

## WRF-Chem Simulation of East Asian Air Quality: Sensitivity to Emissions Distributions

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## Introduction



- Developed finer resolution temporal (i.e. seasonal, day-of-week, diurnal) and vertical scaling for different categories and species of TRACE-P anthropogenic emissions inventory (Streets et al., 2003) in East Asia.
- Conducted two experiments in July of 2001: CTL (control run with default emissions) and SCL (scaling run with the new scaled emissions) to evaluate the roles of temporal and vertical scaling to prediction of NO<sub>2</sub>, SO<sub>2</sub> and O<sub>3</sub>.
- SCL continuous run four months: March, July, October and December of 2001 to evaluate model performance for East Asian air quality in different seasons.

(7 day spin-up, i.e., 22-28, Feb., 24-30, Jul., Sep., and Dec.)

## Model settings and observations data



### ≻Domain:

central: 35.18°N, 110°E 30km (232×172) 28 vertical levels (σ) with 6 within PBL the first model layer at ~37m Parameterizations:

long & shot wave radiation: CAM land surface model: NOAH boundary layer schem: YSU dry deposition: Wesely (1989) photolysis scheme: Fast-J gas chemistry: RACM aerosol scheme: MADE/SORGAM as well as other parameters



### ≻Observations:

The Acid Deposition Monitoring Network in East Asia (EANET)



- Biogenic emissions: calculated "online" within WRF-Chem using Guenther et al. (1994).
- Biomass burning: monthly averaged emissions from Streets et al. (2003) and Woo et al. (2003).
- Volcano SO<sub>2</sub> emissions: monthly averaged emissions at Miyakejima (139.53°E, 34.08°N, 813m MSL and located in the west Pacific Ocean) from Kajino et al. (2004)

placed in the fifth model layer (925hPa) (estimated smoke height: 450-760m)

> Anthropogenic emissions: TRACE-P emissions inventory.





# Diurnal variations for each sector of TRACE-P anthropogenic emissions





- Residential & weekday LDVs have 2 peaks;
- Percentage of LDVs & HDVs for each species was derived from U.S. EPA Nation Emissions Inventory 99.

## Diurnal variations for seven major species of weekday transportation emissions





- CO, NMVOC & NH3 have 2 peaks (LDVs domaints 90%);
- $\triangleright$  SO<sub>2</sub>, NO<sub>x</sub> peaks relatively small;
- $\rightarrow$  PM<sub>10</sub> & PM<sub>2.5</sub> relatively leveled during daytime;
- $\blacktriangleright$  BC & OC use the same profile as PM<sub>2.5</sub>.



| Species                 | Height of Emission Layer (m) |        |         |         |         |  |  |
|-------------------------|------------------------------|--------|---------|---------|---------|--|--|
|                         | 0-76                         | 76-153 | 153-308 | 308-547 | 547-871 |  |  |
| SO <sub>2</sub>         | 5                            | 30     | 35      | 25      | 5       |  |  |
| NO <sub>x</sub>         | 5                            | 40     | 25      | 25      | 5       |  |  |
| СО                      | 5                            | 70     | 20      | 5       |         |  |  |
| NH <sub>3</sub>         | 5                            | 75     | 15      | 5       |         |  |  |
| NMVOC                   | 5                            | 85     | 10      |         |         |  |  |
| PM <sub>2.5</sub>       | 5                            | 45     | 25      | 20      | 5       |  |  |
| <b>PM</b> <sub>10</sub> | 5                            | 55     | 20      | 15      | 5       |  |  |
| BC                      | 5                            | 65     | 20      | 10      |         |  |  |
| OC                      | 5                            | 70     | 15      | 10      |         |  |  |

Derived from U.S. EPA NEI 99;

- SO2: largest in the 3rd model layer, others: maximized in the 2nd layer;
- > All species are small near the surface and above 500m.

## Statistics of daily mean NO<sub>2</sub>, SO<sub>2</sub> & O<sub>3</sub> in Jul., 2001 for SCL & CTL vs. observations



| Site  | Statistics | N      | NO <sub>2</sub> |       | SO <sub>2</sub> |       | <b>)</b> <sub>3</sub> | Bias = $\frac{1}{N} \sum_{i=1}^{N} (P_i - O_i)$               |
|-------|------------|--------|-----------------|-------|-----------------|-------|-----------------------|---|
|       |            | SCL    | CTL             | SCL   | CTL             | SCL   | CTL                   | $GE = \frac{1}{N} \sum_{i=1}^{N} ( P_i - O_i )$               |
| China | R          | 0.38   | 0.36            | 0.54  | 0.54            |       |                       | $\frac{1}{NGE} = \frac{1}{N} \sum_{i=1}^{N} ( P_i - O_i )$    |
|       | Bias       | 0.46   | 2.30            | -1.09 | 1.43            |       |                       | <i>N</i> : the number of observat                             |
|       | GE         | 3.28   | 3.93            | 2.81  | 3.15            |       |                       | <i>P</i> : WRF-Chem prediction<br><i>O</i> : observed values. |
|       | NGE        | 106.22 | 144.27          | 95.91 | 142.54          |       |                       |   |
| Japan | R          | 0.64   | 0.65            | 0.84  | 0.83            | 0.67  | 0.67                  | •   |
|       | Bias       | -0.04  | 0.47            | -0.10 | 0.05            | 2.87  | 2.11                  | •   |
|       | GE         | 0.89   | 1.06            | 0.52  | 0.55            | 8.96  | 8.87                  |   |
|       | NGE        | 82.33  | 114.74          | 92.53 | 109.95          | 42.90 | 42.05                 |   |

$$GE = \frac{1}{N} \sum_{i=1}^{N} (|P_i - O_i|)$$

$$NGE = \frac{1}{N} \sum_{i=1}^{N} (|P_i - O_i| / O_i)$$
*N*: the number of observations;
*P*: WRF-Chem predictions;

- $\triangleright$  SCL simulation for NO<sub>2</sub> & SO<sub>2</sub> is in better agreement with observations at EANET sites in China and Japan, with higher correlation, lower bias, gross error & normalize gross error;
- SCL simulation is close to CTL for  $O_3$  at sites in Japan.

## **Frequency Distributions of NO<sub>2</sub> and SO<sub>2</sub> at EANET sites in China (top) & Japan (bottom) in Jul., 2001**





Over China: SCL frequency of NO<sub>2</sub> lower for lows; SO<sub>2</sub> lower for highs; SCL is better than CTL
 Over Japan: SCL frequencies are in better agreement with observations for NO<sub>2</sub> & SO<sub>2</sub>

## **CTL-SCL: Surface NO<sub>2</sub> difference in Jul., 2001**





- $\triangleright$  differences all positive: CTL allocates more NO<sub>x</sub> emissions in the surface layer
- large in major cities and industrial regions over China: 3-7 ppb
- largest in Beijing: up to 9 ppb
- small in South Korea & Japan

## **CTL-SCL:** Surface SO<sub>2</sub> difference in Jul., 2001





- differences all positive
- ▶ 6~8 ppb over northern and eastern China, Sichuan Basin, up to 10~12 in Chongqing, Taiyuan
- > over 26 ppb in Beijng, Shanghai & Seoul
- less than 10 ppb over Japan

# **Diurnal cycle of surface NO<sub>x</sub> and O<sub>3</sub> at EANET sites in Japan in Jul., 2001**





- daytime: SCL close to CTL, both 0.4 ppb lower than observations at noon;
- nighttime: SCL agree well with observations, CTL significantly overestimates NOx by a factor of 1.2~2.5.
- both realistically predict daily maximum (4:00 pm) and minimum O<sub>3</sub> (7:00 am);
- daytime: SCL close to CTL, both 4 ppb higher than observations after 10: am;
- nighttime: SCL overestimate 2 ppb, CTL underestimate 2 ppb.

# CTL-SCL: Surface daily, nighttime & daytime O<sub>3</sub> difference in Jul., 2001





- daily: -4~-6 ppb in northern & eastern China,
   -8 ppb in Beijing;
- nighttime: larger, -8 ppb over northern and eastern China, -12 ppb in Beijing;
- daytime: within ±2 ppb over vast areas of East Asia -2~-4 ppb in northern & eastern China.
- > reason for negative difference:
  - (1) larger NOx emissions at night for CTL produce high NOx concentrations, titrate more O<sub>3</sub>;
  - (2) large portion of nighttime NOx emissions available for the next day for CTL, close to CTL.



## Statistics of daily mean $NO_2$ , $SO_2 \& O_3$ in Mar., Jul., Oct., and Dec., 2001 (SCL vs. EANET observations)



| NO <sub>2</sub>                   | Statistics              | March   | July  | October   | December   | Four periods   |
|-----------------------------------|-------------------------|---|---|---|--|--|
| China                             | R                       | 0.52  | 0.38  | 0.54  | 0.65   | 0.58   |
|                                   | Bias                    | -0.28   | 0.46  | -1.70   | -4.03  | -1.39  |
|                                   | GE                      | 4.16  | 3.28  | 6.53  | 8.01   | 5.49   |
| Japan                             | R                       | 0.59  | 0.64  | 0.61  | 0.62   | 0.60   |
|                                   | Bias                    | -0.10   | -0.04   | 0.30  | 0.18   | 0.09   |
|                                   | GE                      | 1.03  | 0.89  | 1.03  | 1.00   | 0.99   |
|                                   |                         |   |   |   |  |  |
| SO <sub>2</sub>                   | Statistics              | March   | July  | October   | December   | Four periods   |
| SO <sub>2</sub><br>China          | Statistics<br>R         | March<br>0.55   | <b>July</b><br>0.54   | October<br>0.45   | December<br>0.62   | Four periods<br>0.61   |
| SO <sub>2</sub><br>China          | Statistics<br>R<br>Bias | March           0.55           -2.12  | July<br>0.54<br>-1.09   | October<br>0.45<br>-2.00  | December           0.62           -3.55  | Four periods           0.61           -2.18  |
| SO <sub>2</sub><br>China          | StatisticsRBiasGE       | March           0.55           -2.12           5.33                               | July           0.54           -1.09           2.81                                | October           0.45           -2.00           3.90                               | December           0.62           -3.55           5.03                               | Four periods           0.61           -2.18           4.27                               |
| SO <sub>2</sub><br>China<br>Japan | StatisticsRBiasGER      | March           0.55           -2.12           5.33           0.45                | July           0.54           -1.09           2.81           0.84                 | October           0.45           -2.00           3.90           0.74                | December           0.62           -3.55           5.03           0.56                | Four periods           0.61           -2.18           4.27           0.62                |
| SO <sub>2</sub><br>China<br>Japan | StatisticsRBiasGERBias  | March           0.55           -2.12           5.33           0.45           0.32 | July           0.54           -1.09           2.81           0.84           -0.10 | October           0.45           -2.00           3.90           0.74           0.29 | December           0.62           -3.55           5.03           0.56           0.16 | Four periods           0.61           -2.18           4.27           0.62           0.15 |

Bias = 
$$\frac{1}{N} \sum_{i=1}^{N} (P_i - O_i)$$
  
GE =  $\frac{1}{N} \sum_{i=1}^{N} (|P_i - O_i|)$ 

*N*: the number of observations;*P*: WRF-Chem predictions;*O*: observed values.

| O <sub>3</sub> | Statistics | March | July | October | December | Four periods |
|----------------|------------|-------|------|---------|----------|--------------|
| Japan          | R          | 0.45  | 0.67 | 0.69    | 0.76     | 0.67         |
|                | Bias       | -7.00 | 2.87 | 0.38    | -0.24    | -1.06        |
|                | GE         | 9.73  | 8.96 | 8.17    | 5.16     | 8.04         |

## SCL simulations and observations of NO<sub>2</sub> at EANET sites in Mar., Jul., Oct., and Dec., 2001





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## SCL simulations and observations of SO<sub>2</sub> at EANET sites in Mar., Jul., Oct., and Dec., 2001





## SCL simulations and observations of O<sub>3</sub> at EANET sites in Mar., Jul., Oct., and Dec., 2001





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## **Summary**



- Developed finer resolution temporal (i.e. seasonal, day-of-week, diurnal) and vertical scaling for different categories (i.e., power generators, industry, residential and transportation) and each species for TRACE-P anthropogenic emissions.
- Temporal and vertical distribution play and essential role on air quality modeling in East Asia.New scaled emissions improved WRF-Chem performance in predicting NO<sub>2</sub> and SO<sub>2</sub> (statistics and frequency distribution). The sensitivity is significantly large for NO<sub>2</sub> and SO<sub>2</sub>.
- > Performance of both default and new scaled emissions are statistically similar for  $O_3$ . The sensitivity is relatively weak for  $O_3$ .
- New scaled emissions could well predict spatial and seasonal variation of NO<sub>2</sub>, SO<sub>2</sub> and O<sub>3</sub> over East Asia.