1. Comparison CB-4 and SAPRC mechanisms
2. Improvement of Initial Condition
3. Improvement of meteorological simulations

Daewon W. Byun
S.T. Kim, B. Czader, F. Ngan, D. Lee, X. Li

Institute for Multi-dimensional Air Quality Studies (IMAWS)
University of Houston
1. CB-4 & SAPRC Comparison

- 2000 TexAQS Episode with TEI2000/imputed HRVOC
- 2006 TexAQS-2 Sept 6-8 Episode with TEI2000/imputed HRVOC
- 2006 TexAQS-2 Sept 6-8 Episode with 2005 projected EI
TexAQS 2000 Episode

NOAA Aircraft Canister

Improvement of high O3 predicted by SAPRC more pronounced with CMAQ

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TexAQS 2000
Episode
NOAA Aircraft
Ozone

CAMx with CB-4 well simulated O3 peak but overpredicted with SAPRC
(C) CMAQ CB-4

CMAQ with CB-4 underestimated O3 peak but well predicted with SAPRC

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TexAQS 2000 Episode

NOAA Aircraft

HNO3

CAMx with CB-4 and SAPRC both overpredicted HNO3, including the background

CMAQ with CB-4 overpredicted HNO3 slightly, but SAPRC compared well with obs.
2006 simulations: AQF - F2, 4-km resolution
To compare CMAQ simulations between CB-4 and SAPRC99 for projected EI (lower NOx) at 2005 level

CMAQ4.4, CB4, Projected EI for 2005

CMAQ4.4, SAPRC, Projected EI for 2005

Figure. Spatial plots of daily maximum 1-hour ozone concentrations with (a) CB4 and (b) SAPRC99 chemical mechanisms for August 15th, 2006.

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2006 simulations: AQF - F2, 4-km resolution
To compare CMAQ simulations between CB-4 and SAPRC99 for projected EI (lower NOx) at 2005 level

CMAQ4.4, CB4, Projected EI for 2005

CMAQ4.4, SAPRC, Projected EI for 2005

Figure. Spatial plots of daily maximum 1-hour ozone concentrations with (a) CB4 and (b) SAPRC99 chemical mechanisms for August 16th, 2006.
2006 simulations: AQF - F2, 4-km resolution

To compare CMAQ simulations between CB-4 and SAPRC99 for projected EI (lower NOx) at 2005 level

CMAQ4.4, CB4, Projected EI for 2005

CMAQ4.4, SAPRC, Projected EI for 2005

Figure. Spatial plots of daily maximum 1-hour ozone concentrations with (a) CB4 and (b) SAPRC99 chemical mechanisms for August 18th, 2006.
2006 simulations: AQF - F2, 4-km resolution
To compare CMAQ simulations between CB-4 and SAPRC99 for projected EI (lower NOx) at 2005 level

CMAQ4.4, CB4, Projected EI for 2005

CMAQ4.4, SAPRC, Projected EI for 2005

Figure. Spatial plots of daily maximum 1-hour ozone concentrations with (a) CB4 and (b) SAPRC99 chemical mechanisms for August 21st, 2006.

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In general, SAPRC99 produces higher PAN, HONO, but lower HNO3, HCHO
In general, SAPRC99 produces higher PAN, HONO, but lower HNO3, HCHO.
2. Sensitivity to initial condition

Daily maximum resulted

Clean conditions

January 1, 0:00:00
Min = 0.000 at (72,59), Max = 0.031 at (83,47)

August 24, 2006 0:00:00
Min = 0.043 at (1.4), Max = 0.122 at (29,39)
3. MM5 AQF vs. Assimilation

NCEP NMM (ETA, WRF/NMM) → DataSpider → MM5-REGRID → MM5-LITTLE_R → MM5-INTERPF (Real-Time 3D Objectively Analyzed Meteorological Fields)

CAMS, METARs, NPN profilers, sounding

12-, 4-km domains Multi-step assimilation

REGRID → LITTLE_R → INTERPF → MM5 → NESTDOWN → INTERPB

Intermediate files of REGRID for fine domain

Grid data (EDAS data)

Observations (MADIS + CAMS)

Objectively Analyzed fields

Output in coarse domain
Statistical summary (provided by Dr. XiangShang Li)

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Comparison of Wind

Wind (m/s) 20060831: 6 Houston sites

Time (CST)
Comparison of Wind

Wind (m/s) 20060926 : 6 Houston sites

- 8 MNS
- 8 AQF
- 8 OBS
- 53 MNS
- 53 AQF
- 53 OBS
- 34 MNS
- 34 AQF
- 34 OBS
- 26 MNS
- 26 AQF
- 26 OBS
- 1 MNS
- 1 AQF
- 1 OBS
- 113 MNS
- 113 AQF
- 113 OBS

Time (CST)

0.2 20
MM5 MS-FDDA Assimilation Results

Temperature

8/31

Humidity

9/01
MM5 MS-FDDA Assimilation Results

Temperature

9/26

Humidity

9/26

Regional average (49 sites)

Temperature (°C)

Time (CST)

Obs.  AQF  MNS

Regional average (13 sites)

Relative Humidity (%)

Time (CST)

Obs.  AQF  MNS

Regional average (49 sites)

Temperature (°C)

Time (CST)

Obs.  AQF  MNS

Regional average (13 sites)

Relative Humidity (%)

Time (CST)

Obs.  AQF  MNS

9/27
O3 comparison

8/31  15 CST

9/01  04 CST
O3 comparison

9/01 16 CST

9/01 19 CST
AQF vs MS-FDDA Met.
O3 comparison (Daytime 8/31/06)
O3 comparison

9/26 07 CST

9/26 15 CST
AQF vs MS-FDDA Met.
O3 comparison (Daytime, 9/26/06)
Conclusive Remarks

CB4 vs. SAPRC

- For 2000, CMAQ with SAPRC performed well both O3, HNO3
- CB4 generated more HNO3 less PAN
- SAPRC generated less HNO3 more PAN, thus higher O3 productivity at O3 > 90 ppb
- SAPRC overpredicted medium range O3 a few ppb

- For 2006, CB-4 with 2000 EI and projected 2005 (actually 2003 NOx) compared: show small difference in O3.
- With SAPRC, high O3 enhancement area coincides with the downwind area of high HRVOC emissions.
- SAPRC with 2000 EI overpredicted observation at 60 ppb range, but compared well with O3 > 90 ppb.

MS-FDDA

MM5 multi-stage 4D data assimilation runs are promising, but need to be evaluated and improved further