Predicting Near-Road $PM_{2.5}$ Concentrations: A Comparative Assessment of CALINE4, CAL3QHC and AERMOD

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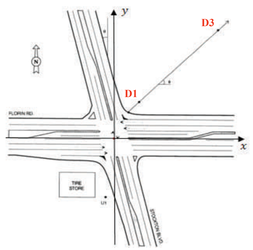
ABSTRACT

Accurately predicting near-road $PM_{2.5}$ concentrations is important for project level transportation conformity and health risk analysis. This study assessed the capability and performance of three dispersion models, CALINE4, CAL3QHC, and AERMOD, in predicting near-road $PM_{2.5}$ concentrations. An intersection in Sacramento, California and a busy road in London, United Kingdom were used as sampling sites to evaluate how model predictions differed from observed $PM_{2.5}$ concentrations. Screen plots and statistical analyses indicated that, at the Sacramento site, CALINE4 and CAL3QHC performed moderately well, while AERMOD under-predicted $PM_{2.5}$ concentrations. For the London site, both CALINE4 and CAL3QHC resulted in *over-predictions* when incremental concentrations due to on-road emission sources were low, while *under-predictions* occurred when incremental concentrations were high. The street canyon effect and receptor location likely contributed to the relatively poor performance of the models at the London site.

STUDY AREAS

For scale: Nearest receptors are approximately 15 m from the road centerline in both cases.

Sacramento Site
Intersection at Florin Rd and Stockton Blvd



There are three receptors: two at location D1 with heights of 3m and 9m, respectively; one at D3 with a height of 3m. In the above reference frame, the (x, y) coordinates of D1 and D3 are (18.3m, 19.4m) and (74.5m, 75.6m). Measurements obtained using a single IMPROVE module (see http://aqp.engr.ucdavis.edu/Documents/1996-Ashbaugh-UCDCaltrans.pdf for details).

London Site
Marylebone Road, London, UK

There is one receptor: the receptor's coordinates in the above reference frame are (0, -13.5m); the height of the receptor is 3m. Measurements obtained using a two tapered-element oscillating microbalance (TEOM) (see Using CALINE Dispersion to Assess Vehicular $PM_{2.5}$ Emissions by Yura et al., 2007).

DISPERSION MODEL DESCRIPTIONS

- **CALINE4** was developed by the California Department of Transportation (Caltrans); It predicts pollutant concentrations for receptors located within 500 meters of the roadway. It models concentrations at a point with coordinates (x, y, z) based on the Gaussian equation:

$$C(x,y,z) = \frac{q}{2\pi u \sigma_y \sigma_z}\left\{\exp\left[\frac{-(z-H)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z+H)^2}{2\sigma_z^2}\right]\right\}\int_{y_1}^{y_2} \exp\left(\frac{-y^2}{2\sigma_y^2}\right) dy$$

- **CAL3QHC** was developed by the U.S. EPA; it is also a Gaussian-based model and was designed to consider vehicular queues at signalized intersections.
- **AERMOD** is also a Gaussian-based model; it was developed by the U.S. EPA and the American Meteorological Society. AERMOD is the EPA-recommended model for evaluating the dispersion of inert pollutants from point, area and line sources under short-range, steady-state conditions.

COMPARATIVE ANALYSES

Data Requirements

	CALINE4	CAL3QHC	AERMOD
Vehicle-Related Data			
Traffic Volume	√	√	√
Emission Factor	√	√	√
Average Total Signal Cycle Length		■	
Average Red Total Signal Cycle Length		■	
Clearance Lost Time		■	
Approach Volume on the Queue Link		■	
Idle Emission Factor		■	
Saturation Flow Rate		■	
Arrival Rate		■	
Meteorological Data			
Wind Speed	√	√	√
Wind Direction	√	√	√
Wind Direction Variation	√	Δ	
Dry Bulb Temperature	√	√	√
Wet Bulb Temperature			^
Dew-Point Temperature			Δ
Atmospheric Stability Class	√	√	
Surface Roughness	√	√	√
Midday Albedo			√
Daytime Bowen Ratio			√
Total/Opaque Sky Cover			√
Sky Cover at layer 1,2,3,4			Δ
Relative Humidity			Δ
Precipitation Amount			Δ
Precipitation Type			Δ
Horizontal Visibility			Δ
Cloud Type			Δ
Sea Level Pressure			Δ
Station Pressure			Δ
Upper Air Sounding			√
Other Data			
Source Height	√	√	√
Mixing Zone Width	√	√	√
Link Geometry	√	√	√
Receptor Coordinates	√	√	√
Settling Velocity	√	√	
Deposition Velocity	√	√	
Longitude and Latitude			√

√ : required input;
Δ : optional input;
■ : required for CAL3QHC's queue algorithm.

Difference Patterns

Basic Statistics: AERMOD Under-Performed Other Models

D_{ij} = modeled concentration - observed concentration (i = model ID; j = sample ID) in ug/m³

	D_{ij}			$\lvert D_{ij}\rvert$		D_{ij}^2	
	Sum	Min	Max	Sum	Average	Sum	Average
Sacramento Site (Sample Size = 29)							
CALINE4	-3.0	-1.5	2.3	18.2	0.628	20.6	0.710
CAL3QHC	-8.3	-5.1	1.2	21.3	0.734	40.5	1.397
AERMOD	-27.4	-8.1	0.8	34.3	1.182	106.4	3.668
London Site (Sample Size = 253)							
CALINE4	-74.9	-11.7	16.6	532.5	2.105	2790.0	11.028
CAL3QHC	20.9	-10.8	10.3	522.5	2.065	2331.7	9.216

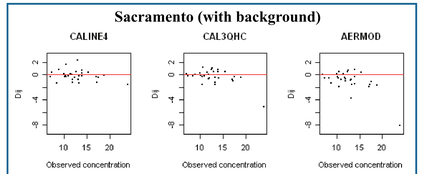
Note: AERMOD was run for Sacramento using detailed local meteorological inputs; AERMOD was not used for the London site due to limited available meteorological data.
As D_{ij} approaches zero, model performance improves. AERMOD did not perform as well as other models.

Portion of Sample Under, Correctly, or Over-Predicted

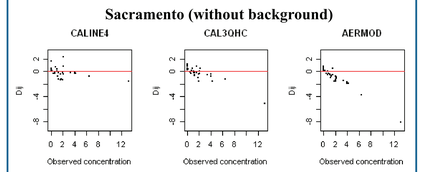
	Sacramento (N = 29)			London (N = 253)		
	$D_{ij} < 0$	$D_{ij} = 0$	$D_{ij} > 0$	$D_{ij} < 0$	$D_{ij} = 0$	$D_{ij} > 0$
CALINE4	18	0	11	140	11	102
CAL3QHC	17	0	12	116	6	131
AERMOD	21	0	8	n/a	n/a	n/a

D_{ij} less than zero indicates under-predicting concentrations. Number counts of positive versus negative D_{ij} suggest a higher number of under-predicted (D_{ij}<0) than over-predicted samples (D_{ij}>0).

Sacramento (with background)

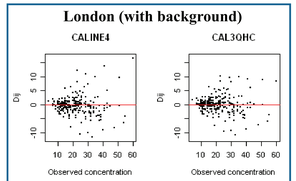


Sacramento (without background)

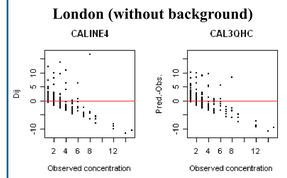


D_{ij} less than zero indicates under-estimation based on the model results; for the Sacramento site (without background), AERMOD produced more under-predictions.

London (with background)



London (without background)



Under-prediction by CALINE4 and CAL3QHC tended to increase with concentrations for the London Site.

Statistical Tests

Test Results for Under- and Over-Prediction Bias

(a) Sacramento Case (N = 29)

	T^*	p-value	Conclusion
CALINE4	-0.6643	0.512	Unbiased
CAL3QHC	-1.3281	0.195	Unbiased
AERMOD	-3.0004	0.0056	**Under-Predict**

One-sample t-test: for the Sacramento case, model results from CALINE4 and CAL3QHC were not biased, while AERMOD under-predicted observed concentrations.

(b) London Case

	Category 1 (N = 74)			Category 2 (N = 58)		
	T^*	p-value	Conclusion	T^*	p-value	
CALINE4	5.353	<0.0001	**Over-Pred**	1.354	0.181	
CAL3QHC	7.236	<0.0001	**Over-Pred**	2.998	0.004	
	Category 3 (N = 53)			Category 4 (N = 68)		
CALINE4	-0.302	0.764	Unbiased	-5.192	<0.0001	
CAL3QHC	0.761	0.450	Unbiased	-5.461	<0.0001	

One-sample t-test using four categories: Category 1 (increment concentration = 1 μg/m³), Category 2 (increment concentration=2 μg/m³), Category 3 (increment concentration = 3 μg/m³), Category 4 (increment concentration > 3 μg/m³). The test statistics suggest that both CALINE4 and CAL3QHC over-predicted for low increment concentrations and under-predicted for high increment concentrations.

Test Results to Assess Bias as Concentrations Increased

	With background			Without background		
	Est. slope	p-value	Conclusion	Est. slope	p-value	
Sacramento site (N = 29)						
CALINE4	-0.062	0.167	$D_{ij} \rightarrow$	-0.131	0.03	
CAL3QHC	-0.176	0.002	$D_{ij} \downarrow$	-0.396	<0.0001	
AERMOD	-0.287	0.0004	$D_{ij} \downarrow$	-0.628	<0.0001	
London site (N = 253)						
CALINE4	-0.005	0.794	$D_{ij} \rightarrow$	-0.806	<0.0001	
CAL3QHC	-0.019	0.319	$D_{ij} \rightarrow$	-0.816	<0.0001	

We tested the statistical significance of the trend that model <u>under-prediction increases with increased concentration</u> (D_{ij} decreases with increasing increment concentrations):

- **$D_{ij} \rightarrow$ means D_{ij} was similar for different observed concentrations;**
- **$D_{ij} \downarrow$ means D_{ij} became smaller when the observed concentration became larger (model under-prediction increases as concentrations increase).**

CONCLUSIONS

- In the Sacramento case, model results paired in space and time from CALINE4 and CAL3QHC matched the observed concentrations moderately well, while AERMOD tended to under-predict near-road $PM_{2.5}$ concentrations.
- In the London case, model results paired in time from CALINE4 and CAL3QHC did not match the observed concentrations well.
- CALINE4 and CAL3QHC produced concentration estimates that were not statistically different; for the Sacramento site, the predicted concentrations from AERMOD were significantly lower than those provided by CALINE4 or CAL3QHC.
- AERMOD allowed for greater resolution in replicating atmospheric conditions; however, it required more meteorological data, some of which was unavailable.
- The monitoring data available for this study (only one location in the London case and two locations in the Sacramento case) enabled us to complete an exploratory assessment but limited our ability to explore how well each model addressed spatial variations in concentrations. Further research is needed to examine model performance at various near-road distances.

Acknowledgements

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