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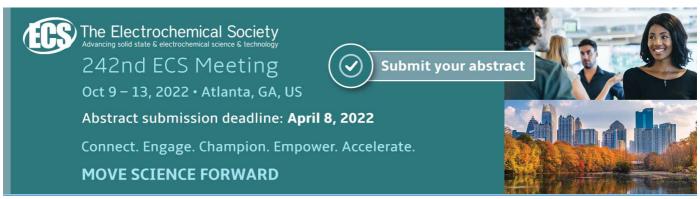
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Evaluation of regional simulation of surface ozone over Southeast Asia using ground-based observation at two existing Global Atmospheric Watch stations

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Abstract. High level of ground level ozone concentrations was found in most of Southeast Asian (SEA) large cities and often exceeded the national ambient air quality standard. Ozone and PM₁₀ are among of the critical air quality parameters that cause the unhealthy air quality index. Effort to mitigate ozone pollution is greatly complicated due to the photochemistry processes therefore photochemical smog modelling has been widely used. Surface ozone simulation in SEA was done using CHIMERE and weather research forecast (WRF) model. Emission inventory of ozone precursors was done for three countries in the domain, i.e. Indonesia, Thailand and Cambodia. Modelling performance evaluation for meteorological parameters and ozone at the SEA big cities was done in another study. This paper focused on the model evaluation conducted at the two remote sites represented by 2 (two) global atmospheric watch (GAW) remote stations of Bukit Kototabang (BKT) and Danum Valley (DNV). Evaluation result showed an overestimation of observed ozone in BKT while a contradictive result was seen in DNV station which was due to the ozone chemistry and inaccurate estimation of emissions (both anthropogenic and biogenic emission). The evaluation conducted at the remote sites was not even better than that conducted previously at the urban areas. Statistically, only mean normalized gross error and unpaired peak accuracy values that satisfy the criteria for surface ozone modelling suggesting major improvement required for ozone precursors emission inventory data.

Keywords: Ozone, GAW, WRF/Chimere, model performance, precursor

Track Name: Atmospheric Chemistry and Physics

1. Introduction

Surface ozone is a secondary pollutant that is known to cause detrimental effects on human health and reduction of agricultural yield [1]. Tropospheric ozone burden increased by 40 % from 1850 to the present day due to anthropogenic activities. Global satellite monitoring showed an increasing trend of ozone levels during the last decade [2]. Rapid development in Asia has been connected to the increase of surface ozone levels especially in the big cities which was affected by the local emission build up as

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well the favourable meteorological conditions [3]. Photochemical smog pollution abatement is greatly complicated in reducing NO_x or VOC due to the non-linear process in the photochemistry. In addition to the good data of monitoring, photochemical smog modelling has been widely used to understand the formation of ozone in an area as well as to simulate effects of precursor emission reduction on surface ozone concentration [4].

For Southeast Asia (SEA), limited studies are available for regional ozone simulation but mainly used the global emission inventory data with the coarse resolution. In addition, the maritime region of Indonesia was not included in the study domain. In this study, new emission inventory (EI) for three countries in SEA namely Thailand, Indonesia and Cambodia were developed [5]. Regional simulation of surface ozone was conducted for 1 year (2007) for SEA domain utilizing the newly developed EI. The evaluation of meteorological model performance and surface ozone modelling at the several SEA urban sites using the existing governmental air quality monitoring networks was done previously [6] suggesting a fair performance. This paper attempts to fill in gaps in evaluating regional model performance at the remote sites. Two existing Global Atmospheric Watch (GAW) stations at Bukit Kotatabang (BKT), Indonesia and Danum Valley (DNV), Malaysia were taken.

2. Methodology

Emission inventory (EI) is a foremost step prior to modelling task. The data for SEA were taken from our previous works including the emission of biomass open burning and fossil fuel combustion [5]. Estimation followed the framework of Atmospheric Brown Cloud Emission Inventory Manual (ABC EIM). Biogenic emission of isoprene, α -pinene, β -pinene, limonene, ocimene, and NO were calculated in the Model of Emissions of Gases and Aerosols from Nature (MEGAN) module provided in CHIMERE model. Data sources of EI and the coverage including species and sources are presented in Table 1. Initially, VOC speciation for anthropogenic emission was done using the available VOC source profile data (presented in Table 1).

Table 1. Emission data sources for the rest of countries in the domain for base year of 2007 (except Indonesia, Thailand, and Cambodia).

Sources			VOC Profile ^a							
	SO_2	NOx	CO	VOC	PM_{10}	PM _{2.5}	BC	OC	CH ₄	
Power generation										[7], [12]
Industry		CGRER ^a [13]						EDGAR ^b [14]	[7], [8], [11]	
Residential										[7], [12]
Transportation										[7], [10]
Biomass open burning	Song <i>et al</i> . [15] and GFED3 ^c [16]						[7], [9]			
Biogenic emission	Calculated by MEGAN model in CHIMERE for 2007					Directly from MEGAN				

Note: ^a – Center for Global and Regional Environmental Research, ^b - The Emissions Database for Global Atmospheric Research, and ^c – The Global Fire Emission Database.

For CHIMERE model, speciated VOC emission was initially converted to Statewide Air Pollution Research Center (SAPRC) using the methodology described in [17]. Further, the SAPRC speciated VOC

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data were then converted to MELCHIOR (CHIMERE) using aggregation factors from [18] for totally 33 species. Ready input emission data were then prepared in netcdf format prior to CHIMERE simulation.

Simulation was done for 1 (one) year starting from 1st January – 31st December 2007. For this study monthly mean concentration of gases and aerosols for period of 1998-2002 for boundary conditions were taken from the global model simulation of LMDz-INCA while the initial condition used interpolation of global concentration fields from the same global model. Detail model set-up for both CHIMERE and WRF is presented in [5].

Bukit Kotatabang GAW station (BKT) is located in the Western part of Sumatra at 864 m above mean sea level (AMSL). This station is centralized at 0° 12′ 07″ (latitude) and 100° 19′ 05″ (longitude) which is surrounded by the tropical forest (see Figure 1). DNV is located 426 m AMSL which is centralized at the latitude of 4° 58′ 53″ North and the longitude of 117° 50′ 37″ East (see Figure 1). This site is situated within the 973 km² forest reserved areas managed by the Sabah Foundation.

For model evaluation and comparison at BKT, we selected the period of January-March and August-October 2007 to represent rainy and dry season, respectively. However, due to observation data completeness only January-March period was considered for DNV station. Statistical measures calculated were Mean Normalized Gross Error (MNGE), Unpaired Peak Accuracy (UPA), and Mean Normalized Bias Error (MNBE) with the criteria suggested by [14]. The definitions of all statistical measures used for the evaluation are presented in table 2 below.

Table 2. Definition of the evaluation statistical measures for ozone simulation.

Parameters	Formula	Suggested criteria
MNGE	$NGE = \frac{1}{N} \sum_{i=1}^{N} \frac{\left M_{i} - O_{i} \right }{O_{i}} \ 100$	Ozone: ≤ +35 %
UPA	$UPA = \frac{M_{\text{max}} - O_{\text{max}}}{O_{\text{max}}} 100$	Ozone: ≤ ±20 %
MNBE	$MNBE = \frac{1}{N} \sum_{i=1}^{N} \frac{M_i - O_i}{O_i}$	Ozone: ≤ ±15 %

Notes:

M-modelled value (model outputs for the first layer in different grids); O-observations; \overline{O} : mean- observation;

N-number of observations.

Source: [18].

3. Results and Discussions

Figure 1 presents the spatial distribution of monthly average ozone of selected months (Jan, March, July and August) over the modelling domain for the year of 2007. In March, higher concentration of ozone was seen over the higher altitude as well as in August. In January and July, higher concentrations of ozone were seen in the lower altitude which seems to be affected by the seasonal weather pattern in the region.

Highest monthly average concentrations found in the domain for January, March and September were 66, 61 and 48 ppb. The maximum hourly concentrations for all months in the year ranged from 67-154 ppb. In January, ozone concentrations were seen high at Surabaya and Hanoi while in other months was seen also in other places such as South Sumatera, West Kalimantan and North Malaysia. Urban plumes from the SEA big cities were also well captured through the model simulation results. Northeast and Southwest monsoon patterns seemed to affect the ozone plume movement in the SEA. In January at the upper latitude, NE monsoon brought pollutants from the origin sources to the southwest direction while at the lower latitude (Indonesia) the plume moved to NE/E direction. In August and November at

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the lower latitude the plume moved NW/W direction while in the upper latitude SW monsoon brought the pollutants to the NE direction.

Ozone concentrations at remote sites of the GAW station at two stations (BKT, Indonesia and DNV, Malaysia) were extracted from the model output and were included in the comparison. The scatter plots of hourly simulated ozone concentrations as compared to the measurements at the two stations are presented in figure 2. At BKT, the correlation coefficient derived from the hourly data presented in the scatter plot was 0.443 while at DNV it was slightly higher of 0.497. Even though better correlation coefficient was seen in DNV (maybe due to shorter period of data), evaluation the two stations showed somehow a contradictive result. Ozone simulation seems to be underestimated in DNV while overestimation was seen in BKT. Inaccurate EI especially the local emission sources might affect these discrepancies for both anthropogenic and biogenic emissions. In addition, complex photochemistry in the region especially under convective dominated meteorology could not be well captured by the models.

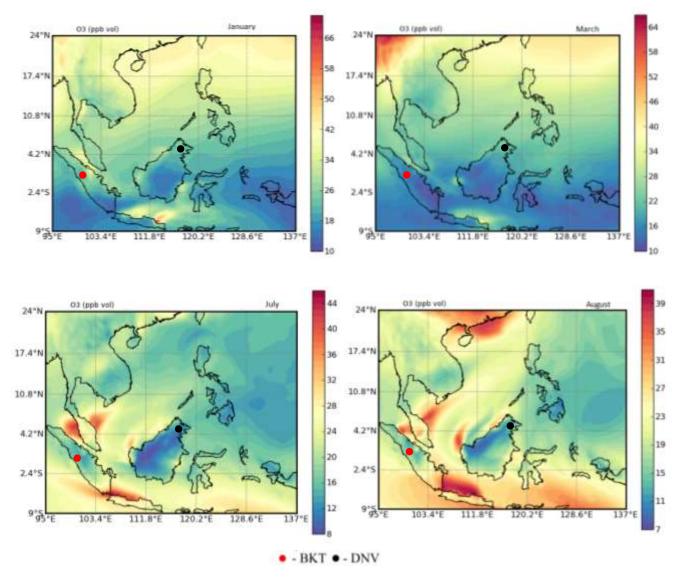
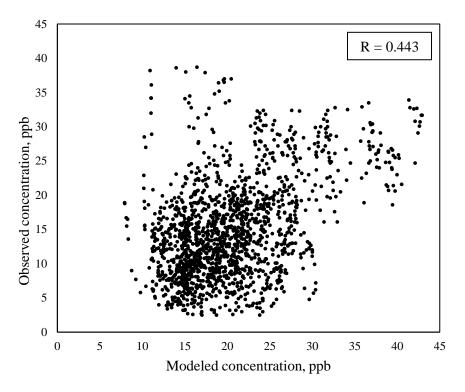


Figure 1. Spatial distribution of ozone for the month January, March, July and August 2007.

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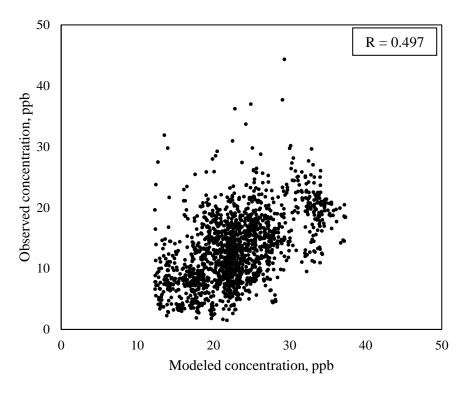
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The next step is to calculate the statistical measures for model performance evaluation (presented in table 3) and the values were then compared to the suggested criteria. At BKT, two parameters (MNGE and UPA) satisfied the criteria while in DNV, only UPA satisfied the criteria. MNBE values at the two sites were well above the suggested criteria. Regional ozone simulation at the remote sites normally performs better than in the urban areas but perhaps inaccurate estimation of both biomass open burning and biogenic emission in Sumatra and Kalimantan would affect this moderate performance.



a) BKT station, Indonesia (period of Jan-March and Aug-Sept)

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b) DNV station, Malaysia (period of Jan – March)

Figure 2. Scatter plots of modelled vs observed ozone concentrations at two GAW stations.

Table 3. Statistical measures analyzed for comparison between model output and observation.

No	Station name	Statistical measures					
	Station name	MNGE (%)	UPA (%)	MNBE (%)			
1	BKT station, Sumatera, Indonesia	34.9	14.7	36.7			
2	DNV station, Sarawak, Malaysia	52.3	-15	40.2			

Note: Bolded values satisfy the criteria below

Criteria for ozone simulation [18]:

MNGE: $\leq +35\%$, UPA: $\leq \pm 20\%$, and MNBE: $\leq \pm 15\%$.

4. Conclusion

Photochemical smog modelling framework of WRF-CHIMERE was applied to simulate surface ozone over SEA. Complete modelling chain starting from emission inventory compilation for ozone precursor, VOC speciation, temporal and spatial distribution was done to prepare model ready input data. Simulated ozone over the higher altitude showed higher concentrations in Jan-Apr than those simulated during the period of May-Aug. Seasonal variation of ozone was successfully simulated that was affected by monthly variation of ozone precursor emission and meteorology. Monsoon circulation affected the ozone plume movement in the domain. In January at the upper latitude, NE monsoon brought pollutants from the origin sources to the southwest direction while in August SW monsoon brought the pollutants to the NE direction. In the same months at the lower latitude (Indonesia) the plume moved to NE/E direction while in August the plume moved NW/W direction. High ozone concentrations over the year were simulated over the equatorial zone. Modeling results were further evaluated using the ground observation available at the two GAW stations in BKT and DNV station. Model results seemed to

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overestimate the observation in BKT and a contradictive result was seen in DNV. However, at least two statistical parameters of MNGE and UPA satisfied the criteria for ozone simulation thus suggesting a moderate model performance as also seen in other big cities. Satellite data that observes the total ozone column can be used to evaluate the model performance especially for the spatial distribution. There are still rooms for improvement such as emission inventory updates, VOC speciation, temporal and spatial distribution of ozone precursor emissions.

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