Implementing an Updated Carbon Bond Mechanism into the Community Multiscale Air Quality Model

Golam Sarwar and Deborah Luecken
United States Environmental Protection Agency
National Exposure Research Laboratory
Research Triangle Park, NC

Greg Yarwood
ENVIRON International Corporation, Novato, CA

Gary Whitten
Smog Reyes, Point Reyes Station, CA

William Carter, University of California, Riverside, CA

Overview of CB-IV Mechanism

- CB-IV was originally developed in late 1980s
  - Gery et al (1989)
- Several updates were made in 1990s
  - PAN chemistry
  - Radical termination reactions
  - Isoprene chemistry
- Two other updates
  - CBM-Z – developed by PNNL in 1999
  - CB-99 and CB-2002 – developed by the UNC
- CB-IV in CMAQ Model warrants updating

Overview of CB05 Mechanism

- Called CB05 mechanism because developed in 2005
- USEPA sponsored the project
- Developed three sets of mechanisms
  - Base CB05 mechanism
  - Reactive chlorine mechanism (optional)
  - Explicit air toxics mechanism (optional)
- Implemented into the CMAQ model
  - Base CB05 Mechanism

Overview of CB05 Mechanism

- Updated rate constants using recent IUPAC and NASA data
- An extended inorganic reaction set
  - Reactions of H_2 for very dry conditions in the upper troposphere
  - Reactions of odd-oxygen for pristine conditions (upper troposphere)
  - Additional NO_3 reactions to improve nighttime chemistry
  - Additional NOx rxns to represent the fate of NOx over multiple days
- Explicit organic chemistry for methane and ethane

Overview of CB05 Mechanism

- Explicit MEO2, MEPX, and FACD
- ROOH, organic acids and peracids
- Internal olefin species - IOLE
- Acetaldehyde - ALD2
- Higher aldehyde species - ALDX
- Higher peroxyacyl nitrate species - PANX
- Lumped terpene species - TERP

Overview of CB-IV and CB05 Mechanisms

	CB-IV	CB05
Number of chemical reactions	93	156
Number of photolytic reactions	12	23
Number of inorganic reactions	45	60
Number of organic reactions	48	96
Number of reactions involving H2	0	2
Number of Species	36	51
Number of primary species	13	19

Additional Species for CB05 Mechanism

Species Name	Description	Species Name	Description
ETHA	Ethane	MEOH	Methanol
IOLE	Internal olefin carbon bond	ETOH	Ethanol
TERP	Terpene	CXO3	Higher acylperoxy radical
ALD2	Acetaldehyde	PANX	Higher peroxyacyl nitrate
ALDX	Higher Aldehyde	MEPX	Methylhydroperoxide
FACD	Formic acid	MEO2	Methyl peroxy radical
AACD	Higher carboxylic acid	ROOH	Higher organic peroxide
PACD	Higher peroxycarboxylic acid		

Overview of CB05 Mechanism

- Evaluated against Chamber Data
  - UNC Chamber Data
  - UCR Chamber Data
- Chemical species mapping was done for CB05

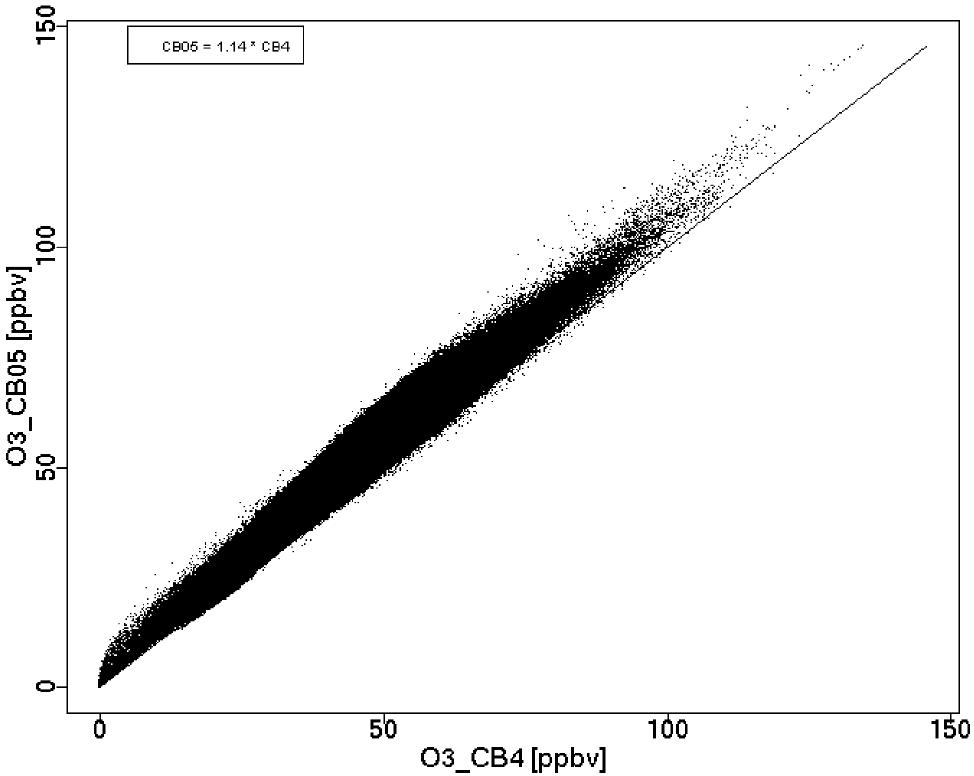
Implementation of CB05 into CMAQ Model

- Implementation was done in several steps
  - It was implemented in a box model (CMAQ version)
  - Rate constants from the box model were compared
  - Box model results were compared to that of OZIP
  - It was then implemented into the CMAQ Model

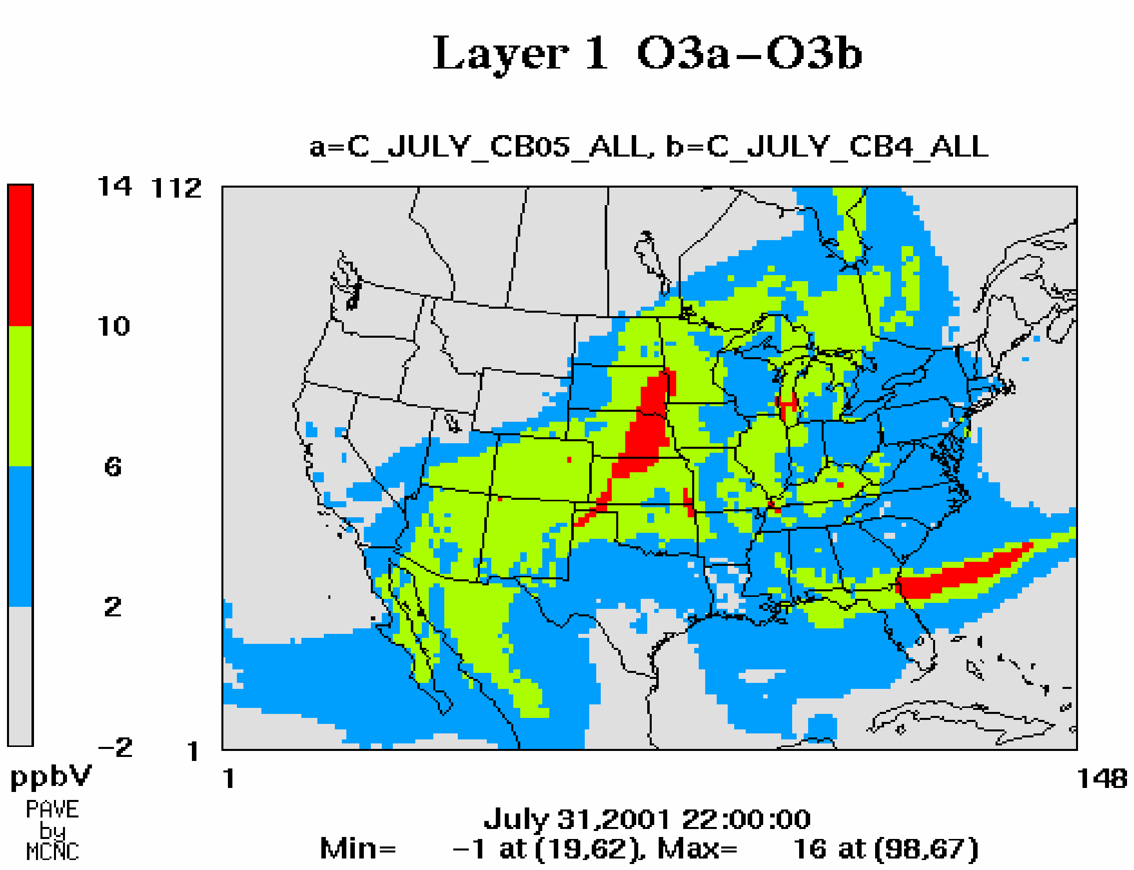
CMAQ Modeling Details

- Number of horizontal grids for conus = 148 X 112
- Horizontal grid resolution = 36-km
- Number of vertical layers = 14
- Chemistry solver – Rosenbrock solver
- New aerosol module (AE4) was used
- Aqueous chemistry was used
- Simulation period: July 1-31, 2001
- Spin up period: July 1-10, 2001

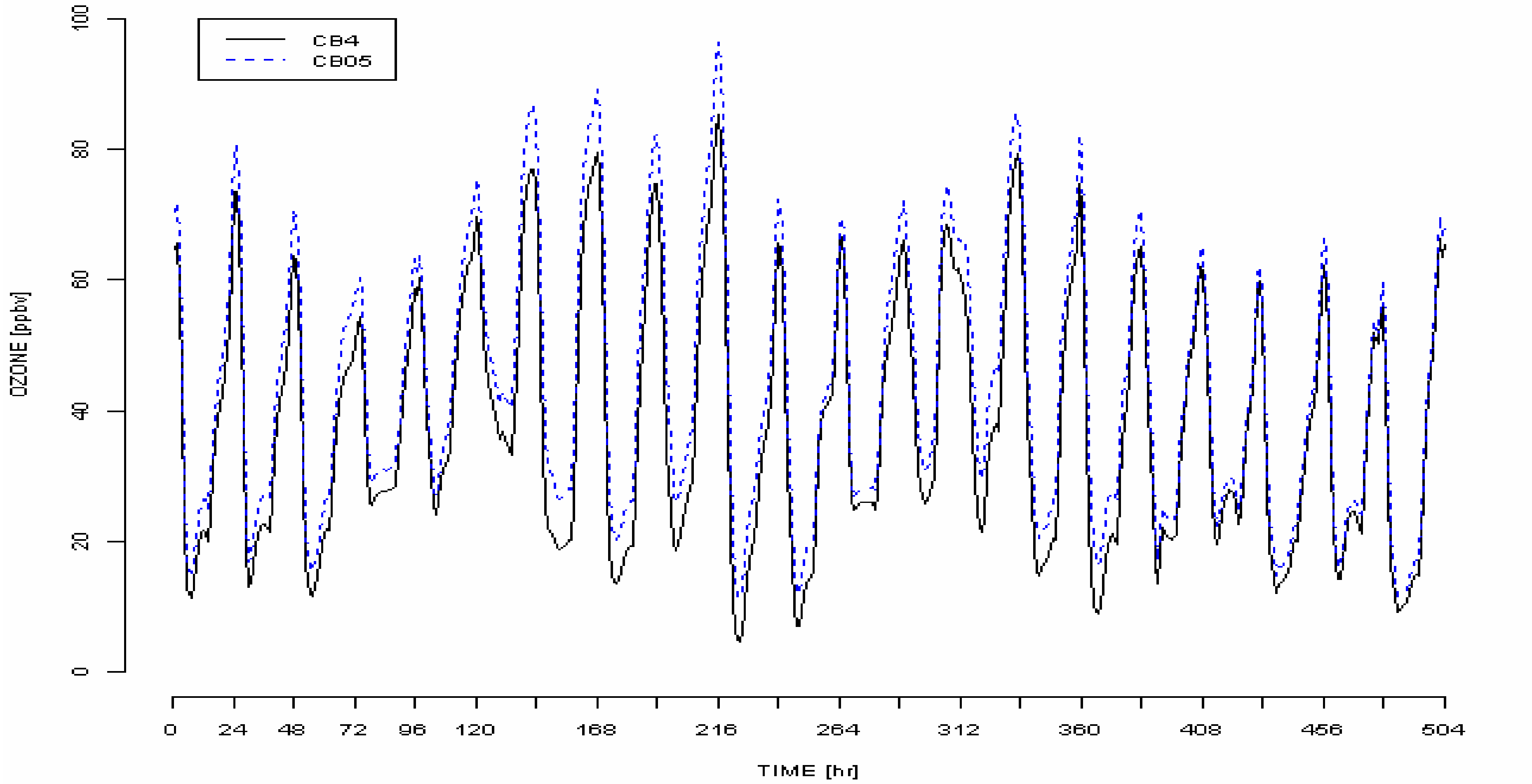
Comparison between CB-IV and CB05 mechanisms O_3 in the first layer



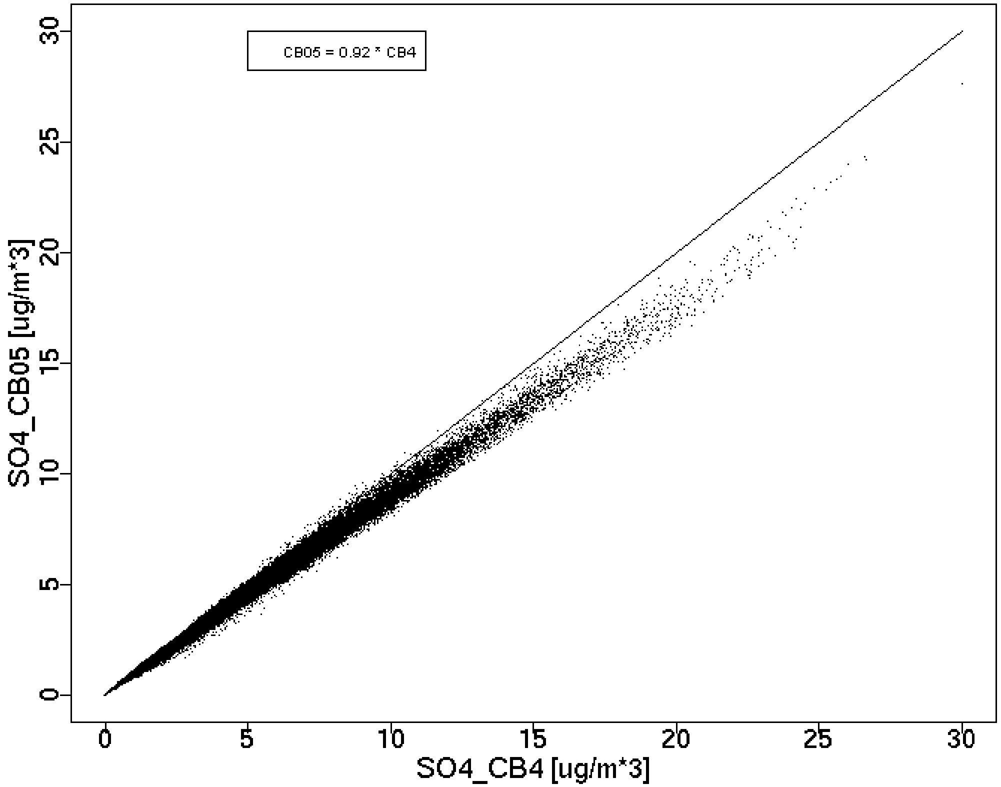
Difference between CB05 and CB-IV mechanisms O_3 in the first layer



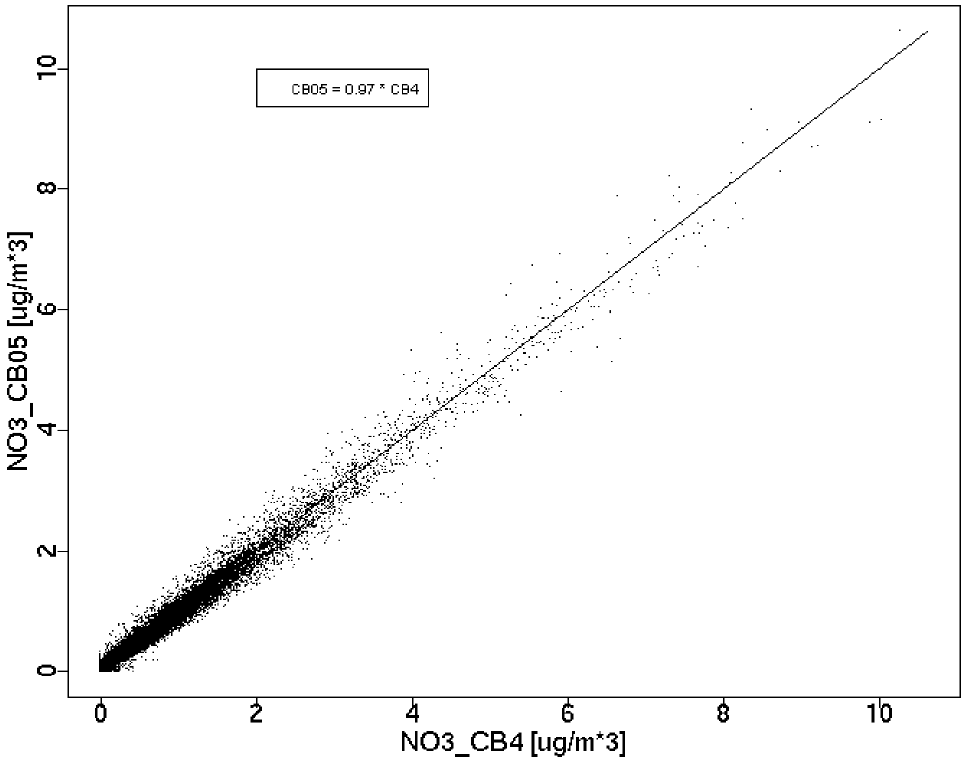
Time series of O_3 at a grid-cell near Houston [grid cell - 80 x 29]



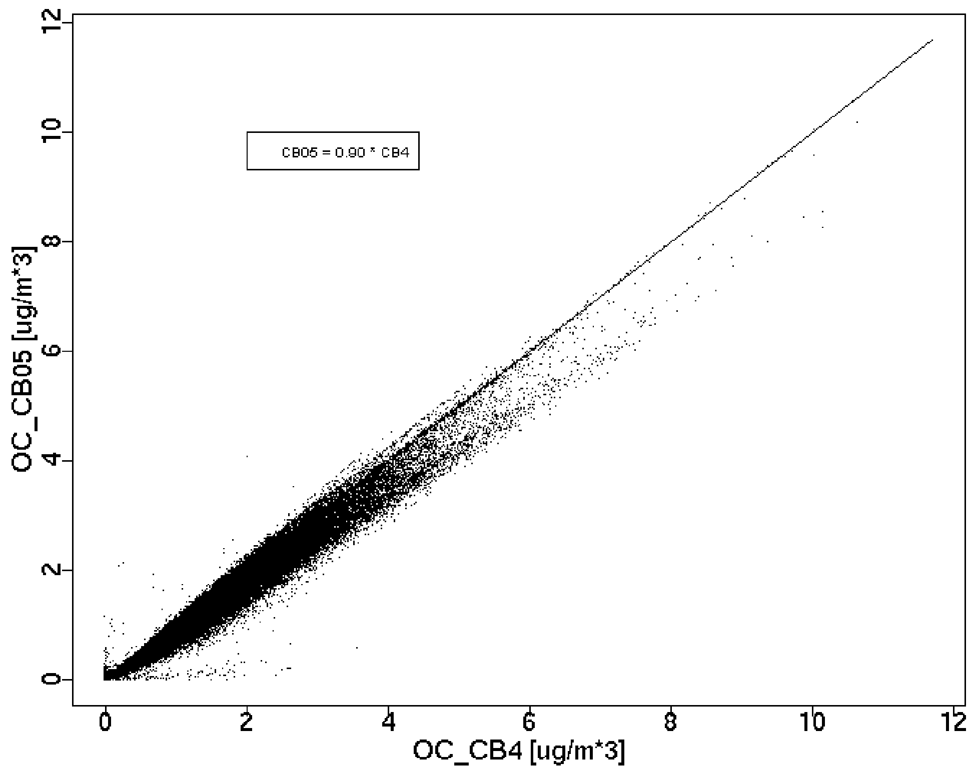
Comparison between CB-IV and CB05 mechanisms daily averaged SO_4 (aerosol) in the first layer



Comparison between CB-IV and CB05 mechanisms daily averaged NO_3 (aerosol) in the first layer



Comparison between CB-IV and CB05 mechanisms daily averaged OC (aerosol) in the first layer



Summary

- Incorporation of CB05 mechanism into the CMAQ Model and comparisons with CB-IV results reveals:
  - Increases in ozone prediction by about 14% when compared to CB-IV, but does not change the time of peak ozone occurrence
  - Decreases in aerosol sulfate prediction by about 8%
  - Decreases in aerosol nitrate prediction by about 3%
  - Decreases in organic aerosol prediction by about 10%
- Model run time increases by about 28%

Disclaimer

DISCLAIMER

The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. This work constitutes a contribution to the NOAA Air Quality Program. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views.