Sensitivity of WRF-Chem model resolution in simulating tropospheric ozone in Southeast Asia

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Abstract. In this paper, WRF-Chem model response to horizontal resolution has been presented in simulating tropospheric ozone distribution during an intense biomass burning across Southeast Asia. Model resolution is varied between 100 km and 20 km. Enhanced fire emissions were also considered in the 20 km resolution simulation. Evaluations were made against observed meteorology such as temperature, relative humidity, wind speed and direction. Spatio-temporal distribution of ozone precursors such as NO2 and CO at the surface retrieved from OMI and MOPITT instruments respectively, were compared against model outputs. Ozonesonde datasets for ozone profile from SHADOZ campaign at Watukosek-Java, Hanoi and Kuala Lumpur were used in evaluating simulated results. All the model simulations adequately represented the observed meteorology. Except in Watukosek-Java where ozone levels were overrepresented, the levels in other locations such as Kuala Lumpur and Hanoi were captured adequately. For model simulations using low-resolution, high-resolution and high-resolution with enhanced fire emissions in Hanoi, Kuala Lumpur and Watukosek-Java region, normalized bias factors are around -0.06, 0.14 and 0.22; 0.01, 0.28 and 0.18, and; 1.20, 3.36 and 3.21, respectively. Normalized root mean square error obtained is as low as 0.09 in Hanoi, and as high as 1.02 in Watukosek-Java region.

Keyword: Ozone, WRF-Chem, resolution, carbon monoxide, nitrogen dioxide, Southeast Asia

1. Introduction
Ozone is a reactive gas and has been favourable to human by forming a protective layer at the stratosphere which prevents harmful solar ultraviolet (UV) radiation from reaching the surface of the Earth, but ground level ozone poses great danger to plants and human health. It is usually a major constituent of smog at the troposphere and formed by photochemical oxidation of volatile organic compounds (VOCs) and/or carbon monoxide (CO) in the presence of oxides of nitrogen (NOx) [1]. Major sources of these precursors are anthropogenic and their increased emissions observed in Southeast Asia could be attributed to rapid growth in the region [1]. Human activities significantly contributing to higher levels of these precursors in the region include transportation, industrial activities, and more predominantly open burning of biomass. While regional ozone concentrations and distribution is
challenging to determine due to the non-linearity in its formation, understanding the distribution of the major precursors - in this study CO and NOx, would provide clarity on the influence of contributing factors such as biomass burning and valuable information in abating air pollution.

Previous reports on regional ozone in some parts of Southeast Asia highlighted that the impact of peat fires and biomass burning emissions in the formation of photochemical smog and increased ground ozone concentrations \[1,2\]. Mohtar et al. also reported seasonal variation of gaseous air pollutants such as ozone in Malaysia attributed to the high level of increased concentrations of precursors in monsoon period \[3\]. Thus far according to our literature survey studies on model sensitivity in simulating the formation and spatial distribution of tropospheric ozone and its precursors across Southeast Asia are very scarce. Therefore, we have used a regional chemical transport model to study the effect of varying horizontal grid resolution and enhanced fire emissions during a period with increased biomass burning haze, in simulating meteorology (temperature, relative humidity, wind speed and direction) and the distribution of ozone and its precursors – CO and NO2.

2. Model data and configuration

2.1. Model set-up

Model response to horizontal grid scale in simulating ozone and its precursors, has been studied using Weather Research Forecasting model coupled with Chemistry (WRF-Chem v 3.9) with a single domain over Southeast Asia. The model horizontal grid resolution was varied between 100 km to 20 km (WRFC_100km and WRFC_20km). For further analysis, fire emissions enhancement are included in the simulation with 20 km grid scale (WRFC_20kmX). The duration of the simulation is 15 days (00:00 UTC 15 June – 00:00 UTC 30 June 2013).

Physics and chemistry models adopted are according to previous work. We used Regional Acid Deposition Model, 2nd generation (RADM2) gas-phase chemistry mechanism combined with Modal Aerosol Dynamics Model for Europe (MADE) and Secondary Organic Aerosol Model (SORGAM). Initial and boundary conditions for meteorological variables were obtained from the National Centre for Environmental Prediction FiNal reanalysis (NCEP-FNL). Initial chemical boundary conditions were set using global chemistry Model for Ozone and Related Chemical Tracers (MOZART) output.

2.2. Emission input

Anthropogenic emissions were obtained from two global emission inventories – Reanalysis of TROPospheric chemical composition over the past 40 years (RETRO) and Emission Database for Global Atmospheric Research (EDGAR). Biomass burning emissions estimated using hotspot datasets obtained from MODIS C6 collection, and the emission inventories were preprocessed into the model using modified PREP-CHM-SRC tool. Biogenic emissions were estimated using the Model of Emissions of Gases and Aerosols from Nature (MEGAN2.1).

2.3. Model evaluation data

We made comparisons between model outputs and satellite retrievals from instruments such as Measurement of Pollution In the Troposphere (MOPITT) and Ozone Monitoring Instrument (OMI) for the distribution of surface CO and tropospheric NO2, respectively. O3 vertical profile from SHADOZ datasets at Hanoi, Kuala Lumpur and Watukosek-Java is used for evaluating simulation results \[4\]. Metric is used for evaluation include correlation coefficient (COR.), root mean square error (RMSE), normalized root mean square error (NRMSE) and normalized mean bias factor (NMBF).

We validated the model outputs using meteorological profiles such as temperature, relative humidity, wind speed and direction at the SHADOZ ozonesondes locations – Hanoi, Kuala Lumpur and Watukosek-Java, observed during O3 measurements initiated at 05:58 UTC 26 June, 03:59 UTC 17 June and 05:30 UTC 26 June 2013 respectively. For temporal evaluation of these meteorological variables, 15-day averaged evaluation of WRF-Chem simulations were made in Singapore and Brunei Darussalam using radiosonde datasets from Department of Atmospheric Science, University of Wyoming \[5\].
3. Model evaluation

3.1. Meteorology evaluation and precursors distribution

The averaged evaluations of meteorological variables in Brunei and Singapore showed that the low and high-resolution simulations were adequately represented (Table 1). This confirmed that the model is suitable to simulate air pollutants formation, transport and distribution in the Southeast Asia.

Meteorology in model simulations evaluated against observations by the SHADOZ ozonesonde instruments in Hanoi, Kuala Lumpur and Watukosek-Java, revealed that variables considered were well predicted in Kuala Lumpur, wind was well represented while Java area has missing data (Table 2).

Time-averaged CO and NO2 distribution from all simulations were compared to retrievals from MOPITT and OMI respectively. The high-resolution simulation with enhanced fire emissions captured the CO distribution better especially across Borneo region (Figure 1). High-resolution simulations presented better detail of tropospheric NO2 across the region with slight overrepresentation than observation in areas where biomass burning was dominant (Figure 2).

Table 1. Mean evaluation of air temperature, relative humidity, wind speed and direction profiles in Brunei (4.93° N, 114.93° E) and Singapore (1.22° N, 103.59° E) between 15th and 30th June 2013.

|        | Brunei COR | RMSE | NRMSE | NMBF | Singapore COR | RMSE | NRMSE | NMBF |
|--------|-------------|------|--------|-------|----------------|------|--------|-------|
| TEMP   | 0.999       | 0.924| 0.016  | 0.999 | 0.849          | 0.817| 0.142  | 0.915 |
| (Celsius) | WRFC_100km  | 1.582| 0.017  | 1.78  | 1.834          | 0.177| 0.186  | 0.178 |
| RH     | 0.858       | 0.171| 0.124  | 0.844 | 0.718          | 0.176| 0.138  | 0.141 |
| (%) WRFC_20km | 14.969   | 0.171| 0.124  | 0.844 | 0.718          | 0.176| 0.138  | 0.141 |
| WSPD   | 0.849       | 0.176| 0.124  | 0.844 | 0.718          | 0.176| 0.138  | 0.141 |
| (m/s)  | 0.181       | 0.176| 0.124  | 0.844 | 0.718          | 0.176| 0.138  | 0.141 |
| WDIR   | 0.757       | 0.203| 0.124  | 0.844 | 0.718          | 0.176| 0.138  | 0.141 |
| (degree) | WRFC_20km  | 0.737| 0.191  | 0.844 | 0.718          | 0.176| 0.138  | 0.141 |

Table 2. Temperature, relative humidity, wind speed and direction vertical profiles evaluation in Hanoi, Kuala Lumpur and Watukosek-Java

|        | Hanoi COR | RMSE | NRMSE | NMBF | Kuala Lumpur COR | RMSE | NRMSE | NMBF | Watukosek-Java COR | RMSE | NRMSE | NMBF |
|--------|------------|------|--------|-------|------------------|------|--------|-------|-------------------|------|--------|-------|
| TEMP   | 0.999      | 0.964| 0.007  | 0.999 | 0.999            | 1.030| 0.010  | 0.999 | 1.209             | 0.012| -0.052 |       |
| (Celsius) | WRFC_100km | 1.824| 0.010  | 0.999 | 0.999            | 1.030| 0.010  | 0.999 | 1.209             | 0.012| -0.052 |       |
| RH     | 0.855      | 0.163| 0.083  | 0.743 | 12.967           | 0.232| 0.133  | 0.818 | 17.175            | 0.215| 0.520  |       |
| (%) WRFC_20km | 11.568   | 0.163| 0.083  | 0.743 | 12.967           | 0.232| 0.133  | 0.818 | 17.175            | 0.215| 0.520  |       |
| WSPD   | 0.846      | 0.201| 0.155  | 0.743 | 12.704           | 0.227| 0.102  | 0.919 | 15.520            | 0.194| 0.517  |       |
| (m/s)  | 0.822      | 0.198| 0.133  | 0.723 | 12.439           | 0.222| 0.094  | 0.919 | 14.241            | 0.178| 0.458  |       |
| WDIR   | 0.960      | 1.070| 1.671  | 0.902 | 2.731            | 0.094| 0.008  |       |                   |       |        |       |
| (degree) | WRFC_100km | 2.417| 0.107  | 0.167 | 0.902            | 2.731| 0.094  | 0.008 |                   |       |        |       |
|        | 0.956      | 0.131| 0.243  | 0.874 | 3.102            | 0.106| 0.014  |       |                   |       |        |       |
|        | 0.960      | 2.588| 0.115  | 0.192 | 0.880            | 3.048| 0.104  | 0.018 |                   |       |        |       |
| WDIR   | 0.691      | 64.135| 0.178  | 0.994 | 9.853            | 0.042| 0.017  |       |                   |       |        |       |
| (degree) | WRFC_20km | 66.737| 0.185  | 0.995 | 9.049            | 0.039| 0.013  |       |                   |       |        |       |
|        | 0.694      | 64.430| 0.179  | 0.993 | 10.455           | 0.045| 0.011  |       |                   |       |        |       |
Figure 1. Surface CO distribution from: top left - MOPITT; top right - WRFC_100km; bottom left - WRFC_20km; bottom right - WRFC_20kmX

Figure 2. Tropospheric NO2 distribution (below 200 hPa) from: top left - OMI; top right - WRFC_100km; bottom left - WRFC_20km; bottom right - WRFC_20kmX
3.2. O3 evaluation

The SHADOZ ozonesondes at three locations in Southeast Asia - Java, Hanoi and Kuala Lumpur, were used to evaluate the vertical profiles of O3 from the model results. Overall, the evaluations revealed that combined enhanced fire emissions and high-resolution improved O3 simulation especially in Hanoi with lowest error and bias. With a more stable meteorology such as wind in Kuala Lumpur, the low-resolution simulation performed better. The performance observed in Watukosek-Java was worse (Table 3).

At Hanoi, O3 mixing ratio observed was around 35 ppbv at the surface and increased rapidly with altitude (Figure 3). The high surface CO mixing ratio in the presence of excess tropospheric NO2 observed in Hanoi could be responsible for the increased tropospheric O3 mixing ratio (Figures 1 and 2). Although the concentration reduced to around 30 ppbv between 850 hPa and 700 hPa, the mixing ratio was steady around 35 ppbv between 650 hPa and 400 hPa before it started increasing up to the stratosphere. High-resolution simulations (WRFC_20km and WRFC_20kmX) had better representation of observed O3 mixing ratios from surface to 850 hPa and from 650 hPa upward. The low-resolution simulation (WRFC_100km) slightly underrepresented the O3 observations near the surface. It was observed that enhanced fire emissions improved model results in high-resolution simulations (Table 3).

At Kuala Lumpur, observed O3 mixing ratio was around 30 ppbv at the surface and slightly reduced upward with noticeable reductions at 850 hPa to 750 hPa and 550 hPa to 400 hPa (Figure 3). The high-

### Table 3. Evaluation of O3 profile between SHADOZ ozonesondes and WRF-Chem simulations in Hanoi, Kuala Lumpur and Watukosek-Java.

| Location         | Simulation | Correlation coef. (r) | RMSE (ppmv) | NRMSE | NMBF |
|------------------|------------|-----------------------|-------------|--------|------|
| Hanoi            | WRFC_100km | 0.938                 | 0.010       | 0.112  | -0.060 |
|                  | WRFC_20km  | 0.857                 | 0.024       | 0.269  | 0.208  |
|                  | WRFC_20kmX | 0.911                 | 0.008       | 0.088  | 0.069  |
| Kuala Lumpur     | WRFC_100km | -0.002                | 0.007       | 0.323  | 0.007  |
|                  | WRFC_20km  | 0.255                 | 0.015       | 0.642  | 0.275  |
|                  | WRFC_20kmX | -0.123                | 0.011       | 0.488  | -0.087 |
| Watukosek-Java   | WRFC_100km | -0.518                | 0.032       | 0.476  | 1.196  |
|                  | WRFC_20km  | -0.372                | 0.069       | 1.023  | 3.355  |
|                  | WRFC_20kmX | -0.333                | 0.064       | 0.956  | 3.213  |

**Figure 3.** Vertical profiles of O3 from SHADOZ and WRF-Chem simulations in: A. Hanoi; B. Kuala Lumpur and; C. Watukosek-Java.
resolution simulations predictions were too high at the surface (> 60 ppbv). This could be attributed to the overrepresentation of tropospheric NO2 in the high-resolution simulations, which is a precursor to O3 formation (Figure 2). Although, the error reduced above 850 hPa, the overrepresentation of O3 mixing ratios was up to the 450 hPa level. Above the 450 hPa, the predictions were below O3 observations. On the other hand, the WRFC_100km had a good result at the surface but slightly lower below 900 hPa. WRFC_100km had similar results to WRFC_20km from 850 hPa upward.

At Watukosek-Java, the ratio of O3 observed at the surface was very high (> 60 ppbv) (Figure 3). Although the surface CO was less compared to Kuala Lumpur and Hanoi, the abundance of tropospheric NO2 could be attributed to the excessive formation of O3 at the surface in Watukosek-Java (Figure 2). From the surface, the O3 abundance was up to 800 hPa before it reduced to around 30 ppbv and the reduction continued from 600 hPa upward. The high-resolution simulations results were very similar to the observations from surface to 800 hPa, but they diverge against observations with O3 mixing ratio increasing from 600 hPa upward. The low-resolution simulation failed to capture the O3 levels observed. WRFC_100km predicted low O3 mixing ratio below 800 hPa and high above 600 hPa.

4. Conclusions

WRF-Chem response to model resolution was assessed in simulating tropospheric O3 in Southeast Asia. All the model simulations adequately represented the observed meteorology (correlation coefficients above 0.9, 0.8, 0.8 and 0.6 for air temperature, relative humidity, wind speed and direction respectively in Tables 1 and 2) and spatial distribution of O3 precursors (CO and NO2) in the troposphere (Figures 1 and 2), except in Watukosek-Java region where ozone levels were overrepresented (Table 3). The levels in other locations such as Kuala Lumpur and Hanoi were captured adequately. Normalized root mean square error was as low as 0.09 in Hanoi, and as high as 1.02 in Watukosek-Java region.

Although high-resolution simulation in this study gave insignificant difference in meteorology and increased error and bias for tropospheric O3, with enhanced fire emissions it represented tropospheric O3 and precursors better in the region. Thus, adopting higher grid scale with higher emission inventories resolution could further improve the regional simulations of tropospheric O3 in Southeast Asia.

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