Surface ozone simulation over Japan using a new atmospheric chemical-transport model (NICAM – CHASER)

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Outline

1. We performed NICAM-CHASER for simulating ozone concentrations in the period of summer 2010
2. We compared them with measurements in three sites Maebashi, Komae and Tsukuba near Tokyo in Japan.
3. To investigate an impact of the meteorological fields to the ozone concentrations, we compared NICAM results in summer 2010 with those obtained by Murata (2014) in 2007.
4. Conclusion
Background

The formation of ozone:

\[ O + O_2 + M \rightarrow M + O_3 \]

Sunlight splits nitrogen dioxide into nitric oxide and an oxygen atom which provides the primary source of the oxygen atoms required for ozone formation.

\[ NO_2 + hv \rightarrow NO + O \]

Ozone formation in the troposphere requires both NOx and VOCs (such as hydrocarbons).

\[ NOx + VOC + hv \rightarrow O_3 + \text{other products} \]

And CO contributes to formation of ozone by NO\(_2\) creation as follow:

\[ HO_2 + NO = NO_2 + OH \]
\[ OH + CO = H + CO_2 \]
\[ H + O_2 + M = HO_2 + M \]

Simplified diagram of the chemical interactions

(Sudo, 2000)
• The Kanto region is the most highly developed, urbanized, and industrialized part of Japan. Its population is over 30 million people.

• Emissions from industrial facilities and electric utilities, motor vehicle exhaust, gasoline vapors, and chemical solvents are some of the major sources of NOx and VOCs.

• In this study, we focus on the Kanto region to calculate the concentration of surface ozone by using Stretch-NICAM (MEXT/RECCA/SALSA, 2013) couples with chemistry module of CHASER.
NICAM

- NICAM (non-hydrostatic icosahedral atmospheric model) by Tomita and Satoh (2004) and Satoh et al. (2008). This new generation GCM has capability of simulating MJO with \( dx=3.5\text{km} \) in a global scale (Miura et al., 2007). Recently, global simulation has been executed using K-computer in Japan with \( dx=870\text{m} \).
- Using a stretched grid system (Tomita, 2008b) compute effective simulations in the target region.

NICAM grid system

Resolution \( \sim \sqrt{\text{S/N}} \)

\( N=10\times4g \)
\( g = \text{Glevel} \)
\( S = \text{Earth surface} \)

Glevel 0
(7141km)

Uniform grid Glevel 6
(112km)

Glevel 6 + Stretch100
\( (dx=11\text{km} \text{ around the stretched center (140E, 35N)}) \)
CHASER

- CHASER (named chemical atmospheric general circulation model (AGCM) for study of atmospheric environment and radiative forcing) by Sudo et al., 2002a, 2002b which is originally coupled with MIROC.

- CHASER has been well validated both in global scale (Sudo et al, 2003; Sudo & Akimoto, 2006) and regional scales that Chatani and Sudo (2011) compared CHASER-simulated ozone with observation over Japan for the period from 1996-2005.

- Chemistry components in this version of CHASER included:
  - 56 chemical species
  - 142 chemical reactions

- The principal objective of CHASER in this study: Calculate the distribution of ozone and its precursors.
Calculated conditions:

Period: Summer (26 July to 9 August) in 2010
Region: Kanto region including Tokyo in Japan
Layers: 40 layers (from 0m – 39620m)
Resolution: $dt = 30s; \text{rlevel} = 2$ (160 regions), $\text{glevel} = 6$ ($dx=11\text{km}$).
Cloud scheme: NSW6 (Tomita, 2008a) without cumulus parameterization
Chemistry: CHASER (Sudo et al. 2002)
Radiation type: MSTRNX (Sekiguchi and Nakajima, 2008)
Emission NOx and CO: Combination EAGrid2000 of Kannari et al. (2007) with REAS(v2.0) by Kurokawa et al. (2013)
Validation data: Atmospheric Environmental Regional Observation System (AEROS) in 2010.
Nudging: by NCEP-FNL (http://rda.ucar.edu/datasets/ds083.2/) available at 1 degree resolution and at six hour intervals.
Anthropogenic emission flux of NOx & CO

**REAS** (Regional Emission inventory in Asia) by JAMSTEC, NIES etc. Resolution: 0.5 degree

**EAGrid** (East Asian air pollutant emission GRID database) by Drs. Kannari, Tonooka, Murano etc. Resolution: 1km (Japan), 0.5 degree (others)
- Air pollution of Ox and CO can distribute beyond nations.
- In this case, Ox and CO are transported from China to Korea and Japan.
- In the Kanto region, maximum Ox in the afternoon on August 1 is mainly caused by domestic pollution.

Our model is not usually regional model. So it can simulate Ox-NOx-CO not only over Kanto/Japan but also over East Asia.
The ozone concentration begins to increase after sunrise around 08:00-09:00 and attains its maximum level in the afternoon until 15:00 mainly due to the photolysis of NO\textsubscript{2}. During the late evening hours 18:00-21:00 the surface ozone concentration tends to decrease and reaches to a minimum.

We compared NICAM at various sites => Choose 3 typical sites for Kanto area
In this study, the maximum concentrations of ozone over the Kanto area of Japan were calculated to be 100 - 150 ppb during the simulation period, which was larger than the Japanese air quality standard for ozone (60 ppb).
Surface NOx in the Kanto region (JST)

<table>
<thead>
<tr>
<th>City</th>
<th>Mean Calculated</th>
<th>Mean Observed</th>
<th>Correlation coefficient (R²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Komae</td>
<td>11.763</td>
<td>29.460</td>
<td>0.155</td>
</tr>
<tr>
<td>Tsukuba</td>
<td>9.959</td>
<td>15.354</td>
<td>0.066</td>
</tr>
<tr>
<td>Maebashi</td>
<td>4.048</td>
<td>14.176</td>
<td>0.076</td>
</tr>
</tbody>
</table>
### Surface CO in the Kanto region (JST)

<table>
<thead>
<tr>
<th>CO</th>
<th>Mean Calculated</th>
<th>Mean Observed</th>
<th>Correlation coefficient (R²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Komae</td>
<td>153</td>
<td>334</td>
<td>0.138</td>
</tr>
<tr>
<td>Tsukuba</td>
<td>138</td>
<td>317</td>
<td>0.272</td>
</tr>
<tr>
<td>Maebashi</td>
<td>112</td>
<td>284</td>
<td>0.003</td>
</tr>
</tbody>
</table>
• Ozone concentrations are high during day time when temperatures are high and solar radiation is intense.

• During the night, ozone is not formed appreciably. While NO and ozone combine to form NO\(_2\) and oxygen until either the NO or ozone is consumed.

• The reduction in NO\(_2\) is due to the production of O\(_3\) by photolysis. While the effect of CO is such that it slowly oxidizes nitrogen monoxide NO to nitrogen dioxide NO\(_2\) and thus indirectly affects the concentration of ozone.

• The concentrations NO\(_2\) and CO were strongly negatively correlated with O\(_3\). Higher concentrations NO\(_2\) and CO are associated with lower ozone concentrations and back, due to photochemical reactions.
Diurnal variation of ozone simulated by Stretch-NICAM-Chem in 2007

[SALSA, 2014]
The performance of simulated Ox in 2010 is worse than that in 2007 because the observed Ox concentrations in 2010 are lower than those in 2007 possibly due to decreasing emission fluxes of NOx and CO and higher temperature in 2007.
Conclusion

• The comparison of calculated and observed ozone as well as its precursors shows that the models appear to reproduce the diurnal variation of observed ozone well.
• Models tends to underestimate the concentration NOx and CO => increase more emission inventory for NOx and CO in the model.
• NICAM –CHASER have succeeded in simulating urban air pollution in regional scale
• NICAM-CHASER model with the stretch-grid system can be applicable for any cities. We will try to adopt it to megacities in East Asia.”
• We will compare NICAM at the western part of Japan as well as other Asian countries.

Thank you very much!
Summer season with strong land-ocean thermal gradients and the resulting mesoscale sea breeze circulation.
• \( O + O_2 + M = O_3 + M \)  
• \( \text{NO}_2 + \text{hn} = \text{NO} + O \)  
• \( O_3 + \text{NO} = \text{NO}_2 + O_2 \)  
• \( \text{RH} + \text{OH} = \text{H}_2\text{O} + \text{R} \)  
• \( \text{R} + O_2 + M = \text{RO}_2 + M \)  
• \( \text{RO}_2 + \text{NO} = \text{NO}_2 + \text{RO} \)  
• The key reaction in the VOC oxidation cycle is the conversion of NO to \( \text{NO}_2 \)  
• \( \text{OH} + \text{HCHO} = \text{H}_2\text{O} + \text{HCO} \)  
• \( \text{HCO} + \text{O}_2 = \text{HO}_2 + \text{CO} \)  
• \( \text{HO}_2 + \text{NO} = \text{NO}_2 + \text{OH} \)  
• \( \text{OH} + \text{CO} = \text{H} + \text{CO}_2 \)  
• \( \text{H} + \text{O}_2 + M = \text{HO}_2 + M \)  
• \( \text{HCHO} + \text{hn} = \text{H} + \text{HCO} \)  
• Another reaction is central to a basic understanding of ozone formation: the \( \text{NO}_2 \) plus radical sink reaction that forms nitric acid.  
• \( \text{NO}_2 + \text{OH} + M = \text{HNO}_3 + M \)  
• (1)  
• (2)  
• (3)  
• (4)  
• (5)  
• (6)  
• (7)  
• (8)  
• (9)  
• (10)  
• (11)  
• (12)  
• (13)
The specific ratio of NO\textsubscript{x} to VOC determines the efficiency of the ozone formation process.

- The relative balance of VOCs and NO\textsubscript{x} at a particular location helps to determine whether the NO\textsubscript{x} behaves as a net ozone generator or a net ozone inhibitor.
- When the VOC/NO\textsubscript{x} ratio in the ambient air is low (NO\textsubscript{x} is plentiful relative to VOC), NO\textsubscript{x} tends to inhibit ozone formation. In such cases, the amount of VOCs tends to limit the amount of ozone formed, and the ozone formation is called "VOC-limited".
- When the VOC/NO\textsubscript{x} ratio is high (VOC is plentiful relative to NO\textsubscript{x}), NO\textsubscript{x} tends to generate ozone. In such cases, the amount of NO\textsubscript{x} tends to limit the amount of ozone formed, and ozone formation is called "NO\textsubscript{x}-limited".
- The VOC/NO\textsubscript{x} ratio can differ substantially by location and time-of-day within a geographic area. Furthermore, the VOC/NO\textsubscript{x} ratio measured near the ground might not represent the ratio that prevails in the air above the ground where most of the tropospheric ozone is generated.
• When using coarse-scale data from a reanalysis or GCM as lateral boundary conditions for a regional model without further constraint, the interior meteorological fields simulated by the regional model can deviate significantly from those of the driving fields. Four-dimensional data assimilation or "nudging" techniques provide one way to constrain the RCM and keep it from diverging too far from the coarse-scale fields.

• the model performs much better during daytime than nighttime for both chemical species and meteorological variables and different combinations of the available PBL and land surface schemes did not reduce the errors.

• Due to the long lifetime of ozone (about a week) in the troposphere, the distribution of ozone concentrations was greatly influenced by the airflow of the anticyclone. The simulated wind direction shows that Japan was under the control of westerly or northwesterly winds from Asia

• In general, the surface ozone exhibits strong diurnal variations, with a mid-afternoon maximum and an early-morning minimum. While the lifetime of NOx in the atmospheric boundary layer (about a day) is too short to allow transport over large distances, its lifetime in the upper troposphere is of the order of 5–10 days, which is sufficient even for intercontinental transport.