HAMPTON UNIVERSITY EASTERN SEABOARD INTERMODAL TRANSPORTATION APPLICATIONS CENTER

FURTHER ANALYSIS OF NO_X AND O_3 DATA, AND THE ACQUISITION, INSTALLATION AND LABORATORY TESTING OF THE PM EQUIPMENT

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FINAL REPORT

ABSTRACT

In the Eastern Seaboard Intermodal Transportation Applications Center at Hampton University, we have started a comprehensive investigation of the emissions around heavily-travelled roadways, shipping channels, airports, and railroads with the purpose of obtaining real time measurements of pollutant concentrations and relating them to real-time weather and traffic information. In the first two cycles of our research program, we built a mobile unit containing a NOx and an ozone analyzer, and a weather station to provide simultaneous measurements of wind speed, wind direction, temperature, and insolation with the concentration measurements. The measured concentrations were compared to the predictions of CALINE4. Considering the effects of $PM_{2.5}$ on public health, for the third research cycle we proposed to include an instrument for the real time measurement of $PM_{2.5}$.

In the last research cycle, as stated below, due to budget constraints, some of the proposed activities could not be undertaken and were replaced by other activities as indicated.

A TEOM 1405-DF dichotomous ambient particulate monitor with a filter dynamics measurement system (FDMS) (Thermo Scientific, Franklin, MA) was purchased, received, set up in the laboratory and tested. To be taken to the measurement locations, this equipment needed to be put on a cart and it needed to be placed in a custom-made outside shelter with an air conditioning and heating unit. Considering the power requirements of the shelter, the PM equipment, O_3 and NO_x analyzers, the computer, and the weather monitoring instruments, a new generator with a higher power rating was, also, needed. Unfortunately, due to the limited funding in the equipment category in the project budget, the hand cart and the outside shelter for the operation of the instrument at the proposed measurement locations could not be purchased in 2011. The outside shelter was received in April 2012. The cart is on order and is not received yet. Recently, the request for the generator was declined by the ESITAC Director making the PM measurements uncertain at this time.

A proposal was submitted to the Virginia Center for Transportation Innovation and Research (VCTIR) to obtain funds for the acquisition of a van suitable for housing all the instrumentation, and for making measurements at any desired location. Although the response was favorable from VCTIR, the approval of the funding could not be finalized until the April of 2012 and the purchase of the van is not expected before fall 2012.

Since the TEOM equipment could not be made functional without the outside shelter, a more powerful generator, and the cart, it was decided to work on improving the data analysis for model validation. The results obtained on NO_2 concentrations could be predicted reasonably well with CALINE4 for upwind receptors, but the difference between predicted and measured concentrations at downwind locations were substantial. Several factors were identified as possible reasons for these discrepancies and these were further investigated.

For this purpose, a new set of data was acquired to evaluate the effect of averaging time on the validity of the model predictions. It was observed that the averaging time did not affect the results significantly. Subsequently, the model variables that are expected to affect the predicted concentrations were investigated by sensitivity analysis.

It was concluded that the only plausible explanations for the observed results seem to be the effect of vegetation between the roadway and the receptors, and the limitation of the CALINE4 reaction scheme.

I. Introduction

In the Eastern Seaboard Intermodal Transportation Applications Center at Hampton University, we have started a comprehensive investigation of the emissions around heavily-travelled roadways, shipping channels, airports, and railroads with the purpose of obtaining real time measurements of pollutant concentrations and relating them to real-time weather and traffic information. In the first two cycles of our research program, we built a mobile unit containing a NOx and an ozone analyzer, and a weather station to provide simultaneous measurements of wind speed, wind direction, temperature, and insolation with the concentration measurements. The measured concentrations were compared to the predictions of CALINE4. Considering the effects of $PM_{2.5}$ on public health, for the third research cycle we proposed to include an instrument for the real time measurement of $PM_{2.5}$. These measurements were expected to provide $PM_{2.5}$ data with superior time and space resolution near roadways, shipping channels, airports, and railroads. This would make it easier to predict the impact of these sources on the air quality in the surrounding areas and plan the placement of buildings that will house sensitive populations such as hospitals, day care centers, retirement and assisted living centers. Also, due to the atmospheric chemistry, it will be more meaningful to measure the particulate matter concentrations simultaneously with NO_x and ozone concentrations with spatial resolution. These simultaneous measurements will enable the use of improved NO_x chemistry for better prediction of the pollutant concentrations by existing models; and will facilitate the validation of the interactive chemistry between the compounds present in the atmosphere.

II. Work Done

In the last research cycle, as stated below, due to budget constraints, some of the proposed activities could not be undertaken and were replaced by other activities as indicated.

1. A TEOM 1405-DF dichotomous ambient particulate monitor with a filter dynamics measurement system (FDMS) (Thermo Scientific, Franklin, MA) was purchased. This equipment is designed to provide long and short term PM concentration measurements for both non-volatile and volatile PM_{10}, $PM_{2.5}$, and PM-coarse (particles between 2.5-10 $\mu g/m^3$) components.

2. The TEOM 1405-DF was received, set up in the laboratory and tested. To be taken to the measurement locations, this equipment needed to be put on a cart and it needed to be held at a moderate temperature interval (46 to 77°F). The manufacturer offers a custom-made outside shelter with an air conditioning and heating unit. This unit by itself requires 2400 W power supply by itself. Considering the power requirements of the PM equipment, O_3 and NO_x analyzers, the computer, and the weather monitoring instruments, it is obvious that the existing generator, which can produce a running power less than 2000 watts, would be inadequate, and a new generator with a higher power rating would be needed. Unfortunately, due to the limited funding in the equipment category in the project budget, the hand cart and the outside shelter for the operation of the instrument at the proposed measurement locations could not be purchased in 2011. The outside shelter was received in April 2012. The cart is on order and is not received yet. Recently, the request for the generator was declined by the ESITAC Director, making the PM measurements uncertain at this time.
3. A proposal was submitted to the Virginia Center for Transportation Innovation and Research (VCTIR) to obtain funds for the acquisition of a van suitable for housing all the instrumentation. Although the response was favorable from VCTIR, the approval of the funding could not be finalized until the April of 2012 and the purchase of the van is not expected before Fall 2012.
4. Since the TEOM equipment could not be made functional without the outside shelter, a more powerful generator, and the cart, it was decided to work on improving the data analysis for model validation.
5. A paper is submitted to the 2nd International Conference on Environmental Pollution and Remediation ICEPR-2012), 28-30, 2012, Montreal, Quebec, Canada. It is accepted for presentation and publication in the proceedings.
6. Three undergraduate engineering students were hired in this research project, providing them the opportunity to have a high quality research experience.

III. <u>TEOM 1405 Setup and Testing</u>

As described above, when the TOEM 1405 could not be operated outside as planned due to lack of equipment funds, it was decided to set up the instrument in the lab to check its operation before the warranty period expires. Chemical Engineering student Avian Lain and Electrical Engineering student LaMarr Hill assisted in the setting up of the TEOM 1405 (Figures 1 and 2). The instrument was operated successfully and subsequently was taken apart to wait for the delivery of the shelter, cart and generator.

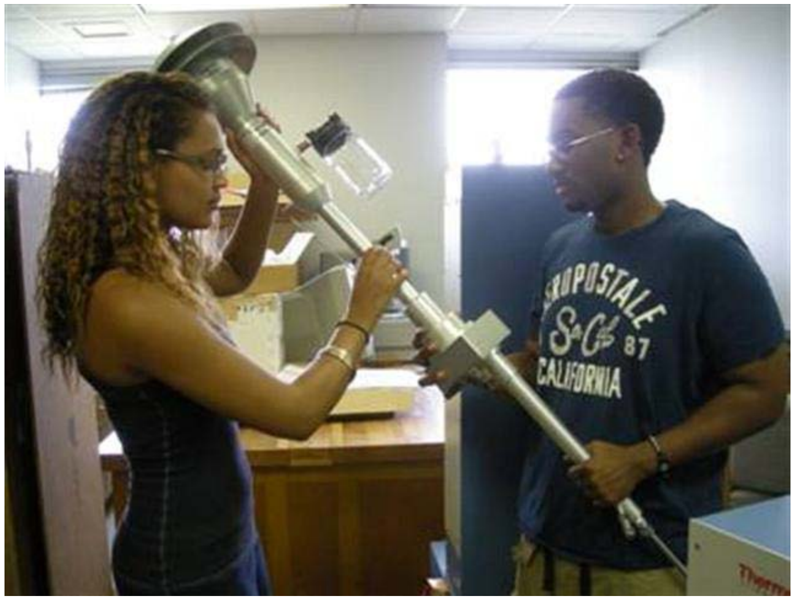

Figure 1. Students Avian Lain and LaMarr Hill installing the sample inlet tube into the section containing the virtual impactor and flow splitter.

Figure 2. Students Avian Lain and LaMarr Hill working on the installation of TEOM 1405.

IV. Further Analysis of NO_x and O_3 Data Obtained in the Previous Research Cycle

IV. i. Summary of Results Obtained in the Previous Research Cycle

The predicted and measured nitrogen dioxide concentrations along with the corresponding values of major variables affecting the results are summarized in Table 1. Wind direction, wind speed, wind direction standard deviation, atmospheric stability, and traffic volume are taken as significant variables. Since the temperature for all experiments were in the upper 20's in °C, temperature was not included in the table. Similarly, other variables such as mixing height and NO_2 photolysis rate constant that are expected to affect the NO_2concentrations were assumed not to differ between measurements and therefore not included in the table. When using CALINE4, 15-minute averages of the weather parameters were used. In most cases the traffic data were obtained before and after all the measurements for a particular day were completed. "Before"data were used for the first two receptors and "after" data were used for the last two. The averages of the "before" and "after" data were used for the two middle receptors.

In Table 1, the wind directions from 355° to 5° and 175° to 185° are considered to represent winds nearly parallel to the roadway as indicated by letter P next to the wind direction. Wind directions from 5° to 175° correspond to cases with receptors (measurement points) are located in downwind positions (indicated by letter D) and the wind directions from 185° to 355° correspond to cases with receptors at upwind positions (indicated by the letter U).

The effect of the traffic volume is through the increased emissions, increased mixing due to mechanical turbulence, and increased vertical thermal dispersion at high vehicle volumes. The last two effects tend to decrease the effect of increased emission.

The effect of wind direction is very significant. When the measurement locations (receptors) are located downwind, the wind creates a plume toward the receptors and carries the emitted and formed species to the receptors. Higher wind speeds create longer and slender plumes, and thus, determine how fast the plume is diluted with the surrounding air. Standard deviation of the wind direction and the atmospheric stability class are also factors determining the dispersion rate.

Nitrogen dioxide concentrations at the receptor locations were observed to be strongly affected by the ambient ozone concentrations. Ozone plays a primary role in the generation of NO_2 from NO. It is also significant in the formation of secondary nitrogen-containing species, thus depleting NO_2. The latter group of reactions is not considered in the estimation of NO_2 by CALINE4.

Table 1 indicates that for most cases with receptors in upwind positions relative to the roadway (wind angles between 5° and 175°), CALINE4 produced concentrations close to the measured ones. When the wind is close to parallel to the roadway (± 5° around 0° and 180°), receptor positions shift frequently between upwind and downwind, producing results that are not very representative of the measurements. At some sampling points located downwind of

Table 1. Summary of results. All concentrations are in ppm, wind direction is in degrees (azimuth measured from north so that 90° indicates wind directly from the east), Wind speed is in m/s, and the traffic count is in vehicles/hour total in both directions.

Run No.	**Pred. NO_2**	**Meas. NO_2**	**Meas. NO_x**	**Meas. O_3**	**wind dir.**	**wind spd**	**st. dev.**	**stability**	**Traffic Volm.**
51910-1	0.17	0.008	0.025	0.02	159.6 D	1.013	19.4	A	4956
51910-2		0.008	0.035	0.005					
52410-1	0.02	0.011	0.048	0.015	104.8 D	0.72	30.8	C	5382
52410-2	0.02	0.009	0.038	0.01	114.2 D	0.628	21.8	C	5540
52410-3	0.02	0.005	0.018	0.015	87.8 D	0.792	42.2	C	5698
52410-4		0.003	0.011	0.016	80.7 D	1.18	38.7		
52510-1	0.137	0.008	0.03	0.019	97.1 D	0.789	38.2	A	5315
52510-2	0.087	0.005	0.025	0.011	111.1 D	0.852	35.2	A	5315
52510-3	0.037	0.005	0.015	0.015	87.9 D	1.21	51.1	A	5034
52510-4	0.027	0.003	0.01	0.014	56.8 D	1.941	35.3	A	5034
52510-5	0.027	0.003	0.008		63.1 D	1.453	37.5	A	4753
52510-6									
52710-1	0.002	0.018	0.045	0.018	209 U	1.22	16.1	B	6654
52710-2		0.018	0.039	0.016	222.2 U	1.938	10.8	B	
52710-3		0.014	0.028	0.014	222.1 U	2.262	7.42	B	
52710-4		0.016	0.026	0.014	225.3 U	2.1	9.29	B	
52710-5		0.016	0.025	0.025	218.9 U	2.023	7.12	B	
60210-1	0.05	0.003	0.007	0.028	228 U	1.654	14.4	A	7041
60210-2		0.002	0.005	0.031					8559

60210-3		0.002	0.007	0.026					6072
60210-4		0.002	0.005	0.026					5281
60310-1	0	0.002	0.004	0.025	239 U	2.09	13.9	C	6246
60310-2		0.002	0.004	0.028	250 U	1.83	21		6246
60310-3		0.002	0.005	0.026	214 U	2.21	18.5		6500
60310-4		0.001	0.004	0.029	223 U	2.16	19.7		6500
60310-5		0.001	0.004	0.029	248 U	2.15	25.9		6754
60310-6		0.002	0.004	0.029					6754
61410-1	0.1	0.003	0.023	0.018	98.7 D	0.82	32.6	A	
61410-2		0.003	0.011	0.021					
61410-3		0.002	0.011	0.015					
61410-4		0.003	0.011	0.014					
61410-5		0.003	0.008	0.015					
61410-6		0.004	0.01	0.025					
61510-1	0.09	0.01	0.038	0.02	114.4 D	0.807	29.7	A	4858
61510-2	0.08	0.01	0.036	0.013	120 D	0.707	20.5	A	4858
61510-3	0.06	0.006	0.018	0.008	118.9 D	0.429	32.6	A	5310
61510-4	0.06	0.006	0.017	0.01	102.5 D	0.633	31.2	A	5310
61510-5	0.05	0.006	0.013	0.011	47.8 D	1.285	36.9	A	5761
61510-6	0.04	0.005	0.009	0.027	83.3 D	1.131	45.8	A	5761
62510-1	0.15	0.015	0.03	0.019	70.5 D	0.753	43.1	A	6837
62510-2	0.11	0.016	0.025	0.017	102.8 D	0.7	40.5	A	6837
62510-3	0.08	0.01	0.015	0.016	95.9 D	1.256	43.7	A	7036
62510-4	0.03	0.007	0.011	0.017	40.1 D	2.063	31	A	7036
62510-5	0.02	0.008	0.012	0.018	39.2 D	2.532	19.6	A	7235
62510-6	0.02	0.007	0.01	0.029	58.5 D	2.44	22.1	A	7235
63010-1	0.01	0.024	0.065	0.012	194.9 U	0.05	41.5	B	6522

63010-2	0	0.019	0.039	0.011					6522
63010-3		0.012	0.024	0.012					6508
63010-4		0.01	0.016	0.015					6508
63010-5		0.008	0.013	0.016					6495
63010-6		0.008	0.014	0.017					6495
70210-1	0.2	0.01	0.023	0.007	147.4 D	0.9	36.1	A	8588
70210-2	0.1	0.009	0.02	0.006	53.6 D	1.58	41.5	A	
70210-3	0.04	0.005	0.01	0.007	28.1 D	2.3	30	A	
70210-4	0.05	0.003	0.006	0.008	65.1 D	2.26	25.3	A	
70210-5	0.02	0.004	0.009	0.008	36.8 D	2.21	25.4	A	
70210-6	0.02	0.004	0.009	0.009	45.7 D	2.7	24.4	A	
70610-1	0.05	0.02	0.031	0.013	201.6 U	0.97	32.5	A	6997
70610-2	0.13	0.034	0.048	0.021	110.4 D	0.7	51.8	A	6997
70610-3	0.03	0.022	0.031	0.015	178.4 P	0.818	54.1	A	6667
70610-4	0.03	0.023	0.032	0.012	160.5 D	1.059	40.7	A	6667
70610-5	0.01	0.021	0.03	0.02	201.7 U	1.982	16.9	A	6894
70610-6	0.01	0.012	0.019	0.033	201.1 U	2.076	12.6	A	6894
70810-1	0.04	0.019	0.056	0.017	89 D	0.682	35.3	B	5847
70810-2	0.03	0.008	0.014	0.02	63.4 D	1.335	34	B	5847
70810-3	0.03	0.008	0.015	0.021	69.8 D	1.165	42.5	B	5596
70810-4	0.03	0.011	0.02	0.022	88.5 D	1.294	41.2	B	5596
70810-5	0.02	0.008	0.013	0.026	69.6 D	1.775	26.4	B	7182
70810-6	0.02	0.007	0.014	0.027	99.6 D	1.719	24.1	B	7182
70910-1	0.14	0.014	0.041	0.026	116.2 D	1.119	18.9	A	6619
70910-2	0.12	0.018	0.037	0.019	113.1 D	0.719	25.1	A	6619
70910-3	0.09	0.009	0.019	0.016	115.3 D	0.86	45.7	A	6900

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70910-4	0.05	0.008	0.016	0.017	69.9 D	1.338	50.3	A	6900
70910-5	0.04	0.007	0.012	0.018	64.9 D	1.544	37.8	A	7358
70910-6	0.02	0.004	0.007	0.022	60 D	2.169	28.8	A	7358
71410-1	0.0	0.005	0.011	0.041	279 U	2.133	23.7	A	7355
71410-2		0.004	0.01	0.042					7355
71410-3		0.004	0.007	0.042					7127
71410-4		0.003	0.006	0.043					7127
71410-5		0.003	0.006	0.042					6898
71410-6		0.003	0.005	0.043					6898
71510-1	0.12	0.041	0.074	0.035	175.9 P	1.293	18.7	A	6196
71510-2	0.12	0.035	0.06	0.041	126.7 D	0.853	39.9	A	6196
71510-3	0.06	0.021	0.033	0.056	143.6 D	0.913	49.4	A	6161
71510-4	0.06	0.016	0.025	0.064	130.1 D	1.088	24.58	A	6161
71510-5	0.04	0.012	0.017	0.069	72.9 D	1.485	32.8	A	6126
71510-6	0.03	0.007	0.012	0.07	111.3 D	1.815	24.6	A	6126

the roadway, predicted values are significantly larger than the measured values. The discrepancy between the measured and predicted values appears to increase as the atmosphere becomes more unstable and as the wind speed decreases. Since the discrepancies at downwind positions are over-predictions and CALINE4 predicts higher concentrations at lower wind speeds the latter observation is expected. The former observation indicates that the actual effect of atmospheric stability may be more significant than predicted by CALINE4 and may reduce the concentrations due to the enhanced dilution of the plume with surrounding air under unstable atmospheric conditions.

There are some limitations in using CALINE4 for the prediction of NO_2 concentrations. CALINE4 gives NO_2 results in increments of 10 ppb and only a few of the measured concentrations are at or above this value. Secondly, the location permitted measurements only up to about 100 meters and for some cases this was not sufficient to obtain accurate background values and this needed the use of extrapolated values in the models. Additionally, for NO_2 predictions, CALINE4 uses a very simple kinetic model involving only three reactions (ozone formation, NO oxidation, and NO_2 photodissociation). Therefore, in comparing the measured concentrations with those predicted by CALINE4, these limitations need to be considered.

CALINE4 was reported to perform best under crosswind conditions with wind speeds greater than 1 m/s. So the over-prediction in our case under these conditions at downwind receptors cannot be easily explained. Considering the complexity of the process, the following reasons for this observation may be suggested:

1. There is a wire fence between receptor positions 1 and 2 with some hedge growth and single line of trees along it. It is possible that this may disrupt the plume extending from the roadway and enhance mixing of the plume contents with the ambient air and reduce the measured concentrations.
2. Since our sampling points were only 1 m above the ground and the roadway is slightly above the measurement points, plume may not reach the sampling points for receptors close to the roadway. Thus, we might not have sampled the gas inside the plume assumed by the CALINE predictions.
3. For measurement sets involving changes in the wind direction and cloud cover, the 15-min average values may not be appropriate because 15 minutes may not be sufficient for the Gaussian distributions assumed by the model to establish. Therefore, use of longer time averages, such as 1-hour averages may be more appropriate for comparison with the model predictions.
4. Formations of secondary nitrogen species except NO_2 are not considered by CALINE4. Therefore the simple reaction mechanism used by CALINE4 may not accurately represent the reactions taking place in the atmosphere.
5. The emission factor calculated by MOVES is based on the local average vehicle mix and may not correspond to the actual mean emission factor that existed during the concentration measurements.
6. The background concentrations used in predictions were taken as the values at a location about 100 m from the roadway median (at the farthest receptor location). At this point, if a steady state concentration value is not reached, extrapolation was used to obtain a rough estimate of the background concentration. Since both ambient NO_x and O_3 concentrations affect the predicted NO_2 concentrations, this could be a source of error in the predictions. Obtaining better background concentration measurements may be difficult due to the limited area available at the current location.
7. Other variables such as deposition velocity and mixing height used for CALINE4 predictions may not accurately represent the actual conditions.

The only way to get more information about the effects mentioned in items 1 and 6 will be to obtain additional measurements at a more suitable location. This will only be possible if all the instruments were installed ia a van and can be taken out of the Hampton University campus. Other items are evaluated further in the following sections.

IV. ii. Effect of Roadway height

To check the validity of the second item given above, CALINE4 was run with different roadway heights at a receptor where significant difference was observed between the measured and predicted NO_2 concentrations. The result is shown in Table 3 below.

Variable	**Variable value**	**Predicted NO_2, ppm**	**Measured NO_2, ppm**
Roadway height	1 m	0.19	0.008
	10 m	0.06	

Although an unrealistically large value was used for the roadway height parameter, the predicted concentration is still about 7 times larger than the measured indicating that suggestion 2 could not have caused the observed result alone.

IV. iii. Effect of averaging period on measured concentrations

CALINE4 is based on the assumption that the concentration distributions in the plume will approximate Gaussian distributions when averaged over time. In our analyses of the NO_x and O_3 data, we had used 15-minute averages of the measured data to compare with CALINE4 predictions. This averaging period might have been too short for comparison with the model estimates. Therefore, we obtained some new data to evaluate the effect of the proper averaging time on the measured concentrations. The results are presented in Table 4.

Table 4. Effect of the averaging time on measured concentrations

15-min avg		**30-min avg**		**45-min avg**		**60-min avg**		**75-min avg**	
NO_2 ppb	**NO_x ppb**	**NO_2 ppb**	**NO_x ppb**	**NO_2 ppb**	**NO_x ppb**	**NO_2 ppb**	**NO_x ppb**	**NO_2 ppb**	**NO_x ppb**
16.42	24.78	18.85	27.52	20.77	29.72	20.87	29.92		
16.66	24.80	16.54	24.79	18.12	26.61	19.74	28.50	20.03	28.90
15.17	22.29	15.91	23.54	16.08	23.96	17.38	25.53	18.82	27.25
13.04	19.38	14.10	20.83	14.96	22.16	15.32	22.81	16.51	24.30

Table 4 shows that the averaging time has some effect on the measured concentrations that are used for comparison with the concentrations predicted by CALINE4; but this effect is not significant enough to explain the observed magnitude of the discrepancies between the measured and predicted concentrations when the receptors are located downwind.

IV. iv. Effect of reaction mechanism and ambient concentrations

A more detailed set of reactions of NO_x in the atmosphere is given below:

1. Nitrogen dioxide formation: $NO + O_3 \rightarrow NO_2 + O_2$

2. Daytime nitric acid formation: $NO_2 + OH + M \rightarrow HNO_3 + M$
3. Ozone formation: $O+O_2+M \rightarrow O_3+M$
4. Photodissociation of NO_2: $NO_2+h\nu \rightarrow NO+O$
5. Nitrate radical formation: $NO_2 + O_3 \rightarrow NO_3 + O_2$
6. Dinitrogen pentoxide formation : $NO_3 + NO_2 + M \leftrightarrow N_2O_5 + M$
7. Nitric acid formation via surface reaction: $N_2O_5 + H_2O$ (surface) $\rightarrow 2HNO_3$
8. Nitrate removal: $NO_3 + NO \rightarrow 2NO_2$
9. Renoxification by surface nitric acid: $NO + HNO_3$ (surface) $\rightarrow NO_2 + HONO$

Only reactions 1, 3, and 4 are considered by CALINE4. The only inputs to CALINE4 that affect the reaction rates are the ambient ozone, NO_2, NO_x concentrations and the photodissociation constant. A sensitivity analysis was performed to test the effects of these variables on the predictions from CALINE4. The results of this sensitivity analysis are presented in Table 5.

Table 5. Effects of ambient concentrations and photodissociation constant on predicted NO_2 concentrations.

Variable	**Variable value, ppm**	**Predicted NO_2, ppm**	**Measured NO_2, ppm**
Ambient O_3 with NO=0.003, NO2=0.003	0.03	0.19	0.008
	0.01	0.19	
	0.3	0.19	
Ambient O_3 with NO=0.03, NO2=0.01,wdir=135	0.3	0.19	
Ambient O_3 with NO=0.05, NO2=0.01,wdir=135	0.3	0.19	
Ambient O_3 with NO=0.05, NO2=0.05,wdir=135	0.3	0.23	
Ambient O_3 with NO=0.05, NO2=0.05,wdir=165	0.1	0.20	
Photolysis rate constant	0.004	0.19	0.008
	0.008	0.19	

The first three rows in Table 5 show no effect of ambient ozone concentration on the predicted NO_2 concentrations. Since CALINE4 may interpret the given low ambient NO and NO_2 concentrations as 0.0, higher values were assigned to them as reported in rows 4, 5, and 6. The only significant effect is observed when ambient NO_2 is increased significantly, but this is mainly due to the additive effect rather than the change in the production rate. Considering that the effect of ambient ozone concentration is most significant at low wind angles, a wind direction of 165° corresponding to a wind angle of about 15° was evaluated. Row 7 indicates that at this wind angle, the ambient ozone concentration has a more significant effect.

The last two rows of Table 5 show that the effect of the photodissociation constant on the predicted concentration under the test conditions is negligible.

All these results indicate that the atmospheric reactions have a slight effect on the CALINE4 predictions under the conditions of the measurement. This is not consistent with the strong correlation that was observed between the concentration of ozone and NO_x compounds during the measurements.

IV. v. Effect of emission factor

Values of the emission factor are obtained from MOVES, which provides these values based on local average vehicle mix. However, the actual value of the emission factor during measurements maybe different from the value provided by MOVES. Therefore, a sensitivity analysis was performed to test the effect of the emission factor on predictions from CALINE4.

Table 6. Effect of emission factor on predicted NO_2 concentration

Variable	Variable value	Predicted NO_2, ppm	Measured NO_2, ppm
Emission factor	1.416	0.19	0.008
	1.0	0.13	
	0.5	0.07	

Table 6 shows that the effect of the emission factor used on the predicted NO2 concentration is significant, even when the emission factor used is reduced threefold, the predicted concentration is still about an order of magnitude larger than the measured value. Therefore, the emission factor used cannot be the sole reason for the observed difference between the measured and predicted values.

IV. vi. Effect of other variables on CALINE4 Predictions

Some other variables that were used in the CALINE4 estimations were varied to show their effect on the predicted concentrations. The results shown in Table 7 indicate that the deposition velocity has the highest impact on the model results, but even a value of 10 predicts a concentration an order of magnitude larger.

Table 7. Effect of various variables that were used as input to CALINE4

Variable	Variable value	Predicted NO_2, ppm	Measured NO_2, ppm
Deposition velocity	0	0.19	0.008
	10	0.08	
Mixing zone width	34	0.19	0.008
	50	0.15	
Mixing Height	1000	0.19	0.008
	500	0.19	

Altitude	6	0.19	0.008
	2	0.19	

V. <u>Conclusions</u>

From the results and discussions above, it is observed that the only variable that can produce predictions close to measured concentrations at downwind receptor locations is the wind direction, but this change will have to put the downwind locations upwind and upwind locations downwind, which would create discrepancies at the upwind receptors. Therefore, the only plausible explanations seem to be the effect of vegetation between the roadway and the receptors (suggestion 1) and the limitation of the CALINE4 reaction scheme (suggestion 4), or a combination of several of the above factors..

VI. <u>Students</u>

Three undergraduate engineering students were hired in this research project, providing them the opportunity to have a high quality research experience. Those students are Ms. Avian Lain, a chemical engineering sophomore, Mr. Ervin Woodfork, a chemical engineering sophomore, and Mr. LaMarr Hill, an electrical engineering junior. The students were trained in the areas of research planning, equipment use, data collection and acquisition. These students are involved in the research projects hands-on, contributing to the setup, calibration, and operation of the analyzers used. Specifically, they worked on the setup, calibration, and operation of the PM analyzer. They participated in the NO_x and ozone measurements for longer time periods, and obtained the traffic volume using the cameras on I-64.

VII. <u>Presentations/Publications</u>

A paper is submitted to the 2nd International Conference on Environmental Pollution and Remediation ICEPR-2012), 28-30, 2012, Montreal, Quebec, Canada. It is accepted for presentation and publication in the proceedings.