Sub-Grid Variability (SGV) Approach to Air Quality Modeling

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February 6, 2007; Cape May, NJ
MARAMA workshop on WOE
Synopsis of Presentation

- CMAQ-AT fine-scale modeling (1-km) for Delaware-Prototype Study
- Sub-grid variability (SGV) – how to Introduce SGV into CMAQ simulations
- Applications of SGV
Fine-scale modeling w/CMAQ for Delaware Prototype Study

Apply fine-scale modeling to:

- capture detailed spatial gradients and temporal variability of air toxics concentration
- identify and characterize the hot spots of air toxics compounds
- provide inputs to exposure modeling
MM5 Configuration

- NCAR-PSU Mesoscale Model Version 5 (MM5)
- 36-, 12-, 4-km runs available for 2001
- 4-km grid scale domain nested down to 1-km grid scale for Delaware domain
- 1-km runs for July 2001
Figure 1. Temperature time series for MM5 predicted and monitored at the New Castle County Airport. Bias = 0.24 K; Gross Error = 2.4 K
Figure 2. Temperature fields interpolated from MM5 (layer 1) to 1.5 m for July 4th 2001 at 6:00 pm EST; left 4-km run and right 1-km run.
Figure 3. Dispersion parameters for July 4th 2001 at 6:00 pm EST:
Left side is 4-km grid; right side is 1-km grid.
Top is PBL height (m); bottom is ustar (m/s).
CMAQ-AT Configuration

- Modified CB-IV treats 20 gas-phase air toxics & provides primary and secondary components of carbonyl compounds

- Modeling from regional to fine scale (Delaware domain) accomplished by 1-way nesting

- 1999 NEI Emissions

- Emissions processed by SMOKE
4-and 1-km Modeling Domains
LUMS POND: Monitored vs Modeled Ozone

Date

Ozone (ppb)

CMAQ-4km
CMAQ-1km
Monitored
LUMS POND: Monitored vs Modeled Isoprene
KILLENS POND: Monitored vs Modeled O3 at 1km grid scale
LEWES: Monitored vs Modeled O3 at 1km grid scale
MLK: Monitored vs Modeled CO at 1km grid scale

Graph showing CO (ppm) over time from 2001-07-01 to 2001-07-15, comparing modeled CO (blue line) and monitored CO (pink line).
MLK: Monitored vs Modeled NO2 at 1km grid scale
Figure 4. CMAQ-AT ozone simulation: July 2nd 2001 at 7:00 pm EST. Top (Lhs: 36-km and Rhs: 12-km); bottom (Lhs: 4-km and Rhs: 1-km).
Figure 5: (a) primary formaldehyde, (b) secondary formaldehyde, (c) isoprene at 4:00 PM EST (July 2nd, 2001)
Figure 6: (a) primary acetaldehyde, (b) secondary acetaldehyde, (c) benzene and (d) CO (5:00 PM EST July 2nd, 2001)
Figure 7: (a) primary acrolein, (b) secondary acrolein
CMAQ simulations using 1 km grid sizes (July 17, 2001)

Layer 1 O3a*1000

Layer 1 NOa+NO2a
Layer 1 FORM PRIMARYa

Layer 1 BENZENEa*1000

a=CCTM_cb4tx1p_DEL_1kmACONC.A2.0

a=CCTM_cb4tx1p_DEL_1kmACONC.A2.010717

July 17, 2001 0:00:00
Min = 0 at (108,85), Max = 6 at (4,125)

July 17, 2001 0:00:00
Min = 0.0 at (104,7), Max = 2.2 at (30,151)
Layer 1 ISOPa*1000

a=CCTM_cb4tx1p_DEL_1kmACONC.A2.010717

July 17, 2001 0:00:00
Min= 0 at (108,86), Max=16 at (107,129)

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er 1 (FORMa-FORM_PRIMARY)

a=CCTM_cb4tx1p_DEL_1kmACONC.A2.010717

July 17, 2001 0:00:00
Min= 2 at (108,3), Max= 8 at (98,156)
Summary of Fine-Scale Modeling

Fine-scale modeling paradigm:
- Captures spatial and temporal variability of the air toxics compounds
- Provides prominent features in concentration fields (helps identify and characterize the hot spots of air toxics compounds)
- Provides evidence of the important role of photochemistry in modeling the carbonyl species
Sub-Grid Variability (SGV)

- SGV is present at all scales

- Factors contributing to SGV:
  - Within-grid source dispersion
  - Spatial heterogeneities from photochemical-dynamic coupling

Methodology for SGV from dispersion of within-grid sources. For this study, we present results for inert species using local scale modeling.

Methodology for SGV from within-grid photochemical reactive-dynamic interactions require coupled chemistry-dynamics modeling. For this study, we present results of 1 km CMAQ to describe SGV for coarser grid sizes.
Assume knowledge of SGV distribution for each model grid, time step

\[ \text{SAC} = C_g \times f_{\text{CSGV}} \]  

- \( C_g \) is gridded concentration (CMAQ….)
- \( \text{SAC} \) is “Concentration adjusted for SGV”
- \( f_{\text{CSGV}} \) is a non-dimensional weighting factor

Investigate: Three options for the non dimensional weighting factor:

- \( f_{\text{CSGV}} = 1 + \text{Coefficient of Variation (COV)} \) \hspace{1cm} (2a)
- \( f_{\text{CSGV}} = 95\text{th percentile of distribution in grid} \) \hspace{1cm} (2b)
- \( f_{\text{CSGV}} = \text{peak of distribution in grid} \) \hspace{1cm} (2c)

Choice of option is application dependent
Contributions to SGV using 1 km CMAQ

- Episodic study (July 2001)
- 36-12-4-1 km one-way nested CMAQ-AT simulations
- 12 km gridded SGVs, SACs from 1 km CMAQ simulations
- Example results for species with differing photo reactivities
Ozone Concentrations for 15th July 20 UTZ

12-km grid

4-km grid

1-km grid
Formaldehyde Concentrations for 15th July 20 UTZ

12-km grid

4-km grid

1-km grid
Benzene (CMAQ): 16th July 2001 at 11:00 UTZ

(A) 12 km  (B) 4 km  (C) 1 km
Benzene (ppb) (Time series for 12 km cells, July 2001)

Black(A)  Red(B)  Green (C)

Standard Deviation (ppb)

1+COV
Benzene SAC (1+COV) for July 2001
Time series & Box plots for HCHO
CMAQ(12), Std Dev, SAC (1+COV)

Grid cells  A&B Urban,  C Rural (see previous slide)
Box Plots for Benzene and Ozone
CMAQ (12), Std Dev, SAC (1+COV)
Grid cell: A, B (Urban) & C (Rural) (see previous slide)
Fig 6.a: O3 95 Percentile

Fig 6.c: O3 Peak-to-Mean

Fig 6.a: O3 Standard Deviation

Fig 6.d: O3 1+COV
Fig 4.a: FORM 95 Percentile

Fig 4.b: FORM Standard Deviation

Fig 4.c: FORM Peak-to-mean

Fig 4.c: FORM 1+COV
Fig 5.a: Benzene 95 Percentile
Fig 5.b: Benzene Standard Deviation
Fig 5.c: Benzene Peak-to-Mean
Fig 5.d: Benzene 1+COV
Summary of SGV

- SAC introduced as 1+COV
- SAC characteristics vary for different pollutant species
- SAC characteristics vary across model domain, e.g., urban SAC differ from rural results
- SGV for scales < 1 km not represented
Application of SGV to WOE in Modeled O3 Attainment Demonstrations
Application of SGV in WOE Analyses

Modeling guidance
- Relative Reduction Factor (RRF) is a single number
- Does not account for SGV inherent in grid modeling

SGV
- Application of SACs to the RRF can provide a range of future design values (DVF).
- Exploratory studies are needed to determine what statistic provides a reasonable range of values for the RFF.
- Upper bound of the DVF favors greater protection
- One possible approach for determining RRF range discussed
Some Statistics based on DE-Prototype Study
RRFs based on CMAQ Modeling for the 8-Hr Ozone SIPs

RRF estimation

- No fine-scale modeling is available
- A number of approaches are possible (e.g., roll-back)
- A simple approach is considered here

Range 2009 CMAQ concs

$$\text{RRF} = \frac{\text{Range 2009 CMAQ concs}}{\text{Range of 2002 CMAQ concs}} = [l,u]$$

l : lower bound
u : upper bound
RRF Estimation, Cont’d

- RRFs estimated by accounting for variations in modeled concentrations
- for cells in design value monitors and neighboring cells calculated
- for Base year modeled concentrations exceeding
  - 70 ppb
  - 85 ppb
  - 85 ppb – top 10 values
# RRFs in 9 Cells around Brandywine, New Castle County

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## RRFs in 9 Cells around Killens Pond, Kent County

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Ozone Trends in Delaware

For 1996-2006 Period
Kent County Killens Pond 1996 – 2006 Hourly O3 Trends

Kent County - ln(O3)

Noise and high frequency filtered

residue
New Castle County Brandywine 1996 – 2006 Hourly O3 Trends

New Castle County - ln(O3)

Noise and high frequency filtered

residue
Sussex County Seaford 1996 – 2006 Hourly O3 Trends

Sussex County - ln(O3)

Noise and high frequency filtered

Residue