smaller range, they were used in all the CALINE4 input calculations. A more detailed comparison between PM_{2.5} and PM₁₀ box model emission factors and AP-42 is shown in the original Caltrans report (9).

EMFAC is another emissions estimation program that is issued by the California Air Resources Board, and emission factors calculated by this program were also compared to the box model results. For the EMFAC calculations, temperatures of 80, 85, and 90°F were used for humidity levels of 30 and 40%. The EMFAC emission rates varied only by speed, and did not vary according to temperatures or humidity change. The EMFAC calculated emission rates are shown in Table 4 below.

Table 4 EMFAC calculated emission factors

Traffic Speed (Miles per Hour)	Emission Rate (mg/VKT ^a)
15	45.98
20	36.66
25	30.45
30	25.48
35	22.37

^a milligrams of PM_{2.5} per vehicular kilometer traveled

The average value for the EMFAC emission rates was approximately 34.6mg/VKT, which is significantly lower than the values calculated through the box model and AP-42 approach. EMFAC is not as accurate in this case because of the very small and specific area (the intersection of Florin Road and Stockton Boulevard) being modeled. No traffic volumes are entered into EMFAC because it uses regional modeling information to estimate the traffic flow for a particular county, or city, in California. Therefore this type of model is best used over larger geographical regions and not on small scale levels, such as an individual intersection.

DATA ANALYSIS

In previous CALINE4 studies, the validation of pollutants such as carbon monoxide and oxides of nitrogen was performed by graphing the predicted versus the observed values and calculating the percentage of the points within a factor-of-two envelope. If at least 75% of the graphed points fell within the envelope, the predicted CALINE4 values were determined to be valid (8). For this analysis, the data were similarly entered into CALINE4, and the results tabulated. Figure 1 shows the predicted versus observed PM_{2.5} concentrations for all three receptors. Roughly 80% of the data are within the factor-of-two envelope.

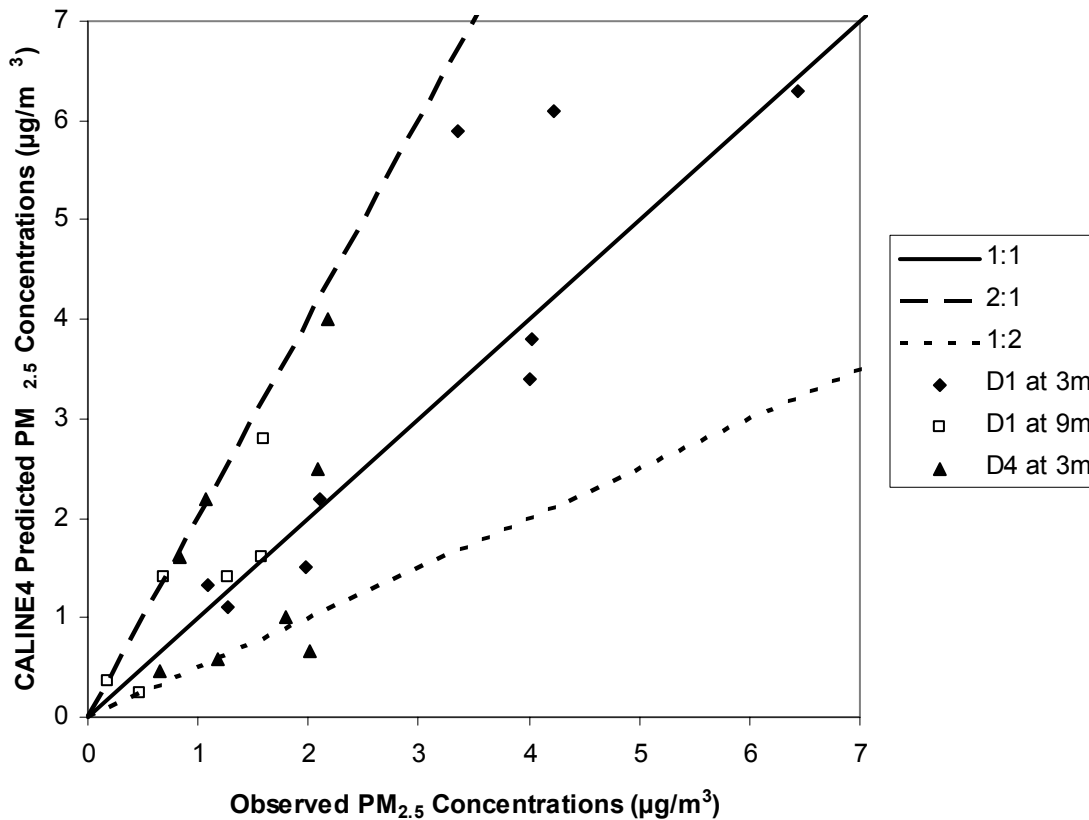


FIGURE 1 CALINE4 predicted PM_{2.5} concentrations vs. observed PM_{2.5} concentrations.

The performance of each individual receptor is shown below in Table 5.

TABLE 5 Percentage within factor-of-two envelope

Receptor	% within envelope
D1 at 3m	100.0
D1 at 9m	66.6
D4 at 3m	66.6

Although 80% overall is considered acceptable, when data are separated not all of the receptors performed as well individually. CALINE4 produced the best estimates for the closest receptor to the roadway positioned at the lowest height (D1 at 3m). This finding is consistent with other CALINE4 studies (8) where predicted concentrations become more accurate as the receptor is closer in proximity to the roadway edge. Predictions were not as close to the receptor D1 at 9m and D4 observed values of PM_{2.5} concentrations. For the D1 values, the errors may be associated with the difficulty in measuring observed PM_{2.5} concentrations at this receptor. The observed concentrations at D1 were small, with most samples being around or below 1.0µg/m³. Because of these small values, this receptor was most affected by low wind speeds, and many data points were excluded due to zero, or negative values. Almost half the sample was eliminated due to zero value concentrations. For the D4 receptor at 3m, 66.6% of the samples fell within the factor-of-two envelope. This receptor was located over 70m from the roadway, which is towards the outer bounds of the recommended maximum CALINE4 prediction area. At distances far from the emission source, wind direction, speed, and variations can greatly influence dispersion. The PM_{2.5} samples collected at D4 may have been influenced by these meteorological factors, any may also have been influenced by emissions from nearby roads and business. The results for D4 are not in the acceptable 75% envelope; however, they are closer than expected given the large distance from the roadway.

To examine the over-predictions and under-predictions of the CALINE4 program, the residuals were plotted for each sample period, shown in Figure 2 below. The residual is equal to the observed PM_{2.5} concentration minus the predicted PM_{2.5} concentration (i.e., a negative residual is the result of a CALINE4 over-prediction).

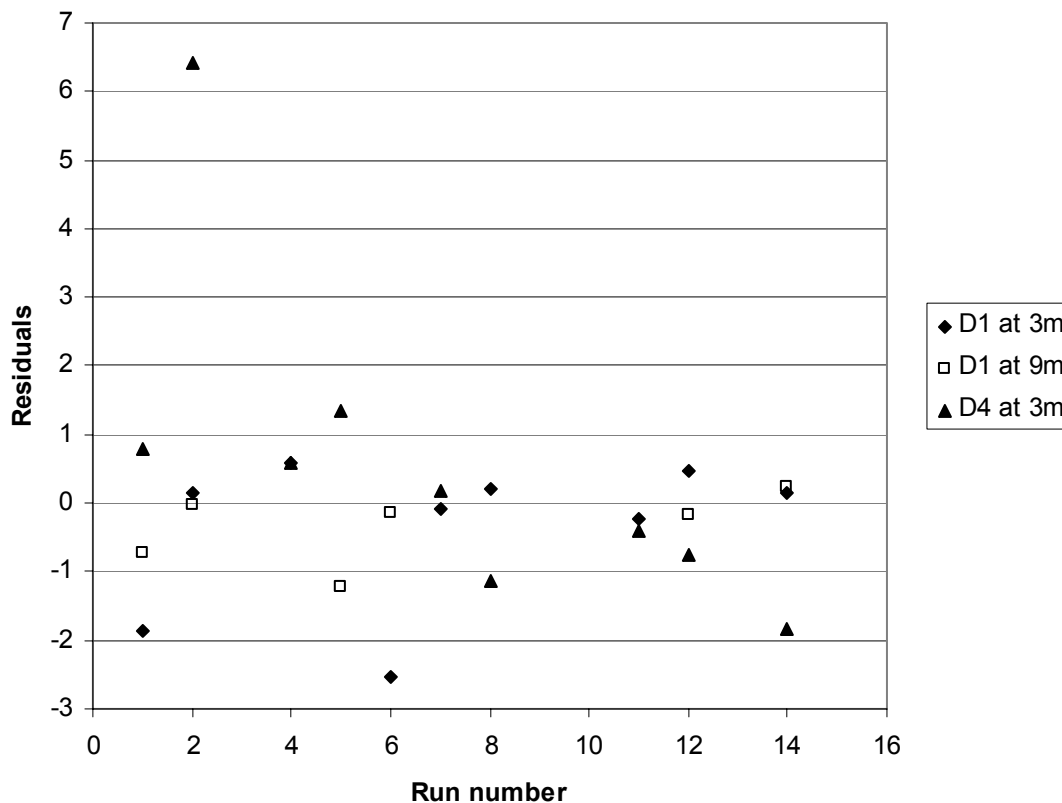


FIGURE 2 PM_{2.5} residuals for the three receptors.

For the closest receptor to the roadway (D1 at 3m), the variation in the residuals is approximately equal, with roughly the same amount of under and over prediction. However, for the same location, but at a greater height (D1 at 9m), CALINE4 over-predicted all but one sample. The range in magnitude for these two receptors was also different. For the receptor closest to the ground, the residuals ranged from 0.5 to $-2.5\mu\text{g}/\text{m}^3$; however, for the higher receptor, the variation was only 0.2 to $-1.2\mu\text{g}/\text{m}^3$. Because the samples at D1 at 9m were few in number and small in concentration, the results from receptor D1 at 9m should be considered only as suggestive. For the receptor located furthest from the roadway (D4 at 9m), the residuals were evenly distributed between over-predictions and under-predictions.

In previous CALINE4 validation experiments (for carbon monoxide and nitrogen oxides), the findings tended to suggest a pattern of larger over-prediction (from 12% to 15%) when compared to the range of under-prediction (from 1% to 7%) (8). This study has a slightly different pattern of findings in that, with the exception of D1 at 9m, CALINE4 predictions appear to be almost equal in terms of both magnitude and number of over and under-predictions. The predictions for receptor D1 at 9m were consistently larger than the observed values at that location, which may be due to other conditions, such as vehicular induced turbulence. Also, according to previous CALINE4 studies (8), as the variability of the wind increases, so should the residuals; however, this pattern is not strongly exhibited in any of the three receptors (Figure 3).

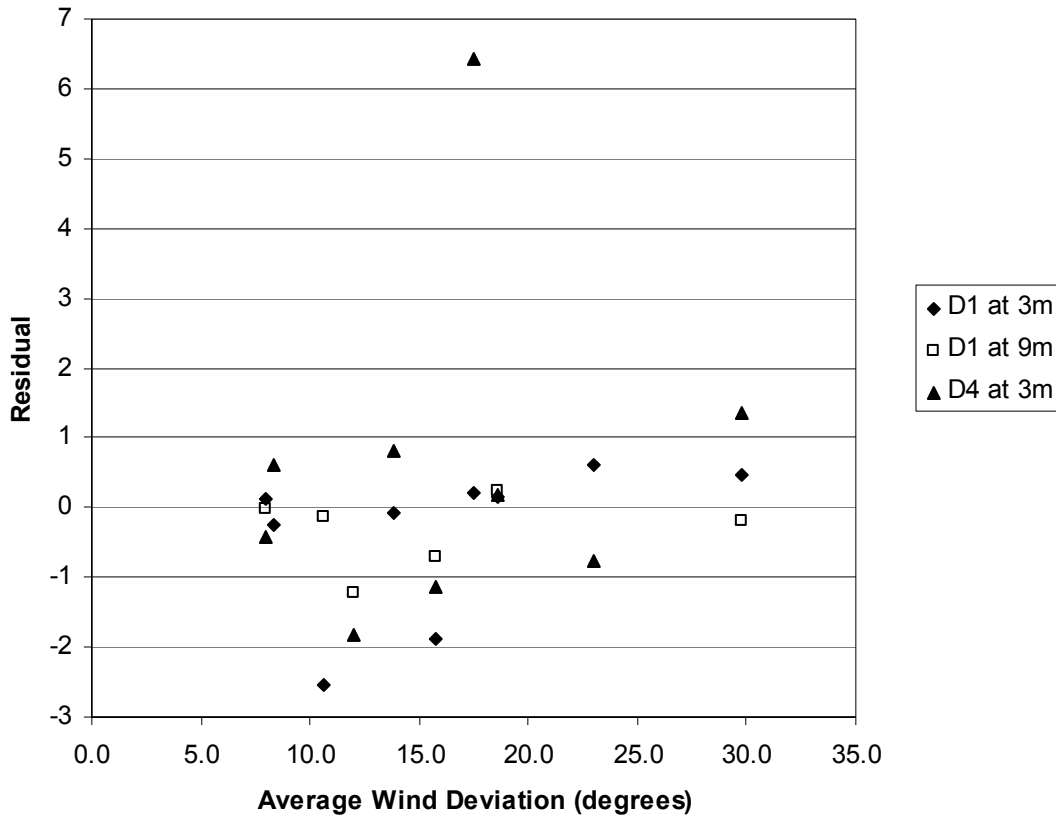


FIGURE 3 PM_{2.5} residuals vs. average wind deviation.

The data set used in this evaluation was small, and it is uncertain if the results obtained would be typical of all PM_{2.5} predictions from CALINE4. Many of the points were discarded because the measured contribution from the roadway to the ambient concentrations was less than or equal to zero. We wanted to find alternate methods of validating CALINE4 PM_{2.5} modeling because of these limitations so we used reverse dispersion to compare observed emission rates (estimated from upwind and downwind mass flux) to emission rates predicted from observed concentrations. Using the observed PM_{2.5} emission factors and the CALINE4 predicted PM_{2.5} concentrations, the CALINE4 dispersion factor was calculated as,

$$DF = \frac{C_c}{EF_{obs}} \quad (2)$$

where,

DF = CALINE4 dispersion factor

C_c = CALINE4 predicted PM_{2.5} concentration

EF_{obs} = Observed emission factor

Each observed PM_{2.5} concentration (at each receptor) was then divided by its corresponding CALINE4 dispersion factor to produce the CALINE4 predicted emission factor.

$$EF_{pred} = \frac{C_{obs}}{DF} \quad (3)$$

where,

EF_{pred} = Emission factor as predicted by CALINE4

C_{obs} = Measured PM_{2.5} concentration

CALINE4 predicted emission factors were calculated for each data point collected, and are shown in Table 6.

TABLE 6 Emission factors predicted from observed incremental concentrations and CALINE4 reverse dispersion

Run	D1 at 3m (g/VMT) ^a	D1 at 9m (g/VMT)	D4 at 3m (g/VMT)
1	0.048	0.034	0.033
2	0.118	0.114	0.097
4	0.127	0.000	0.057
5	-	0.130	0.124
6	0.038	0.061	0.000
7	0.083	0.000	0.156
8	0.124	0.000	0.590
11	0.040	0.000	0.096
12	0.072	0.029	0.180
14	0.018	0.032	0.023

- indicates missing or discarded data

^a milligrams of PM_{2.5} per vehicular kilometer traveled

Using the values in Table 6 with the observed emission rates from Table 2, a two-tailed t-test was performed. The null hypothesis was that the mean of EF_{pred} was equal to EF_{obs} . The resulting means and standard deviations of the emission factors are shown in Table 6.

TABLE 7 T-test for emission factors

	Mean Emission Factor (g/VMT)	Standard Deviation (g/VMT)	Number of Samples (n)
EF_{pred}	0.091	0.110	29
EF_{obs}	0.084	0.056	30

Using the data in Table 7, it was concluded that there is a 74% probability of observing a difference as large as 0.007 g/VMT between the two emission rates when the true difference is zero. Therefore the hypothesis that the predicted emission rates matched the observed emission rates cannot be rejected.

CONCLUSIONS AND DISCUSSION

Although many functions of CALINE4 have been validated, the program's capability to model PM_{2.5} had not yet been assessed. In this study, we used a previously collected PM_{2.5} data set for input into CALINE4, and compared the predicted PM_{2.5} concentrations to the observed data. The results indicated that for areas close to the emission source and near to the ground, CALINE4 will produce PM_{2.5} predictions similar to observed concentrations. However, for points higher from the ground, or further from the emission source, the CALINE4 predicted results decreased in accuracy, and fell outside of the desired factor-of-two prediction envelope. Although each receptor performed differently, combining the results from the receptors indicated a satisfactory overall factor-of-two percentage of approximately 80%. An additional reverse dispersion test was used to compare observed PM_{2.5} emission factors to factors predicted in the CALINE4 model. This additional test suggested close correlation between the observed and predicted data; however, it does not conclusively prove the validity of the CALINE4 PM_{2.5} predictions.

This analysis provides some evidence that CALINE4 can be used to reasonably predict PM_{2.5} concentrations. There are, however, some limitations that require further research. First, the data set used was small, and therefore many of the tests performed have low statistical power. The low number of data limits the overall generalizability of the findings. Second, past CALINE4 validation tests for carbon monoxide and nitrogen oxides occurred under much windier conditions and therefore distinct emissions and ambient air concentrations could be established. However, this data set was sampled under low wind conditions (most < 3m/sec), and as a result it was hard to accurately predict ambient air PM_{2.5} concentrations. On balance, the study results suggest that CALINE4 may be able to reasonably predict PM_{2.5} under conditions near the roadway and close to the ground, but it is recommended that this analysis be rerun with additional, larger, data sets in order to more accurately verify the model.

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RESPONSE TO REVIEWERS

Reviewer 1, Point 1:

“It should mention the measuring methods and the relative accuracy of the measured results.”

Response: A proper citation to the methods of collection for both particulate matter and meteorological conditions is now given on page 2.

Reviewer 1, Point 2:

“It should describe the possible influence of other background sources on the results of the farther away receptors, and how this can influence the confidence on these results.”

Response: Sentences have been added on page 6 to speculate that other nearby traffic sources and meteorological effects would have been the main influences on the further away receptors.

Review 2, Point 1:

“The paper should describe more clearly and in more detail how the emission factors were calculated and how those emission factors compare to MOBILE6.2 or EMFAC emission factors.”

Response: The reviewed draft refers the reader to Ashbaugh (1996) for a complete description of the calculated emission factors; however, additional paragraphs on pages 3, 4, and 5 have now been added in the paper. This addition describes how the box model emission factors were calculated, and how they compare to both AP-42 emission factors, as well as EMFAC emission factors.