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Comparison of AERMOD Performance using Observed and Prognostic Meteorological Data

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Abstract

This study is aimed to compare the performance of AERMOD dispersion model by using actual and prognostic meteorological data in predicting ground level sulfur dioxide (SO_2) concentrations and spatial dispersion in the largest petrochemical industrial complex in Thailand. Three SO_2 monitoring stations having the highest percentage of data completeness were selected among the air quality monitoring network in the study area to serve the evaluation purpose. Emission data in this study comprised of 472 combustion stacks and 11 roads. Those emissions were assumed as constant value for each source over the simulated period. The observed air quality and meteorological data in May, 2013 were then also selected due to the occurring of hourly extreme concentration (episode) of SO_2 as well as having highest completeness of measured data. Hourly meteorological data during this period obtained from direct measurement and prognostic meteorological data were used as input independent variables in the model simulation. Evaluation of model performance was accomplished by statistical comparison between observed and modeled SO_2 concentrations. Results from statistical analysis indicated that there were no different between predicted SO_2 concentrations from using of prognostic and actual meteorological simulations. However, predicted SO_2 concentrations by AERMOD from both meteorological data provide over-estimate results when compare with those monitoring results.

Keywords: AERMOD; Maptaphut industrial area; Prognostic meteorological simulations; SO_2

1. Introduction

As we all know, since the industrial revolution to the present is the time when mankind has caused most air pollution problems because of the consumption of energy in the household, transport, industry and agriculture (Pochanart, 2012). Air pollution is a common problem, especially in large cities around the world (Sienfeld, 1986). There are ozone (O_3), total suspended particulates (TSP), particulate matter (PM), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), carbon monoxide (CO), lead (Pb) and other toxins affect health (Seangkiatiyuth *et al.*, 2011). At present, the problem of air pollution is one of a major environmental problem in Thailand. The problem is caused by several reasons. One of the major reasons is significantly increasing of industrial development in order to serve the rapidly growing populations and economics (Rakphong, 2009). Major sources of air pollution in Thailand are vehicles and industrial plants. Vehicles cause air pollution problems particularly in large community areas. However, the biomass burnings and fugitive emissions also played an important role of emission sources in some areas. Air pollution from industrial plants is space-specific problems, but it spreads to surrounding areas, both rural and urban, and affecting health of people in the community.

According to the third national economic and social development plan (1972-1976), the Industrial Estate Authority of Thailand has selected potential areas for setting up industrial estates and export industrial zones in the suburbs of Bangkok, vicinity and provinces around the country to make an industrial estate a tool for local and urban development.

Maptaphut industrial area (MA) is the largest industrial complex in Thailand (Chusai *et al.*, 2012). It is located in Rayong province in the Eastern region of Thailand (about 179 km from Bangkok). At present, the complex consists of five industrial estates namely Map Ta Phut, East Hemaraj, Asia, Padaeng, and RIL industrial estates and the seaport. As in March 2016, there are many types of factory located in MA including petrochemical industry (75.0%), coal-fired power plant (1.5%), metal industry (7.4%), natural gas power plant (11.4%), gas separation plant (2.8%), and oil refinery (1.9%) (ONEP, 2016). There has been concern about many air pollutants over this area due to rapid urbanization and industrial growth. The MA has been designated as the pollution control area by the Thai's government in 2009 (ONEP, 2009). The cause of concern was air quality management for the area is known to be difficult, due to lack of understanding of emission characteristics from different sources or sectors, for instance, industrial, power plant, transportation, and residential (Chusai *et al.*, 2012). SO_2 is one of major air pollutant resulted to deterioration of ambient air quality (US EPA, 2016). It mainly emits as a result of combustion of fossil fuel. It also releases from industrial processes such as petrochemical industries and power plants, etc. The distribution of SO_2 not only depends on the emission of SO_2, but also is affected by meteorological conditions (Calkins *et al.*, 2016). It dissipates in the atmosphere cause global warming and acid rain (US EPA, 2016).

The AMS/EPA Regulatory Model (AERMOD) was developed in the United States in 1991 by the American Meteorology Society (AMS) and United States Environmental Protection Agency (US EPA). It has been applied to evaluate the dispersion of particle and gaseous emissions (Carbonell *et al.,* 2010; Chusai et al., 2012; Ma et al., 2013, Calkins *et al.,* 2016; Tartakovsky *et al.,* 2016). The major part of the AERMOD modeling developed and differentiated from other models is the application of the Planetary Boundary Layer (PBL) principle and advanced methods for complex terrains. The AERMOD modeling is a steady-state plume model. It is assumed that the Stable boundary layer (SBL) has a Gaussian concentration distribution. The convective boundary layer is a Gaussian spread horizontally. The convective boundary layer (CBL) in the horizontal will be Gaussian distribution, but in the vertical will be Bi-Gaussian distribution. However, the limitation in using the Gaussian equation accurately to simulate gas dispersion is due to a low wind speed or calm wind less than 0.5 m/s (Schnelle and Dey, 2000), which is not significant to mathematical evaluation. AERMOD is a mathematical model used to estimate air pollution distribution, distances not exceeding 50 km from a variety of sources. The model uses meteorological data prepared from AERMET pre-processor. AERMET is a process for predicting changes in altitude meteorological variables by means of similarity or scaling length based on surface meteorological data include wind speed, wind direction, turbulence and temperature. AERMAP is a terrain preprocessor that characterizes the terrain and generates receptor grids, discrete receptors, and elevation for AERMOD. AERMET uses meteorological data (surface and upper air meteorological data) and surface characteristics to calculate boundary layer parameters needed by AERMOD (US EPA, 2004). At present, meteorological data used to prepare AERMET to serve the regulatory air model simulations in Thailand i.e. for Environmental Impact Assessment (EIA) were obtained from direct measurement from the Thai Meteorological Department (for upper and surface data) and some were from the Pollution Control Department (for surface data). However, the upper-air data are only measured by one station (Bangkok) for using nationwide. As for surface data, even though they are measured on the provincial scale, the representativeness of the station and large amount of missing data are major constraint for these measured meteorological data. This problem is the major constraint of using air dispersion modeling in Thailand and many developing countries. A problem emerges when trying to estimate the convective mixing height because upper air meteorological data are required. In Thailand, upper air soundings with the required frequency (twice daily) are only available at Bangkok (about 120 km from the study area). Under these conditions, an upper air estimator (UAE) that can estimate the convective mixing heights is required. Generally, the results of 3D meteorological meso–scale models such as MM5 (PSU/NCAR, 2005) or WRF–ARW (Advanced Research WRF) (PSU/NCAR, 2010) are used to fill in to complete the upper air characteristics.

To overcome this problem, a prognostic meteorological data are used to support the model simulation. However, it should be noted that the processed meteorological data may not represent the actual conditions experienced at the area accurately (Chen *et al.,* 2011). Therefore, it is important to determine whether the prognostic meteorological data can be used to substitute the measured data as well as giving the similar predicted concentrations when applying as input data for the air dispersion model simulations.

This study is aimed to evaluate and compare the performance of AERMOD dispersion model in predicting ground level concentrations of air pollutant using an actual and prognostic meteorological data. To serve this major objective, simulations of SO_2 concentrations in MA were conducted. Emission data consisted of 472 combustion stacks and 11 roads located in the study area. Predicted results from both actual and prognostic meteorological input were compared with measured ambient SO_2 concentrations obtained from an intensive ambient air monitoring station network. Performances of model simulations were evaluated through statistical analysis. The anticipated benefits of this study will be much useful in identifying the appropriateness of using actual and prognostic meteorological data and examine the ability to use interchangeable for inputting hourly meteorological data to reduce the cost of data acquisition for AERMOD to being utilized for further air pollution management and control.

2. Methodology

2.1 Model configuration

AERMOD dispersion model version 9.4 is used in this analysis. The modeling domain covers an area of 16 × 16 km^2 with a horizontal and vertical grid spacing of 100 m. Study domain is centered at 12.71066 °N (latitude), 101.13273 °E (longitude). Topographical characteristics of the study domain are derived from the Shuttle Radar Topography Mission (SRTM3) with a resolution of 90 m. These data are used as input data for AERMAP analysis. SO_2 emissions

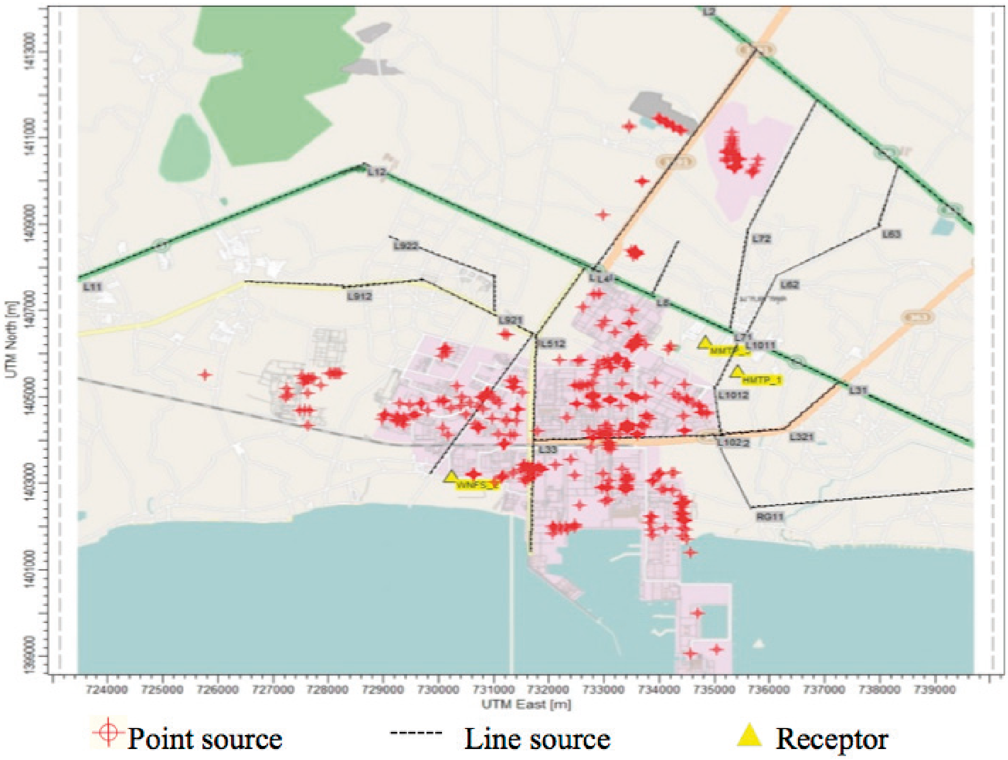


Figure 1. Study domain in a radius of 8 km from center of the MA

from point and line sources located within the study domain are used as emission input for the simulation of AERMOD.

Emissions of SO_2 from industrial sources are derived from the database of the year 2016 of the Office of Natural Resources and Environmental Policy and Planning (ONEP). These data consisted of geographical coordinates, stack height (m), stack diameter (m), exhausted temperature (K), stack exit velocity (m/s) and SO_2 emission rate (g/s) of each stack. As for line sources, these data were obtained from previous study by Thepanondh (2009) and Thawonkaew (2016). Totally, there were 472 stacks and 11 roads with a total SO_2 emission of 1732.70 g/s are used as emission input in this analysis. Spatial distribution of emission sources is illustrated in Figure 1.

2.2 *Meteorological data*

The hourly surface and upper air meteorological of the year 2013 were selected in this analysis. Those meteological data were prepared in each file format that is suitable to be used with the MM5 to produce a MM5 met.SFC and MM5 met.PFL files (Brode, 2008). The prognostic (predicted) meteorological data were generated and defragmented by the Mesoscale Meteorological Model (MM5) in SAMSON (for surface meteorological data) and TD-6201 (for upper meteorological data) formats suitable to be used with AERMET processor. The observed data such as surface characteristics and standard meteorological observations (e.g. wind field) can also be used as input directly into MM5. AERMET then calculates the PBL parameters (Monin-Obukhov length; L, convective velocity scale; w*, surface friction velocity; u*, temperature scale; 2*, mixing height; Z_i. These parameters are then passed to the INTERFACE where similarity expressions (in conjunction with measurements) are used to calculate vertical profiles of wind speed, lateral and vertical turbulent fluctuations, potential temperature gradient, and potential temperature. For calculation of similarity theory scaling parameters (L, u*, and w*) and other parameters can be found in user guide of AERMOD and AERMET (US EPA, 2004). As for measured meteorological data, the data at surface level (10 m height from the ground) were obtained

(a) (b)

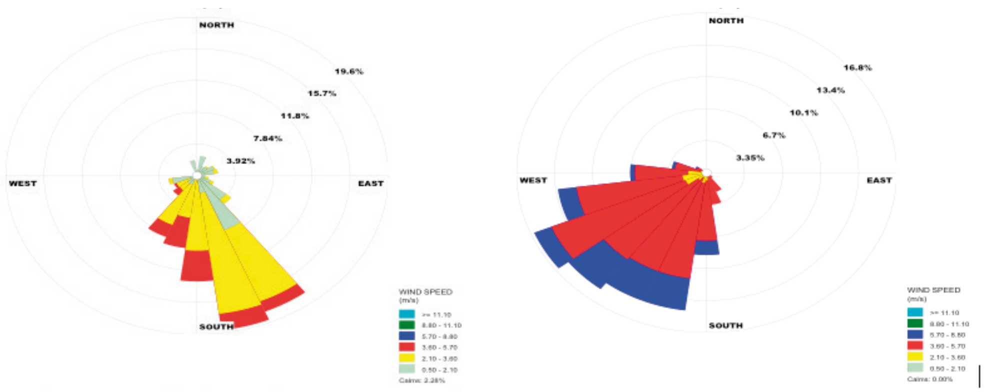


Figure 2. Wind rose in May 2013 of (a) measured meteorological data and (b) prognostic meteorological data.

from direct measurement at the HMTP ambient air monitoring station located within the study domain. However, since there were no available of measured upper meteorological data within the study area, these data were derived from the measurement in Bangkok (about 120 km in the northwestern direction of MA). Monitoring of meteorological data at 10 m height were compared with the results obtained from MM5 simulation at the same level. Comparison of predicted and measured meteorological data by using the wind speed and wind direction data were illustrated as wind rose as show in Figure 2. There were differences in wind direction in which mostly of prevailing wind obtained from measured data were these blown from south-southeast while the prevailing winds from south-southwest were predicted from the MM5 model. MM5 also predicted higher values of wind speed as compared with those obtained from direct measurement. The difference between prognostic and measured meteorological characteristics may be caused by the influenced from nearby building located in the vicinity of the meteorological monitoring site. These prognostic and measured meteorological data were used as input data to evaluate for their sensitiveness in predicting ground level concentrations of SO_2 in the study domain in the next step.

2.3 *Ambient SO_2 measured concentration data*

Ambient air quality data were acquired from top three monitoring stations namely Health Promotion Hospital Maptaphut (HMTP), Wat Nong Fap School (WNFS), and Muang Mai Maptaphut (MMTP) taking into consideration the highest number of available data. SO_2 ambient monitoring data during the period from 1-31 May 2013 were selected for model evaluation purpose due to the occurrence of hourly extreme concentration (episode) of SO_2 as well as availability (completeness) of measured data from every monitoring station as summarized in Table 1.

2.4 *Performance evaluation*

Evaluation of model performance was accomplished by statistical comparison between observed and modeled SO_2 concentrations covering the period from 1 – 31 May 2013. Statistical tools used to serve this purpose were Observed Mean (O_{mean}), Predicted/modeled Mean (P_{mean}), Observed Standard Deviation/sigma (O_{std}), Predicted/modeled Standard Deviation/sigma (Pstd), Pearson correlation coefficient (r), Root Mean Square Error (RMSE), Index Of Agreement (IOA), Fractional Bias (Fb), Fraction Variance (Fs) and the Robust Highest Concentration (RHC). Predicted results under the simulations with the observed and prognostic meteorological data over the modeling period on an hourly basis were compared with measured SO_2 concentrations. Statistical indicators used in this evlation were followed the previous studies by Cox and Tikvart (1990) and Tunlathorntham and Thepanondh (2017) as shown in Equations (1) - (10).

Table 1. Completeness of measured SO_2 concentration data (%) from monitoring stations

Months	Monitoring stations / Receptors		
	HMTP	**FCRzC**	**WNFS**
JAN	48.25	90.32	99.87
FEB	65.18	94.49	100.00
MAR	42.20	90.99	100.00
APR	93.47	94.86	99.58
MAY*	**98.92**	**95.03**	**99.87**
JUN	85.00	95.28	100.00
JUL	66.26	91.67	97.98
AUG	77.96	94.49	98.79
SEP	87.64	93.47	98.89
OCT	86.16	93.68	4.70
NOV	95.69	94.03	0.00
DEC	96.24	81.32	68.15

* Reference month have the highest percentage of data completeness

$$O_{mean} = \frac{1}{N}\sum_{i=1}^{N} Oi \qquad \text{(Eq.1)}$$

$$P_{mean} = \frac{1}{N}\sum_{i=1}^{N} Pi \qquad \text{(Eq. 2)}$$

$$O_{sid} = \sqrt{\frac{1}{N}\sum_{i=1}^{N} (O_i - O_{mean})^2} \qquad \text{(Eq. 3)}$$

$$P_{sid} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N} (P_i - P_{mean})^2} \qquad \text{(Eq. 4)}$$

$$r = \frac{N(\sum_{i=1}^{N}(O_i P_i) - (\sum_{i=1}^{N}(O_i)(\sum_{i=1}^{N}(P_i)}{\sqrt{[N(\sum_{i=1}^{N}(O_i{}^2) - (\sum_{i=1}^{N}(O_i)^2][N(\sum_{i=1}^{N}(P_i{}^2) - (\sum_{i=1}^{N}(P_i)^2]}} \qquad \text{(Eq. 5)}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N} (P_i - O_i)^2} \qquad \text{(Eq. 6)}$$

$$IOA = 1 - \frac{\sum_{i=1}^{N}(O_i - P_i)^2}{\sum_{i=1}^{N}(|P_i - O_{mean}| + |O_i - O_{mean}|)^2} \quad \text{(Eq. 7)}$$

$$Fb = 2\frac{(O_{mean} - P_{mean})}{(O_{mean} + P_{mean})} \quad \text{(Eq. 8)}$$

$$Fs = 2\frac{(O_{std} - P_{std})}{(O_{std} + P_{std})} \quad \text{(Eq. 9)}$$

$$RHC = C(R) + (\overline{C} - C(R)\ \mathrm{In}\ (\frac{(3R - 1)}{2})) \quad \text{(Eq. 10)}$$

Where

Oi = Observed data

Pi = Predicted modeled data

C(R) = the R^{th} highest concentration

$\overline{C}$ = the mean of the top R-1 concentrations

3. Results and Discussion

3.1 *Sulfur Dioxide (SO_2) concentrations*

Predicted ground level concentrations of SO_2 at three receptors were simulated from AERMOD model using both observed and prognostic meteorological data. Predicted data were on an hourly basis were compared with those measured data during the same period (1-31 May 2013). It was found that AERMOD over-estimated SO_2 concentrations at two receptor points namely HMTP and MMTP for both simulations under actual and prognostic meteorological input. However, predicted concentrations at WNFS were slightly lower than their measured data. Overall performances of the model were evaluated using fractional bias (Fb) and fractional variance (Fs). The values can be varied between -2 and 2, with a negative value indicating over-prediction and good performance is indicated by a value closed to zero (Jittra and Thepanondh, 2015). Highest values of Fb were found at HMTP while the lowest values were observed at WNFS. There were no differences between Fb calculated from the model simulations under actual and meteorological scenarios. Root Mean Square Error (RMSE) is an estimator of the overall deviations between the observed and predicted values (Jittra and Thepanondh, 2015).

Smaller of the value indicates a better performance of the model. By using this statistical tool, it was confirmed that predicted SO_2 concentrations at WNFS were well agreed with those measured data. The values of RMSE from both actual and prognostic meteorological conditions were even lower than their standard deviation (S.D.) indicated that predicted results

Table 2. Performance evaluation statistics for SO_2 concentrations

Monitoring stations	No. of samples	Mean	S.D.	r	RMSE	IOA	Fb	Fs	RHC
1. HMTP									
Observed	744	6.39	9.23	-	-	-	-	-	92.78
Prognostic Met	744	42.44	24.86	0.83	40.29	0.38	-1.48	-0.92	137.92
Actual Met	744	42.68	24.94	0.83	40.54	0.38	-1.48	-0.92	138.80
2. WNFS									
Observed	744	3.70	3.30	-	-	-	-	-	21.01
Prognostic Met	744	2.67	9.75	0.42	8.93	0.42	0.32	-0.99	145.97
Actual Met	744	2.68	9.75	0.42	8.92	0.42	0.32	-0.99	146.13
3. MMTP									
Observed	744	13.21	13.15	-	-	-	-	-	88.0
Prognostic Met	744	35.13	36.60	0.96	32.64	0.64	-0.91	-0.94	151.66
Actual Met	744	35.36	36.86	0.96	32.99	0.63	-0.91	-0.95	151.70
All stations									
Observed	2232	7.77	10.28	-	-	-	-	-	91.23
Prognostic Met	2232	26.75	31.34	0.93	29.11	0.59	-1.10	-1.01	182.95
Actual Met	2232	26.91	31.53	0.93	29.36	0.59	-1.10	-1.02	182.29

Note: S.D.; Standard deviation, r; Correlation coefficient, RMSE; Root mean square error, IOA; Index of agreement, Fb; Fractional bias, Fs; Fractional variance, RHC; Robust highest concentration

were no biased toward over- or under-predicted concentrations. Results of statistical analysis to evaluate performance of the model are presented in Table 2.

The quantile–quantile (Q–Q) plots can examine the model bias over the concentration distribution of their data. Figure 3 (a) presents the Q–Q plots between observed and modeled values (actual and prognostic meteorological data) of SO_2 concentrations at every station (receptors). This Q–Q diagram indicated that AERMOD performed over-prediction for all monitoring stations. Figure 3 (b) presents the Q–Q plots between actual and prognostic meteorological data for predicted SO_2 concentrations. The over- predicted results were probably originated as results of over-estimation of SO_2 emission inventory. The ability of the model to predict extreme end concentrations (episode) of SO_2 were evaluated by comparing high end percentiles (90^{th}, 95^{th}, 99^{th}, 99.5^{th}, 99.9^{th}), maximum and the robust highest concentration (RHC) of measured and predicted SO_2 data as illustrated in Figure 4. It was found that predicted results from both simulations under actual and prognostic meteorological scenarios were about 2 times higher than measured data.

Therefore, it can be concluded that AERMOD did not perform well in predicting SO_2 concentrations in this study. Beside the problem with emission input, this problem

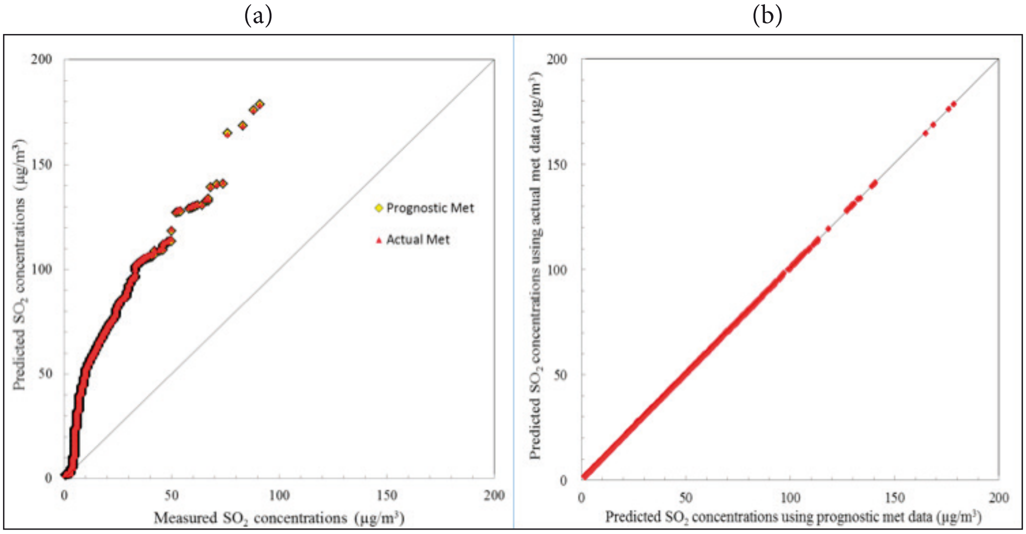


Figure 3. Q–Q plots of SO_2 concentrations between (a) observed and modeled results (actual and prognostic meteorological simulations) and (b) actual and prognostic meteorological simulations

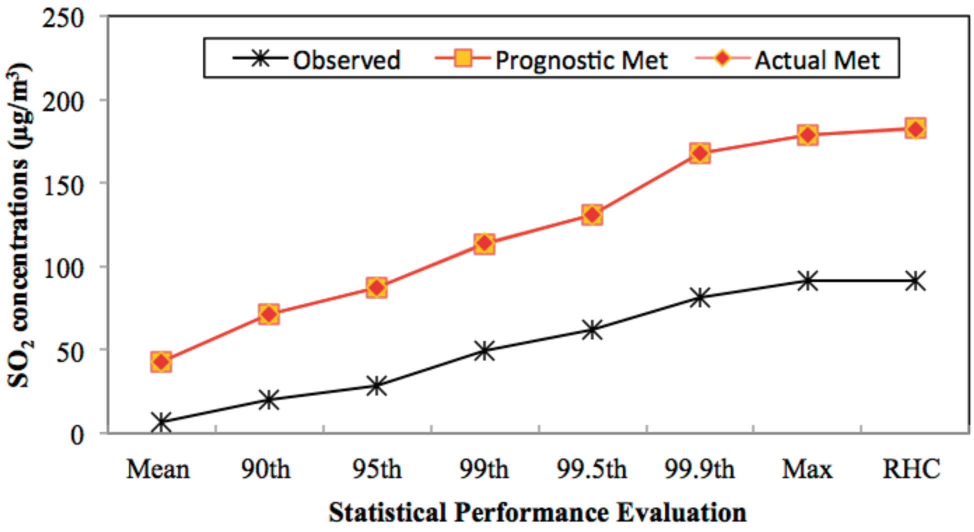
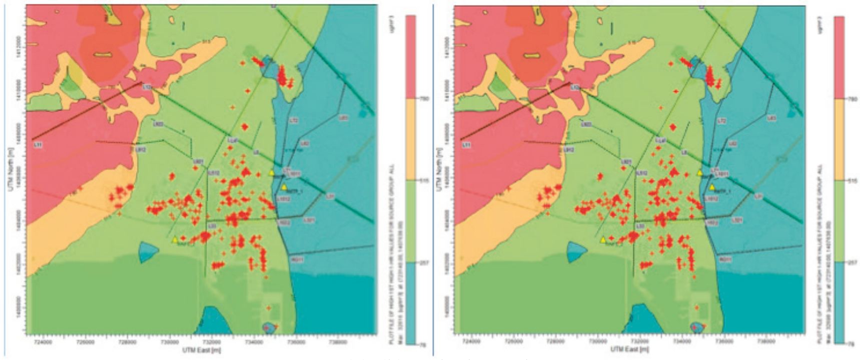


Figure 4. Mean, percentiles, maximum, and RHC for predicted and observed SO_2 concentrations for all stations

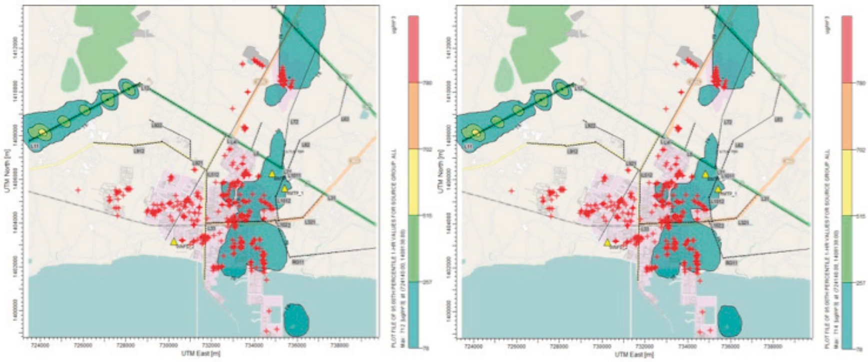
could also be contributed by low concentrations of measured SO_2 data, particularly the present of "zero" concentration and a more serious problem where atmospheric reactions or deposition mechanisms may not be included in the model (Chen *et al.,* 2011; Seangkiatiyuth *et al.,* 2011), which made it difficult to compare measured and predicted results and performed statistical analysis. Comparison of SO_2 concentrations for three different times using both hourly MM5 model-generated meteorological output and observed meteorological data were illustrated in Table 3 and Figure 5. The results revealed that there were no differences between predicted. SO_2 concentrations under actual and prognostic meteorological simulations.

Table 3. Comparison of SO_2 concentrations for the entire year 2013

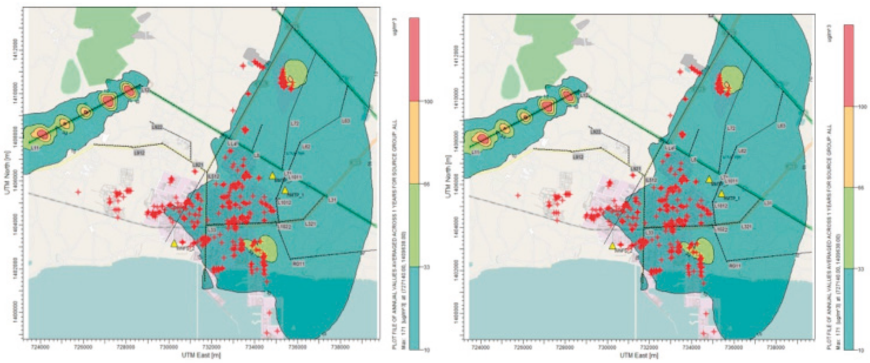
Type of meteorological data for modeling	**Concentration (μg/m³)**		
	Max. (1-hr)	**95^{th} percentile (1-hr)**	**Annual**
Prognostic data	32,698	714	171
Observed data	32,616	712	171



Δ (a), (b) 1st highest 1-hr



Δ (c), (d) 95th percentile of 1-hr



Δ (e), (f) Annual average concentrations

Figure 5. Comparison of plot file of SO_2 concentrations (μg/m³) between measured (a,c,e) and prognostic meteorological simulations (b,d,f)

This finding indicated that the prognostic (modeled) meteorological data can be used to substitute or replace meteorological data obtained from direct measurements in this study area. Small difference in predicted SO_2 concentrations simulated using actual and prognostic meteorological data could be resulted by the influences of similar upper air which play more important role in AERMOD than surface air data. Figure 5 (a & b) illustrate the spatial distribution of the highest 1-hour average concentration for each Cartesian grid. High concentrations were occurred in the northwest direction of the emission sources due to the influence of the wind blew from SE direction. In order to evaluate whether these high concentrations were probably occurred only for couple hours, we also evaluate for the 95th percentile of the predicted data as shown in Figure 5 (c & d). The results clearly indicated that the affected areas were those located in the northern direction from the emission sources can be considered as the affected zone from the industrial complex. These areas are located downwind from the major prevailing wind (southern wind) of the study area. These data were relevant with the wind rose diagram over the whole year of the study area. Furthermore, little difference in SO_2 levels may be due to other parameters are not considered (surface characteristics, cloud cover, precipitation, etc.), which may also significantly affect model results (Touma *et al.,* 2007; Chen *et al.,* 2011).

4. Conclusions

AERMOD air dispersion model was evaluated for its performance to predict ground level SO_2 concentrations using actual and prognostic meteorological data. Study area was Maptaphut industrial area, Thailand. SO_2 emission data comprised of 472 stacks and 11 roads located in the study domain. These emissions were assumed as constant value for each source over the simulated period. Predicted results were compared with those observed data from top three receptors, having the highest percentage of data completeness in the year 2013 selected among the Maptaphut ambient air monitoring stations. Wind rose analysis showed that the prevailing wind directions were from the southern direction. The difference between prognostic and measured meteorological characteristics may be caused by the influenced from nearby building located in the vicinity of the meteorological monitoring site. The maximum and minimum values of both wind speed and temperature are not significantly different. Comparisons of modeled and observed results indicated that were the differences results indicated that were the differences between the modeled and observed values. Predicted SO_2 concentrations from using both actual and prognostic meteorological data were higher than measured SO_2 ground level concentrations for AERMOD air dispersion model. Therefore, AERMOD models did not perform well in predicting SO_2 concentrations (over-prediction) for this study. This problem could have been caused by low concentrations of measured SO_2 data, which made it difficult to compare the results from the predicted and observed. Only WNFS station was considered best performing due to the highest completeness of measured SO_2 concentration data. Major finding from this study can be concluded that predicted SO_2 concentration obtained from prognostic meteorological simulation were not difference with simulation using actual meteorological data. Therefore, these data can be used interchangeably for preparation of meteorological input for AERMOD model in this study. This study will be much useful in identifying the appropriateness of using actual and prognostic meteorological data and examine the ability to use interchangeable for inputting hourly meteorological data to reduce the cost of data acquisition for AERMOD. It should be noted that one of the difference between the predicted SO_2 concentrations with those measured data may be attributed by the choice of metrological model used in the analysis. Further model comparison study using new generation of meteorological model such as WRF model could be interested for better explanation of the meteorological characteristics in this study area. The Advanced Research WRF system (WRF-ARW 3.1) can be used as an alternative meteorological driver for MM5 in the air quality modelling. The WRF-ARW system is a non-hydrostatic model (with a hydrostatic option) using terrain-following vertical coordinate based on hydrostatic pressure (Gsella *et al.*, 2014). It is considered by NCAR as the successor of MM5, since further development of MM5 has come to an end in favor of WRF.

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