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EVALUATION OF DISPERSION MODEL PERFORMANCE IN PREDICTING SO_2 CONCENTRATIONS FROM PETROLEUM REFINERY COMPLEX

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ABSTRACT: The AERMOD and CALPUFF air dispersion models are tested for their performance in predicting ground level concentration of sulfur dioxide in Thailand. Emission data used in this study are obtained from petroleum refinery complex. Predicted results are compared with those measured data using the year 2012 as a reference year. A set of statistical parameters are employed to evaluate model performance. Overall results indicated that both AERMOD and CALPUFF can provide good results. However, AERMOD can perform better in predicting of extreme end of the concentration distribution at the receptor sites. The maximum ground level concentrations of sulfur dioxide within the modeling domain are about 359 and 456 µg/m^3 for AERMOD and CALPUFF simulations, respectively. This result indicates that CALPUFF provides more conservative of maximum result than predicted data from AERMOD. The decision to select an appropriate dispersion model in the study is accomplish by using the Multi-Criteria Attribute (MCA) analysis. Result from MCA supports that AERMOD is more appropriate to be applied for study of air dispersion in this area than CALPUFF system.

Keywords: AERMOD, CALPUFF, Sulfur dioxide, Multi criteria attribute, Thailand

1. INTRODUCTION

Sulfur dioxide (SO_2) is one of a group of highly reactive gasses 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 [1].

The steady-state model AERMOD and Lagrangian puff model CALPUFF are the U.S. Environmental Protection Agency preferred models for demonstrating regulatory compliance in the near field (less than 50 km) and far field (more than 50 km), respectively [2]. However, CALPUFF also be recommended to use for the analysis of air pollution dispersion in the vicinity of emission source in case of complex terrain and wind characteristics. AERMOD assumes that a plume disperses in the horizontal and vertical directions resulting in Gaussian concentration distributions. It does not track the contribution or carry-over of plume from previous hours. Consequently, each hour a plume is dispersed in the direction of that hour’s meteorology in a straight-line trajectory [3]. AERMOD’s concentration algorithm 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 (PBL) through which plume material travel directly from the source to the receptor [4]. CALPUFF is a multi-layer, multi-species, non-steady state 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 [5]. It is an atmospheric source-receptor model recommended by the U.S. Environmental Protection Agency for use on a case-by-case basis in complex terrain and wind conditions [6]. In Thailand, both models are regulated as preferred model for an environmental impact assessment (EIA) process. In this study, performances of these models are evaluated for sulfur dioxide dispersion as resulted from emission of petroleum refinery complex in the Eastern seaboard area of Thailand. This study is aimed to evaluate performance of AERMOD and CALPUFF air dispersion models by comparing model predictions with field measurements. Finally, decision of model selection, based on its appropriateness is analyzed by multi-criteria attribute (MCA) analysis using results from statistical analysis of model performance evaluation.

2. METHODOLOGY

In this study, measured data of ambient sulfur dioxide concentration, obtained from 3 monitoring stations, located in the surrounding area of petroleum refinery complex are used in the analysis. These data are available on an hourly basis. Measured data in the year 2012 and 2013 are used to compare with those modeled data. Emission data are obtained from 13 stack emission sources. Total emission rate of sulfur dioxide is about 120.7 g/s. Emission rate is calculated using amount of sulfur containing in fuel oil and fuel gas on a daily basis. Details of emission data used in this study are summarized in Table 1. Meteorological data, used for both models are obtained from simulation of MM5 meteorological modeling (the fifth-generation NCAR / Penn State mesoscale model). The gridded data needed by both models are selected from Digital Elevation Model (DEM) data and the terrain data are collected from the Shuttle Radar Topography Mission (SRTM3/SRTM1) database.

2.1 Model Configuration

AERMOD (version 8.7) and CALPUFF (version 5.8) of Lakes Environment are used in this study. AERMOD modeling domain is designed for radius of 20 km with the finest grid spacing of 90 m. A 30-km × 30-km model domain having grid spacing of 100 m is established for CALPUFF. Both models are centered approximately on the stack which having highest emission rate. The regulatory modeling options in this research use the default mode of operation for the urban options of dispersion coefficient. Sulfur dioxide ambient concentrations are calculated in 1 hour period on elevated terrain height option. The maximum one-hour concentration for the year 2012 and 2013 at each of the receptor sites are calculated together with the maximum group level concentration within modeling domain to evaluate ability in predicting high concentration of the model

2.2 Model 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 [7]. In this study, performance of AERMOD was examined for each case using the following statistical parameters: Observed Mean (O_{mean}) Eq.(1), Predicted/modeled Mean (P_{mean}) Eq.(2), Observed Standard Deviation/sigma (O_{std}) Eq.(3), Predicted/modeled Standard Deviation/sigma (P_{std}) Eq.(4), Pearson Correlation Coefficient (r^2) Eq.(5), Root Mean Square Error (RMSE) Eq.(6), Index Of Agreement (IOA) Eq.(7), Fraction Bias (Fb) Eq.(8), Fraction Variance (Fs) Eq.(9) and Robust Highest Concentration (RHC) Eq.(10). Equations used to calculate for these statistical parameter are as presented below:

Table 1 Characteristics of stack emission sources in this study

Source ID	Height (m)	Temperature (Kelvin)	Diameter (m)	Velocity (m/s)	Emission rate (g/s)
A-C (3 stacks)	140	573.15	2.93	9.49	13.44, 1.85, 11.59
D-E (2 stacks)	140	593.15	2.23	26.77	2.93, 2.93
F-G (2 stacks)	140	593.15	3.05	7.18	0.000025, 0.0000215
H-J (3 stacks)	140	505.15	3.03	7.49	1.53, 0.84, 0.69
K-L (2 stacks)	140	502.15	3.13	7.38	31.23, 31.23
M (1 stacks)	140	503.15	2.9	8.59	22.4

$$O_{mean} = \frac{1}{N}\sum_{i=1}^{n} Oi \quad (1)$$

$$P_{mean} = \frac{1}{N}\sum_{i=1}^{n} Pi \quad (2)$$

$$O_{std} \quad \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(Oi - \text{Omean})^2} \quad (3)$$

$$P_{std} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(Pi - \text{Pmean})^2} \quad (4)$$

$$r^2 = \frac{N(\sum_{i=1}^{N} OiPi) - (\sum_{i=1}^{N} Oi)(\sum_{i=1}^{N} Pi)}{\sqrt{[N(\sum_{i=1}^{N} Oi^2) - (\sum_{i=1}^{N} Oi)^2][N(\sum_{i=1}^{N} Pi^2) - \sum_{i=1}^{N} Pi)^2]}} \quad (5)$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(Pi - Oi)^2} \quad (6)$$

$$IOA = 1 - \frac{\sum_{i=1}^{N}(Pi - Oi)^2}{\sum_{i=1}^{N}(|Pi - Omean| + |Oi - Omean|)^2} \quad (7)$$

$$Fb = 2\frac{(Omean - Pmean)}{(Omean + Pmean)} \quad (8)$$

$$Fs = 2\frac{(Ostd - Pstd)}{(Ostd + Pstd)} \quad (9)$$

$$RHC = C(R) + (C^{-} - C(R)\ln(\frac{(3R-1)}{2}) \quad (10)$$

Where
Oi = Observed data
Pi = Predicted modeled data
C(R) = the R^{th} highest concentration
C^{-} = the mean of the top R-1 concentrations

The performances of model are tested by comparing the predicted pollutant concentrations of SO_2 with those measured actual values (hourly mean concentrations) at three ambient air quality stations. Comparisons are performed by characterizing the bias. For this purpose, three metrics relating to the bias, the mean bias (e.g., the mean difference between the modeled and the observed data), the root mean square error (RMSE), and fractional bias (Fb) are chosen. 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 which comprised of bias (the extent of over or under estimation) and variance (precision) [8]. The fractional bias is presented because it is the statistic recommended by U.S.EPA. Fractional bias is symmetrical and bounded with values ranging between +2 (extreme under prediction) and -2 (extreme over-prediction). The U.S.EPA guidance for selecting the best performing air dispersion model 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 [9]. 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.

3. RESULTS AND DISCUSSION

For the paired ensemble means performance objective, the dataset was based on the union of the predicted and observed concentrations [10]. In this study, only predicted and observed concentration pairs greater than zero were considered. Missing data of measured concentrations were replaced by average values of the hour before and after that missing time. Results of statistical analysis are summarized in Table 2 and Table 3. Results from statistical evaluation indicated that there were differences between the model and observed values. However, these differences were much lower than their respective predicted standard deviations (RMSE < Pstd), indicating that accurate results were being shown by the model. Generally, both models performed well for the prediction of average concentration at every monitoring site; at least to within the accuracy of the observations (standard deviation). In general, it is found that AERMOD is more accurate than CALPUFF (as determined by fraction bias and root mean square error). AERMOD also provides better result than CALPUFF in determining of robust highest concentration (RHC). 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 [11]. Results from robust highest concentration indicated that AERMOD provided slightly better result in predicting extreme end of SO_2 concentration than CALPUFF (percentage of overall difference in RHC from AERMOD was about 33 % while this value from CALPUFF prediction was about 35%). However, both models do not perform well in predicting the extreme concentration at station “A”. These results can be explained by the fact that station “A” is located very close to emission sources in the model simulations. This assumption is supported by the conceptual framework of a Lagrangian puff model which is better suited for long range transport where winds vary spatially across the model domain. Hence, Lagrangian puff models may be preferable for dose reconstruction where model domains can be large and where the assessment question is an unbiased estimate of concentration in time and space [10].

It was found that the values of Fb calculated from predicted data from both model were positive values indicating under-prediction of the simulated results. Good performance was identified with value close to zero. The maximum Fb were found for simulated data at station "A" while the best model performances were found at station "B" (Fb = 0.21 and 0.35 for AERMOD and CALPUFF simulations, respectively) as shown in Fig 1. Generally AERMOD also provided lower values of RMSE from the observed values than those obtained from CALPUFF calculations as presented in Fig.2.

Table 2 Comparisons of model performance in predicting high concentration (unit:µg/m^3)

Model	Monitoring site	RHC	
		measured	predicted
AERMOD	A	129.94	151.55
	B	91.54	38.4
	C	24.47	17.76
CALPUFF	A	129.94	46.64
	B	91.54	94.63
	C	24.47	33.68

Table 3 Comparisons of overall performance of the models using statistical analysis

Model	Monitoring site	Omean (µg/m^3)	Pmean (µg/m^3)	Ostd	Pstd	r^2	RMSE	IOA	Fb	Fs
AERMOD	A	4.05	5.77	4.17	10.45	0.81	9.76	0.82	0.71	0.19
	B	2.92	9.25	1.2	7.55	0.91	4.3	0.93	0.21	0.16
	C	4.43	3.52	6.08	2.47	0.88	3.47	0.77	0.56	0.48
CALPUFF	A	4.05	4.23	4.17	4.72	0.87	28.38	0.48	1.45	1.28
	B	2.92	13.39	1.2	16.84	0.96	9.3	0.89	0.35	-1.34
	C	4.43	4.93	6.08	4.99	0.86	6.71	0.66	0.77	-0.15

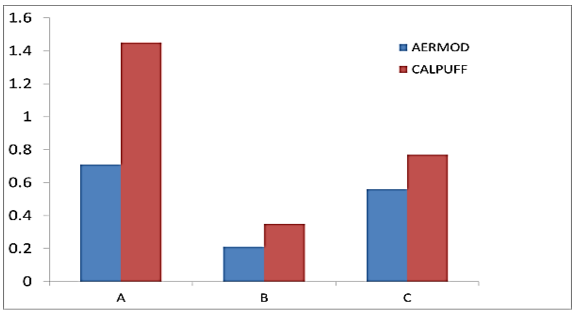


Fig 1 Model performance evaluation using Fb

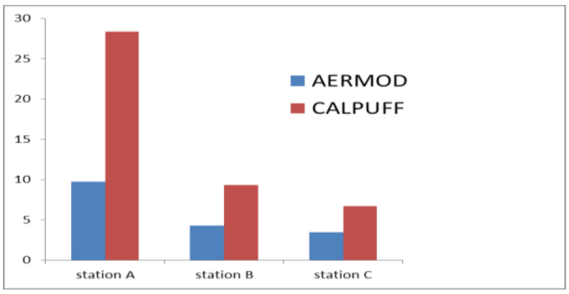
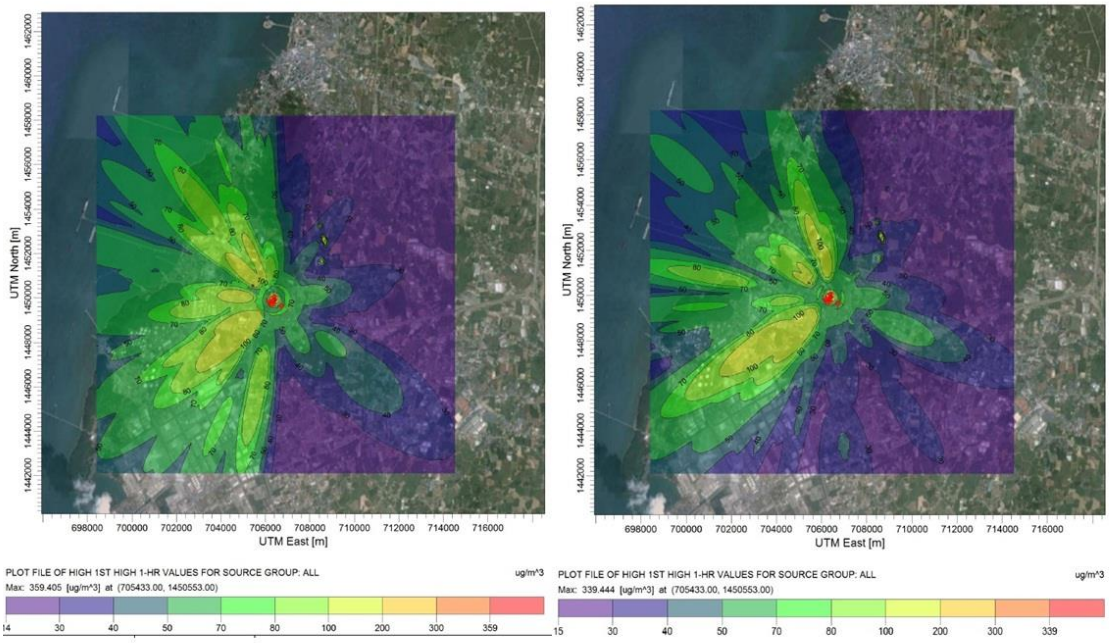


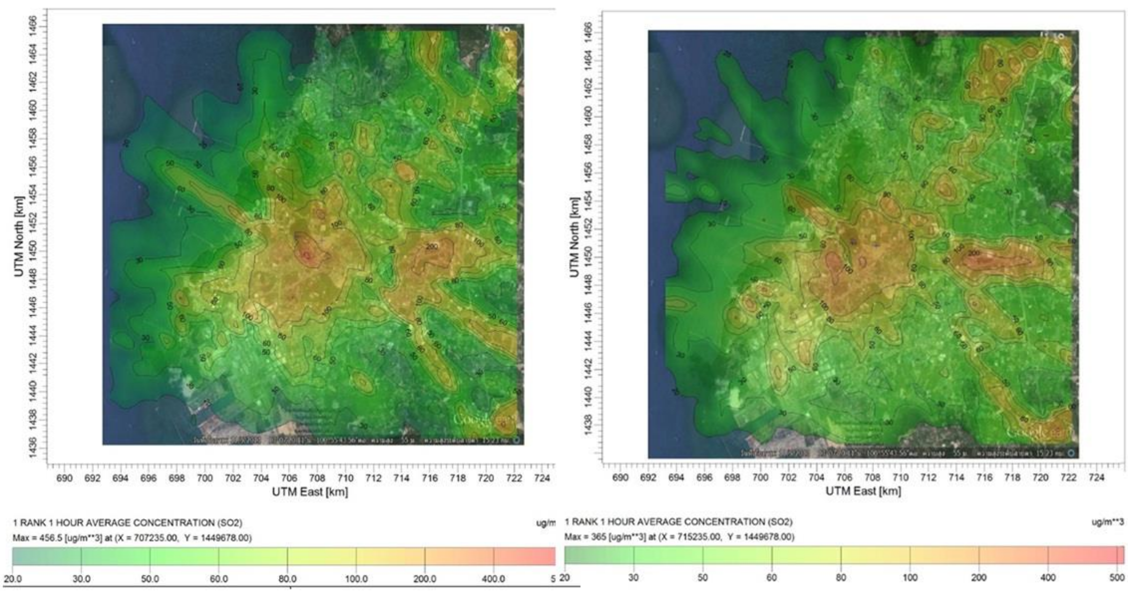
Fig 2 Model performance evaluation using RMSE

The maximum ground level concentrations of sulfur dioxide within the modeling domain in the year 2012 are 359 and 456 µg/m^3 for AERMOD and CALPUFF simulations, respectively. CALPUFF also provides higher predicted maximum concentration than AERMOD in the simulation year of 2013 (AERMOD = 339 µg/m^3, CALPUFF = 365 µg/m^3). Results of the maximum concentration in each grid cell from simulation of both models are illustrated in Fig 3 and Fig 4. This finding indicates that the predicted maximum ground level concentrations within modeling domain computed from AERMOD are slightly lower than those obtained from CALPUFF simulations.



(2012) (2013)

Fig 3 Plot file of the highest 1-hr concentration of SO_2 in µg/m^3 (AERMOD result)



(2012) (2013)

Fig 4 Plot file of the highest 1-hr concentration of SO_2 in µg/m^3 (CALPUFF result)

The decision to select an appropriate dispersion model in the study is accomplish by using the Multi-Criteria Attribute (MCA) analysis. MCA approach is a tool to calculate overall scores and rankings based on the scores given for each individual option [12]. This assessment method does not try to monetize everything, but to supply and unrefined view on the many different dimensions of the multiple effects of a certain policy/project option. In this study, 4 criteria are set for selection of the most appropriate model. They are 1) availability of meteorological data; 2) percentage of difference of measured and predicted RHC; 3) index of agreement and 4) factional bias. Each criterion is weighted as 25% of the total score. Details of score given to each criterion are as described in Table 4. Availability of meteorological data for using in CALPUFF model was given as 50% while the meteorological data for AERMOD was rated as 75%. In Thailand, the number and spatial distribution of meteorological monitoring stations may be limited. Therefore, data of observed wind characteristics varied spatially across the model domain are insufficient for CALPUFF simulation. Result of the MCA analysis indicates that AERMOD is more appropriate choice for model selection in this study as shown in Table 5. It should be noted that even though the availability of meteorological data were weighted as the same score for AERMOD and CALPUFF, total score of MCA of AERMOD was still slightly higher than the total score of CALPUFF.

Table 4 Criteria and indicators for scoring

Score	% difference in RHC	IOA	Fractional bias
100	0 - 20	0.8 - 1.0	< 0.2
75	20 - 50	0.6 - 0.8	0.2 - 0.5
60	-	-	0.5 - 0.75
50	50 -75	0.5 - 0.6	0.75 -1.0
25	75 - 100	-	-
10	>100	< 0.5	> 1.0

Table 5 MCA analysis for the selection of appropriate model

Criteria	Score	AERMOD	CALPUFF
Data availability (Meteorological data)	25	18.75	12.5
% Difference of RHC	25	18.75	18.75
IOA	25	18.75	18.75
Fractional bias	25	15	12.5
Total	100	71.25	62.5

Predicted results are compared with those measured data using the year 2012 as a reference year. In this study, measured data of ambient air concentration, obtained from 3 monitoring stations on an hourly basis were used for model validation.

A set of statistical parameters are employed to evaluate model performance. Overall results indicated that both AERMOD and CALPUFF can provide good results. However, AERMOD can perform better in predicting of extreme end of the concentration distribution at the receptor sites. Overall predicted results obtained from AERMOD simulations were shown to have less bias with those measured results as compared with predicted data from CALPUFF and may be considered as the appropriate calculation for prediction of annual average concentration. As for selection of appropriate model, the multi criteria attribute (MCA) analysis is applied here to assist as a decision tool for evaluation. Result from MCA also supports that AERMOD is more appropriate to be applied for study of air dispersion in this area than CALPUFF system.

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