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Performance Evaluation of AERMOD and CALPUFF Air Dispersion Models in Industrial Complex Area

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ABSTRACT: AERMOD and CALPUFF air dispersion models were evaluated for their performance in predicting nitrogen dioxide (NO_2) and sulfur dioxide (SO_2) in Maptaphut industrial area in Thailand. Emission data were obtained from 292 point sources in the study domain. Modeled results were compared with those measured data from 10 receptor sites. Evaluation of model performance was carried out by using statistical analysis. Overall results revealed that AERMOD provided more accurate results than CALPUFF model for both NO_2 and SO_2 predictions. As for the highest value, results from robust highest concentration analysis indicated that AERMOD had better performance in predicting extreme high-end concentration than CALPUFF.

KEYWORDS: AERMOD, CALPUFF, air dispersion, Maptaphut

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Introduction

Air pollution is an important issue to which people have paid considerable attention. Air pollution can pose risks to both public health and welfare. Economic growth typically increases fuel consumption to support human-related activities that induce more emissions into the atmosphere. In Thailand, a large number of power plants and industrial facilities are present and the industrial growth continues.[1] Energy consumption in industrial facilities has accounted for more than half of the total national fuel consumption. Industrial facilities in Thailand have a relatively large contribution to total national emissions for some emission species (eg, 30%–50% for NO_x and over 90% for SO_2).[2]

Oxides of nitrogen (NO_x) are a very interesting and important family of air-polluting chemical compounds. NO_x represent a family of seven compounds. However, Environmental Protection Agency (EPA) regulates only nitrogen dioxide (NO_2) as a surrogate for this family of compounds because it is the most prevalent form of NO_x in the atmosphere that is generated by anthropogenic activities. NO_2 is not only an important air pollutant by itself but also reacts in the atmosphere to form the tropospheric ozone (O_3) and acid rain.[3]

The chemical mechanism of NO_x (NO and NO_2) formation during combustion results from hundreds of elementary chemical reactions. Depending on the temperature range, stoichiometric ratio, and type of nitrous species present in the combustion zone, it is possible to distinguish predominant groups of chemical reactions, which are called the mechanisms of nitrogen oxide formation. Usually, the type of flame determines the conditions of the predominant mechanism of NO_x formation.[4]

Sulfur dioxide (SO_2) is one of a group of highly reactive gases known as "oxides of sulfur." The largest sources of SO_2 emissions are from fossil fuel combustion at power plants and other industrial facilities. Smaller sources of SO_2 emissions include industrial processes such as extracting metal from ore and the burning of high sulfur-containing fuels by locomotives, large ships, and road equipment. SO_2 is also linked with a number of adverse effects on the respiratory system.[5]

The Maptaphut industrial area (MIA) was established in 1988 as part of the economic policy of the Thai government to develop the eastern seaboard. The Industrial Estate Authority of Thailand (IEAT), a state enterprise under the Ministry of Industry, was assigned by the government to implement this policy. Currently, the MIA serves as a significant manufacturing base for petrochemical, chemical, iron, and metal, as well refineries.[6] In order to support air quality management in this area, the Thai government declared the MIA as a pollution-controlled zone in 2009. This designation requires the IEAT and entrepreneurs to seek for proper measures to limit and control emissions to the environment. NO_2 and SO_2 are air pollutants required by the government for consideration when assessing the impacts of an industrial facility in order to acquire a permit for operation in this pollution-controlled zone. Furthermore, they are also the parameters that are required to be assessed when planning for future expansion of industrial activities in the MIA.

The government has encouraged the study of air emissions assimilative capacity using air dispersion model in this area. Efforts have been made to assess the status of air quality using both direct measurement and predicted data from air quality model. Evaluation of assimilative capacity of air pollution in this area can assist in area-based management of pollution problems together with individual emission source control through the implementation of emission standards.

In Thailand, AERMOD and CALPUFF air dispersion models are regulated as preferred models for an environmental impact assessment (EIA) process. In Maptaphut area, AERMOD had been utilized by several studies. Chusai et al[7] used AERMOD to evaluate dispersion of NO_2 and SO_2 and relative roles of emission sources over this area. This study reported that predicted data of both pollutants were underestimated when compared with those observed data. Results also indicated that petrochemical industry played the major contribution in annual average area-wide concentrations of NO_2 and SO_2 in this area. A study of AERMOD tiering approach for NO_2 prediction in this industrial area was conducted by Tunlathorntham and Thepanondh.[8] Three methods were tested for their performance in modeling NO_2 concentrations (Tier I: total conversion of NO_x to NO_2; Tier II: NO_2/NO_x ratio of 0.60; and Tier III: ambient O_3 concentrations were used for calculation using the plume volume molar ratio method). The results indicated that Tier I provided less bias with those measured data as compared with other tiers. It also performed very well in predicting the extreme end of NO_2 concentrations. This study recommended that Tier I was an appropriate method for the prediction of the annual average as well as in determining the maximum ground-level concentration of NO_2 in the MIA.

However, with regard to the uncertainties of the dispersion models, it is quite important to evaluate the performance of the model before being used in a specific site. This study is intended to evaluate the performance of these air dispersion models by comparing model predictions with field measurements in predicting NO_2 and SO_2 concentrations. Two years of monitored data from 10 receptor sites in the study area were used for intensive evaluations of model performances. This study provides useful information and example of the procedure to identify the model performance prior to being utilized for further management of air pollutions.

Materials and Methods

Study area. MIA is the biggest petrochemical-based industrial estate in Thailand, which is located in Rayong province, East of Thailand. This industrial estate is located at a latitude of 13′16″N and longitude of 100′93″E. This is an area potentially affected by air pollution problems including particulate matter and volatile organic compounds, especially, nitrogen dioxide (NO_2) and sulfur dioxide (SO_2) that are the main pollutants of this area.

Air dispersion model. AERMOD (AMS/EPA Regulatory Model) is relatively a recent model developed by the American Meteorology Society (AMS) and United States Environmental Protection Agency (US EPA) for regulatory purposes. AERMOD is a steady-state model that assumes that a plume of emissions disperse in the horizontal and vertical directions resulting in Gaussian (ie, bell shaped) concentration distributions. The concentration algorithm of AERMOD considers the effects of vertical variation of wind, temperature, and turbulence profiles. These profiles are represented by equivalent values constructed by averaging these values over the planetary boundary layer through which the plume material travels directly from the source to the receptor.[9] It is recommended by the US EPA for examining the effects of sources on receptor that are generally within 50 km of the source.[10]

Two preprocessors, AERMAP and AERMET, are required in order to run AERMOD. AERMAP is a terrain preprocessor that characterizes the terrain and generates receptor grids, discrete receptors, and elevation for AERMOD. Note that in AERMOD, when specifying discrete receptors, it is necessary to specify the position of a source relative to the receptor is assigned.[11] Gridded terrain data are used to calculate a representative terrain-influenced height (hc), associated with each receptor location, and to calculate the dividing streamline height. The gridded data needed by AERMAP is selected from digital elevation model (DEM) data. The elevation for each specified receptor is automatically assigned through AERMAP. For each receptor, AERMAP passes the following information to AERMOD: the receptor's location (xr, yr), its height above mean sea level (zr), and the receptor-specific terrain height scale (hc).[12]

CALPUFF (California Puff Model) was developed by Sigma Research Corporation (currently part of Earth Tech, Inc.) sponsored by California Air Research Board. CALPUFF is an atmospheric source–receptor model recommended by the US EPA for use on a case-by-case basis in complex terrain and wind conditions.[13] CALPUFF is a multilayer, multispecies, nonsteady-state Lagrangian puff dispersion model. Dispersion is simulated for discrete "puffs" of species emitted from modeled sources. The puffs are tracked until they have left the modeling domain while calculating dispersion, transformation, and removal along the way.[10] A puff model releases emissions periodically.[14] CALPUFF is intended for use on modeling domains from tens of meters to hundreds of kilometers from a source.

The CALMET model used for generating meteorological input data for the CALPUFF model calculates hourly wind and temperature fields on a three-dimensional (3D) gridded modeling domain. In addition, it produces mixing height, surface characteristics, and dispersion properties.[15]

Emission quantities and CALMET outputs are the input data into the CALPUFF model. Finally, the CALPOST program is a postprocessor for results from CALPUFF simulations.[16]

Data collection. The surface and upper air data were obtained from simulations of MM5 meteorological modeling for the years 2012 and 2013. Meteorological data contained hourly wind speeds, temperature, cloud covers, ceiling heights, surface pressures, and relative humidity. Ambient air quality data in this analysis were obtained from Pollution Control Department, Maptaphut Industrial Estate (IEAT), and BLCP Power Plant. Totally, there were 10 air-monitoring stations located in the surrounding area of the industrial complex whose data were collected on an hourly basis used in this study. These stations are generally located in the community area objected to evaluate health impact possibly caused by industrial emission. As for quality control of data, all the analyzer from every stations were daily calibrated by standard gas following the guideline of the ambient air-monitoring station designated by the Pollution Control Department of Thailand.

Oxides of nitrogen (NO_x) and sulfur dioxide (SO_2) emission data of each stack were obtained from the Office of Natural Resource and Environment Policy and Planning of Thailand. These data were reported by each factory for the process of EIA and were used as emission limit for each individual emission sources during its operation period. Totally, there were 292 stack sources with the height of stacks ranging from 3 to 200 m. Total emissions of NO_x and SO_2 used as input data in this study were 2,021 and 2,025 g/second, respectively (Fig. 1).

Model configuration. Air pollutant concentrations were calculated in one-hour period on elevated terrain height and urban area option. Data periods read from meteorological data files started from the first hour in January 1, 2012, to the 24th hour in December 31, 2013. The gridded data needed by AERMET and CALMET were selected from DEM data, and the terrain data were collected during the Shuttle Radar Topography Mission (SRTM3).

Domain site of AERMOD and CALPUFF was designed for a radius of 10 km with the finest grid resolution being 500 × 500 m. Meteorological data were simulated from the NCAR MM5 (fifth-generation mesoscale model) prognostic meteorological model for this study area. The domain size was 50 × 50 km with a grid resolution of 4 km was used in MM5 simulation. The surface and profile meteorological data were the default of AERMET format from MM5-preprocessed meteorological data. As for CALPUFF, the meteorological data were the default of CALMET format from MM5-preprocessed meteorological data.

Performance evaluation. Numerous steps have been taken to ensure that the best model is properly used for each regulatory application and that the model is not arbitrarily imposed. Two types of performance measures are identified: (1) measures of difference and (2) measures of correlation.

Measures of difference represent a quantitative estimate of the size of the differences between predicted and observed values. Measures of correlation indicate quantitative measures of the association between predicted and observed values.[17]

In this study, model performance was evaluated using several statistical measures. They were observed mean (Omean), predicted/modeled mean (Pmean), observed standard deviation/sigma (Ostd), predicted/modeled standard deviation/sigma (Pstd), root mean square error (RMSE), index of agreement, fractional bias (Fb), fractional variance (Fs), and the robust highest concentration (RHC). The performances

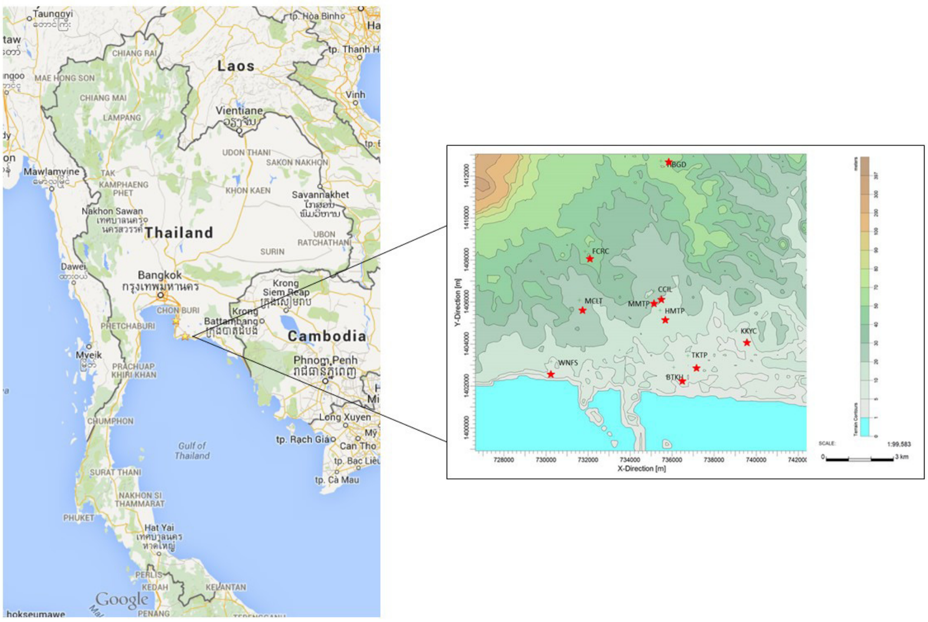

Figure 1. Location of air quality monitoring stations.

of the AERMOD and CALPUFF were tested by comparing the predicted pollutant concentrations of SO_2 and NO_x with those measured actual values (hourly mean concentrations) at 10 ambient air quality stations. Comparisons were performed by characterizing the bias. For this purpose, three metrics relating to the bias, the mean bias (eg, the mean difference between the modeled and the observed data), the RMSE, and the fractional bias (Fb), were chosen. Mean value was selected in this study due to normal distribution characteristic of the data. The mean bias is easily understood and preserved the sign of bias. The RMSE is a measure of the deviations from the 1:1 relationship and preserves the scale of the original measurements. It is derived from the mean square error that comprised bias (the extent of over- or underestimation) and variance (precision).[18] The fractional bias is presented because it is the statistic recommended by US EPA. Fractional bias is symmetrical and bounded with values ranging between +2 (extreme underprediction) and −2 (extreme overprediction). The US EPA guidance for selecting the best performing air dispersion model[19] stated that although a completely objective basis for choosing a minimum level of performance was lacking, accumulating results from a number of model evaluation studies suggested that a factor of two is a reasonable performance target a model should achieve before it is used for refined regulatory analysis. The guidance goes on to recommend the fractional bias as a screening tool for evaluating whether a model should be eliminated from consideration. The fractional variance (Fs) is also presented in the model evaluation in this study. The RHC is preferred to the actual peak value and represents a rounded estimate of the highest concentrations, based on a tail exponential fit to the upper end of the distribution. With this procedure, the effect of extreme values on model comparison is reduced.[20]

Results and Discussion

Nitrogen dioxide. In this study, full conversion of NO_x to NO_2 (100% conversion) was used as an assumption for NO_2 prediction taking into consideration the result from the previous study by Tunlathorntham and Thepanondh.[8] Hourly emission characteristics for point source were used in AERMOD and CALPUFF air dispersion model. The model was simulated covering the years 2012 and 2013. The hourly average ambient ground-level concentrations of nitrogen dioxide at each of the monitoring sites were computed, and the results were compared with those measured data. Statistical evaluations of model performances for NO_2 prediction are presented in Table 1.

Generally, both models provided quite similar results in predicting average concentrations of NO_2 (41.0 and 40.2 μg/m^3 for AERMOD and CALPUFF, respectively). These results agreed with the average concentration from observed data (39.8 μg/m^3). There were differences between the model and observed values. However, these differences were much lower than their respective standard deviations (sigma) (RMSE < standard deviation), indicating that skill was being shown by both models. Generally, AERMOD performed well for the prediction of the average concentration at every monitoring site, at least to within the accuracy of the observations (standard deviation) except at TKTP and CCIL. The fractional bias (Fb) and fractional variance (Fs) varied between −2 and 2, with a negative value indicating overprediction and good performance indicated by a value close to zero. The maximum Fb and Fs were found for simulated data at CCIL station (Fb = −1.08) and KKYC station (Fs = 1.38). This poor agreement might result from missing of monitored data. The best model performances were found at BTKH (Fb = 0.05) and HBGD stations (Fs = −0.02), respectively.

RMSE is an estimator of the overall deviations between the observed and predicted values. Smaller values of RMSE indicate a better performance, and it is not biased toward models that overpredict or underpredict. In this study, AERMOD were in good agreement with ambient air concentrations of NO_2 than CALPUFF at all monitoring stations.

The quantile–quantile (Q–Q) plots for each model and field study are developed from the ranked and paired distributions of observations and predictions. The sorted predicted concentrations were plotted against the sorted observed values (independent of time) using a Q–Q plot diagram in order to examine the model bias over the concentration distribution. Comparisons of modeled and observed NO_2 concentrations at each site are presented in Figure 2.

Q–Q plots were prepared using the model predicted and observed values of the NO_2 concentrations. The Q–Q diagram indicated that AERMOD performed quiet well and provided high correlations with the observed NO_2 concentrations than CALPUFF for all monitoring stations. It was found at the high observed NO_2 concentrations that CALPUFF performed overprediction for all monitoring stations.

As for the evaluation of model performance in predicting air pollution episodes, RHC analysis was used to determine the ability of the model in predicting extreme end of the concentration distribution. Generally, AERMOD provided better performance than CALPUFF in evaluating extreme concentration of NO_2. Comparisons of the observed and predicted results for the overall parts of the concentration distribution indicate that AERMOD performed quite well in predicting the average, RHC, 90th percentile to 99.9th percentile, and maximum concentration. As for CALPUFF, the model could work well in predicting average, RHC, and 95th percentile of concentrations but did not provide optimum results in predicting the upper-end statistic as illustrated in Figure 3.

The ratio (predicted/observed) of the average concentration indicated that there was a little bias for the model calculation in predicting the average concentration (Fig. 4). AERMOD was found to provide less accuracy at TKTP and CCIL stations for both the average and the extreme concentration distributions. However, AERMOD provided better performance at the other monitoring stations. AERMOD

Table 1. Performance evaluation statistics for nitrogen dioxide concentration.

MONITORING SITE	NO. OF SAMPLES	MEAN	STANDARD DEVIATION	r^2	RMSE	IOA	Fb	Fs	RHC
1. HMTP									
Observed	11165	50.7	70.32	–	–	–	–	–	67.11
AERMOD	11165	54.4	35.05	0.99	7.74	0.99	−0.07	0.67	77.40
CALPUFF	11165	40.8	40.59	0.99	21.54	0.98	0.22	0.54	64.96
2. FCRC									
Observed	7858	38.9	80.73	–	–	–	–	–	52.32
AERMOD	7858	27.9	29.61	0.91	19.30	0.99	0.33	0.93	39.28
CALPUFF	7858	38.2	41.70	0.97	25.13	0.98	0.02	0.64	58.20
3. BTKH									
Observed	8638	44.9	76.04	–	–	–	–	–	59.97
AERMOD	8638	42.7	25.20	0.99	3.72	0.99	0.05	1.00	59.55
CALPUFF	8638	34.3	32.96	0.99	16.25	0.99	0.27	0.79	53.18
4. WNFS									
Observed	5526	36.3	82.91	–	–	–	–	–	47.73
AERMOD	5526	27.4	27.63	0.95	16.82	0.99	0.28	1.00	38.98
CALPUFF	5526	45.8	35.42	0.99	20.22	0.98	−0.23	0.80	72.03
5. MMTP									
Observed	8187	49.7	72.01	–	–	–	–	–	68.18
AERMOD	8187	60.6	40.47	0.97	13.33	0.99	−0.20	0.56	84.02
CALPUFF	8187	48.8	48.93	0.99	22.76	0.98	0.01	0.38	81.78
6. KKYC									
Observed	9921	31.1	89.09	–	–	–	–	–	44.22
AERMOD	9921	25.7	16.09	0.99	7.74	0.99	0.19	1.38	38.40
CALPUFF	9921	36.8	35.19	0.98	16.75	0.99	−0.16	0.87	59.36
7. MCLT									
Observed	7776	29.7	89.44	–	–	–	–	–	40.94
AERMOD	7776	20.8	23.70	0.89	13.73	0.99	0.35	1.16	28.33
CALPUFF	7776	34.7	42.29	0.97	28.76	0.97	−0.15	0.71	53.79
8. TKTP									
Observed	7553	18.7	99.85	–	–	–	–	–	27.31
AERMOD	7553	31.9	22.18	0.99	17.28	0.99	−0.52	1.27	45.64
CALPUFF	7553	29.4	30.26	0.99	21.86	0.98	−0.44	1.06	50.90
9. HBGD									
Observed	6709	75.1	54.04	–	–	–	–	–	99.83
AERMOD	6709	65.3	48.39	0.98	11.55	0.99	0.14	0.11	95.54
CALPUFF	6709	50.4	55.25	0.99	31.55	0.95	0.40	−0.02	81.21
10. CCIL									
Observed	5467	15.8	102.44	–	–	–	–	–	21.64
AERMOD	5467	53.3	31.76	0.92	40.46	0.94	−1.08	1.05	78.74
CALPUFF	5467	49.1	44.25	0.99	46.28	0.93	−1.02	0.79	84.23
All stations									
Observed	78800	39.8	82.01	–	–	–	–	–	63.91
AERMOD	78800	41.0	30.97	0.99	5.35	0.99	−0.03	0.90	64.99
CALPUFF	78800	40.2	40.97	0.99	15.50	0.99	−0.01	−0.66	69.64

Abbreviations: r^2, correlation coefficient; RMSE, root mean square error; IOA, index of agreement; Fb, fractional bias; Fs, fractional variance; RHC, robust highest concentration.

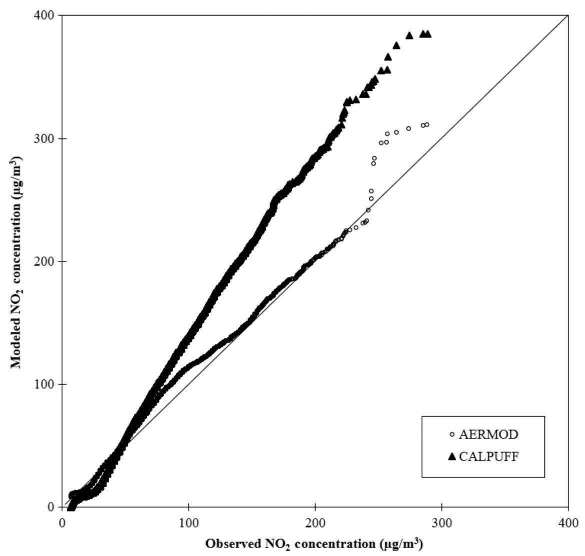

Figure 2. Q–Q plots between observed and modeled (AERMOD and CALPUFF) concentrations of NO_2 at all monitoring sites.

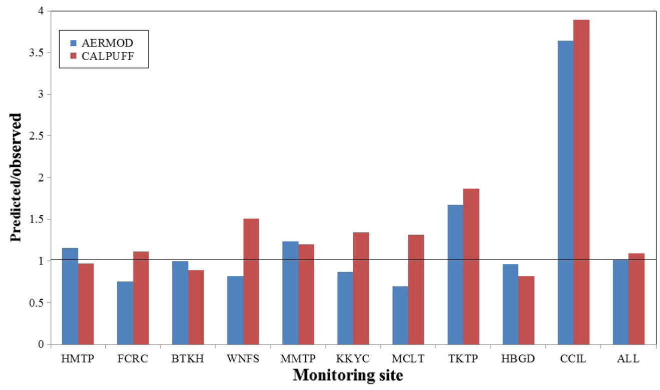

Figure 4. Ratio (predicted/observed) of NO_2 average concentration.

was found to provide better average concentration than the CALPUFF model when comparing with the average concentration from the observed values.

Sulfur dioxide. Hourly average ground-level concentrations of sulfur dioxide at each of the monitoring sites were computed. Results were compared with those measured data and are summarized in Table 2.

The average concentration of the measured data was 24.5 µg/m^3, while the average concentrations from AERMOD and CALPUFF predictions were 36.8 and 38.6 µg/m^3, respectively. Similar to the NO_2 performance evaluation, the differences between the model predicted and observed values were much lower than their respective standard deviations (sigma) (RMSE < standard deviation), indicating that skill was being shown by both models. Generally, AERMOD performed well for the prediction of average concentration at every monitoring site, at least to within the accuracy of the observations (standard deviation) except at HMTP, MMTP, TKTP, and HBGD. The maximum Fb and Fs were found for simulated data at TKTP station (Fb = −1.61) and WNFS (Fs = 1.38). Similar to the poor agreement in NO_2 prediction, this problem might originate from the missing observed data at these stations. The best model performances were found at HMTP station (Fb = −0.19, Fs = 0.12). Smaller values of RMSE indicate a better performance, and it is not biased toward models that overpredict or underpredict. In this study, AERMOD was in good agreement with ambient air concentrations of SO_2 than CALPUFF at all monitoring stations.

Comparisons of modeled and observed SO_2 concentrations at each site are presented in Figure 5. Q–Q plots were prepared using the model predicted and observed values of the SO_2 concentration. The Q–Q diagram indicated that AERMOD performed quiet well and provided high correlations with the observed SO_2 concentrations than CALPUFF for all monitoring stations. It was found that the observed SO_2 concentration, CALPUFF, failed in predicting the high concentrations.

Generally, AERMOD provided better performance than CALPUFF in the evaluation of extreme concentration of SO_2. Comparison of the observed and predicted results for the overall parts of the concentration distribution indicated that AERMOD performed quite well in predicting the average, RHC, and 90th percentile to 99.9th percentile. As for CALPUFF, the model could perform quite well in predicting the average, RHC, and 90th percentile of concentrations but did not provide optimum results in predicting the upper-end statistic as illustrated in Figure 6.

The ratio (predicted/observed) of the average concentration indicated that there was a little bias for the model calculations at predicting the average concentration (Fig. 7). AERMOD was found to provide less accuracy at BTKH, TKTP, and HBGD stations for both the average and the extreme concentration distributions. However, AERMOD provided better performance at the other monitoring stations. It was found that AERMOD provided better average

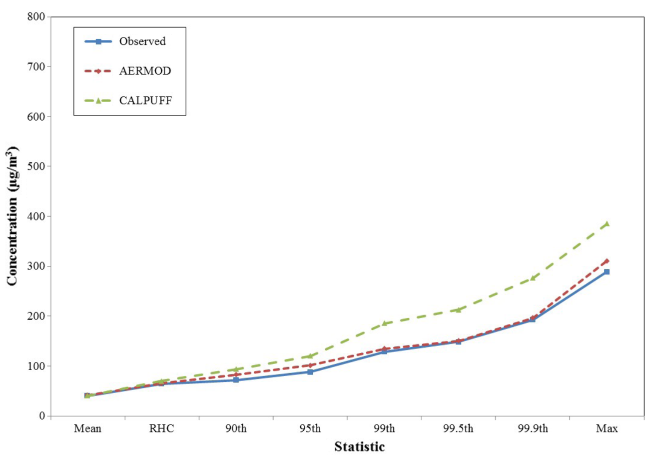

Figure 3. Mean, RHC, percentile statistic, and maximum for predicted and observed NO_2 for all sites.

Table 2. Performance evaluation statistics for sulfur dioxide concentration.

MONITORING SITE	NO. OF SAMPLES	MEAN	STANDARD DEVIATION	r^2	RMSE	IOA	Fb	Fs	RHC
1. HMTP									
Observed	5483	44.0	78.38	–	–	–	–	–	64.32
AERMOD	5483	54.8	29.21	0.99	14.53	0.99	−0.22	0.91	72.16
CALPUFF	5483	53.2	69.62	0.98	41.72	0.94	−0.19	0.12	92.14
2. FCRC									
Observed	4565	14.7	103.67	–	–	–	–	–	19.71
AERMOD	4565	22.9	37.94	0.99	28.97	0.98	−0.43	0.93	38.65
CALPUFF	4565	28.6	42.15	0.99	35.53	0.97	−0.64	0.84	49.62
3. BTKH									
Observed	2836	15.2	102.95	–	–	–	–	–	19.61
AERMOD	2836	52.0	29.66	0.91	39.82	0.96	−1.10	1.11	69.23
CALPUFF	2836	49.2	60.99	0.98	61.93	0.89	−1.05	0.51	85.23
4. WNFS									
Observed	13061	11.6	106.86	–	–	–	–	–	19.15
AERMOD	13061	28.8	17.74	0.89	19.59	0.99	−0.85	1.43	45.55
CALPUFF	13061	30.5	23.18	0.92	23.48	0.99	−0.90	1.29	49.36
5. MMTP									
Observed	7755	59.6	66.64	–	–	–	–	–	86.09
AERMOD	7755	43.8	31.44	0.97	18.11	0.98	0.31	0.72	63.75
CALPUFF	7755	37.3	48.10	0.90	32.05	0.96	0.46	0.32	63.45
6. KKYC									
Observed	4072	9.9	108.25	–	–	–	–	–	13.29
AERMOD	4072	22.2	17.86	0.90	15.90	0.99	−0.76	1.43	33.90
CALPUFF	4072	36.8	45.13	0.99	46.79	0.94	−1.15	0.82	63.75
7. MCLT									
Observed	4342	9.4	109.04	–	–	–	–	–	14.12
AERMOD	4342	13.0	29.15	0.98	13.67	0.99	−0.33	1.16	21.34
CALPUFF	4342	28.2	46.17	0.99	40.60	0.96	−1.00	0.81	48.80
8. TKTP									
Observed	3147	4.7	113.31	–	–	–	–	–	6.56
AERMOD	3147	35.8	20.69	0.91	35.64	0.97	−1.54	1.38	51.99
CALPUFF	3147	43.7	54.41	0.99	63.30	0.90	−1.61	0.70	75.69
9. HBGD									
Observed	2193	19.1	99.66	–	–	–	–	–	27.66
AERMOD	2193	64.7	54.81	0.93	55.66	0.89	−1.09	0.58	105.23
CALPUFF	2193	60.6	68.58	0.99	64.53	0.87	−1.04	0.37	104.95
10. CCIL									
Observed	3477	41.4	78.92	–	–	–	–	–	57.55
AERMOD	3477	59.2	36.71	0.99	18.37	0.98	−0.35	0.73	81.58
CALPUFF	3477	50.1	67.10	0.98	46.32	0.93	−0.19	0.16	86.84
All stations									
Observed	50931	24.5	97.03	–	–	–	–	–	41.47
AERMOD	50931	36.8	29.10	0.98	13.88	0.99	−0.40	1.07	62.76
CALPUFF	50931	38.6	49.14	0.98	27.24	0.97	−0.44	0.65	66.93

Abbreviations: r^2, correlation coefficient; RMSE, root mean square error; IOA, index of agreement; Fb, fractional bias; Fs, fractional variance; RHC, robust highest concentration.

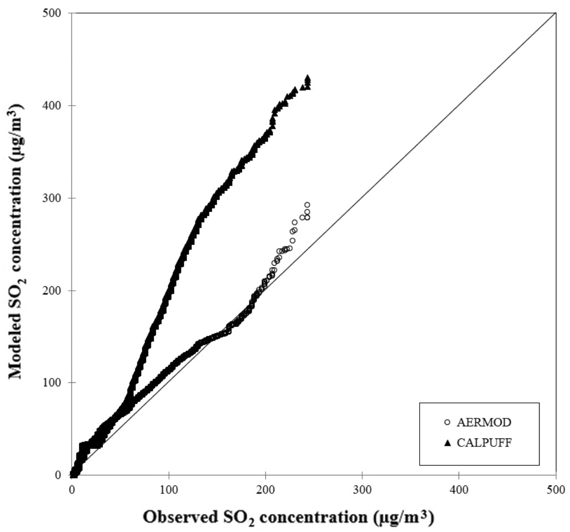

Figure 5. Q–Q plots between observed and modeled (AERMOD and CALPUFF) concentrations of SO_2 at all monitoring sites.

concentration when compared with the average concentration from the observed values than the CALPUFF model. Better performance of AERMOD in this study might result from short distances (<3 km) between emission sources and discrete receptors (monitoring station). Since CALPUFF is recommended for long-range transport (source–receptor distances of 50 km to several hundred kilometres) of emissions from sources, it might not perform well in predicting ambient air concentrations in the areas close to the emission sources.

Conclusions

The applicability of a model in general depends on many reasons, but the accuracy of a model is one of normally determined by an evaluation procedure that involves the comparisons of the modeled concentrations with measured air quality data. Choice of model selection greatly depends on several reasons such as availability and quality of input data and intended use of model result. In this study, AERMOD and CALPUFF air dispersion models were simulated to predict nitrogen dioxide (NO_2) and sulfur dioxide (SO_2) concentrations for the years 2012 and 2013. The study domain was MIA that is the largest petrochemical complex in Thailand. Modeled results were compared with observed concentrations measured from the Maptaphut ambient air quality monitoring network (10 stations).

In comparing the AERMOD and CALPUFF models, it was found that both models produced comparable results when observing differences in predicted and actual data. Fractional bias (Fb) of the modeled and the observed NO_2 data were mostly within the factor of 2, indicating that both models performed quite well in predicting ground-level concentrations of this air pollutant. On the other hand, at some monitoring stations, both AERMOD and CALPUFF models did not perform well in predicting SO_2 concentrations. This problem could have been caused by low concentrations of measured SO_2 data, which made it difficult for comparisons of modeled and observed results. Overall results indicate that there was less bias from AERMOD predictions compared with CALPUFF results. AERMOD also provide better results in predicting extreme end of concentration distributions than modeled data obtained from CALPUFF. Therefore, it can be concluded from this study that the AERMOD dispersion model is more appropriate for air quality management in this industrial area than the CALPUFF model. AERMOD has shown the ability to provide a suitable model for conducting dispersion modeling from point sources in Maptaphut with good model skill for estimating hourly concentrations of NO_x and SO_2. In conclusion, taking into consideration that there are needs to collect data on ambient ground-level concentrations from the areas within the vicinity of the industrial complex, AERMOD is more suitable for application than the regional CALPUFF model in this study.

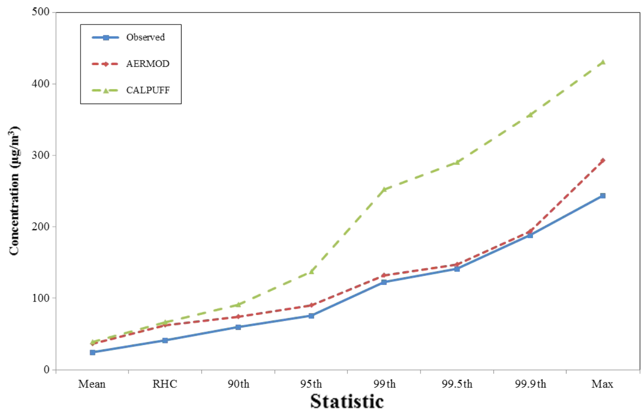

Figure 6. Mean, RHC, percentile statistic, and maximum for predicted and observed SO_2 for all sites.

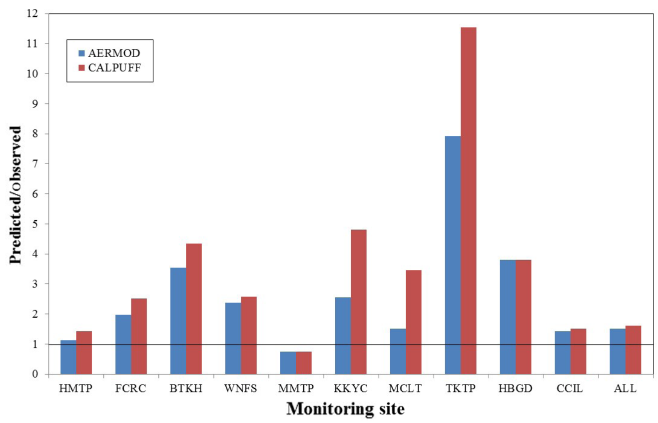

Figure 7. Ratio (predicted/observed) of SO_2 average concentration.

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Author Contributions

Conceived and designed the experiments: ST. Collected data: NP. Analyzed the data: NJ. Wrote the first draft of the manuscript: NJ. Contributed to the writing of the manuscript: ST, NP. Agreed with manuscript results and conclusions: ST. Jointly developed the structure and arguments for the paper: ST. Made critical revisions and approved the final version: ST. All authors reviewed and approved the final manuscript.

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