Implementation of the CB05 Chemical Mechanism into WRF/Chem

Jerold A. Herwehe[1], Ying Pan[2], and Yang Zhang[2]

[1]NOAA/OAR/ARL/Atmospheric Sciences Modeling Division, Research Triangle Park, North Carolina
(In partnership with the U.S. Environmental Protection Agency; E-mail: herwehe.jerry@epa.gov)
[2]North Carolina State University, Raleigh, North Carolina

Introduction

A new Carbon Bond chemical mechanism was developed in 2005, called CB05 (Yarwood et al., 2005), to supersede the default Carbon Bond version IV (CB4) mechanism used in the Community Multiscale Air Quality modeling system (CMAQ; see Byun and Schere, 2006). With around 60 additional reactions, CB05 provides a more detailed representation of urban chemistry while improving the treatment of biogenics, toxics, and species key to the formation of particulate matter and acid deposition (Sarwar et al., 2008).

The Weather Research and Forecasting with Chemistry (WRF/Chem; see Grell et al., 2005) model has online coupled chemistry and meteorology, which is useful for studying two-way interactions between chemistry, aerosols, meteorology, and radiation. WRF/Chem includes chemical mechanisms such as RADM2 and CBM-Z, but starting with Version 2.2, the Kinetic PreProcessor (KPP; see Damian et al., 2002; Sandu and Sander, 2006) was included in the standard model release. The KPP reads text input files and generates efficient chemistry integration code, thus significantly reducing the effort required to add new or modify existing chemical mechanisms in an air quality model. When the option is enabled, KPP is connected to WRF/Chem by the WRF-Chem/KPP coupler (WKC) which generates the necessary interface routines between WRF/Chem and the KPP-generated modules based on the WRF/Chem registry and the KPP input files (Salzmann and Lawrence, 2006).

Purpose

The purpose of this study is to implement the CB05 chemical mechanism into WRF/Chem V2.2 utilizing the KPP, ultimately to aid comparison with the air quality predictions from the CMAQ modeling system using CB05 and driven by meteorology from WRF-ARW. This presentation is a progress report.

Approach

Three major steps are required to add a new chemical mechanism into WRF/Chem using the KPP: 1) create the necessary KPP input files describing the mechanism, 2) modify the WRF/Chem registry and several pertinent program modules in the **`chem`** subdirectory to account for the new mechanism, and 3) develop a program to produce WRF/Chem-ready emissions files speciated for the new mechanism.

KPP Input for CB05 in WRF/Chem

Several text-formatted input files are needed by KPP to add the CB05 mechanism as optional package "cb05_kpp" in WRF/Chem. Descriptions of the main cb05_kpp files that were created under subdirectory **`chem/KPP/mechanisms/cb05`** follow:

- **`cb05.def`** — Used to define special reaction rates (none currently specified for cb05_kpp).
- **`cb05.eqn`** — Equation file containing all mechanism reactions and rate coefficients, with CH_4 implied at 1.7 ppmv but not explicitly included.
- **`cb05.kpp`** — Specifies mechanism name, numerical precision, solver file, whether to perform a stoichiometric check, and other parameters.
- **`cb05.spc`** — Defines all species used by the chemical mechanism.

KPP Input for CB05 in WRF/Chem (contd.)

- **`cb05_wrfkpp.equiv`** — An interface file listing species that have different names in WRF/Chem and KPP; For cb05_kpp, longer than normal list due to reuse of many pre-existing species names in WRF/Chem to conserve run-time memory requirements; Examples of species name mapping from CB05 in KPP to the WRF/Chem chem array are **`oh`** to **`ho`**, **`form`** to **`hcho`**, **`etoh`** to **`c2h5oh`**, and **`pna`** to **`hno4`**.

WRF/Chem Modules for CB05

Despite the advantages of using KPP to add a new chemical mechanism to WRF/Chem, implementation of CB05 required two new source code modules and the modification of several existing modules, all (except **`registry.chem`**) located in the **`chem`** subdirectory. Changes to affected modules are described below:

- **`registry.chem`** — After reusing as many of existing species in WRF/Chem as feasible, added remaining CB05 species here for chem array, and added mechanism package name ending in _kpp (cb05_kpp in this case); Added new emission variables e_aldx, e_par, e_sulf, and e_terp, new non-transported species hco3, cxo3, ror, tolaer, cslaer, xylaer, terpaer, and sulaer, and new gas variables aldx, panx, and terp; Note that ho, ho2, c2o3, to2, and cro are currently advected in WRF/Chem but not in CMAQ.
- **`chemics_init.F`** — Added cb05_kpp case to call initialization of CB05 gas-phase chemistry and optional debug printing of species index numbers.
- **`chem_driver.F`** — Added cb05_kpp case that specified no aerosol coupling (for now), a minimum mixing ratio of 1×10^{-30} to match CMAQ V4.6, and added additional CB05 emissions species to emis driver call.
- **`emissions_driver.F`** — Added references to four new emitted species and cb05_kpp case to call CB05-specific anthropogenic and biogenic emissions routines.
- **`module_cb05_addemiss.F`** (new) — This module is based upon WRF/Chem's module_cbmz_addemiss.F; Contains subroutines cb05_addemiss_anthro and cb05_addemiss_bio.
- **`module_cb05_initmixrats.F`** (new) — Based on WRF/Chem's module_cbmz_initmixrats.F, this contains specification of the same default mixing ratio profiles as used in CMAQ V4.6 for idealized initial conditions (ICs) and boundary conditions (BCs) with interpolation to the WRF-Chem vertical grid; BCs include boundary-specific (i.e., differing) south-east-north-west profile values, also the same as used for CB05 in CMAQ V4.6.
- **`module_dep_simple.F`** — Added cb05_kpp case, currently with nonzero deposition velocities for sulf, ch3oh, c2h5oh, open, aldx, panx, and terp.
- **`module_input_chem_data.F`** — Modified to call CB05 IC/BC specification routines and read all CB05-speciated emissions data.

Emissions Preparation for WRF/Chem

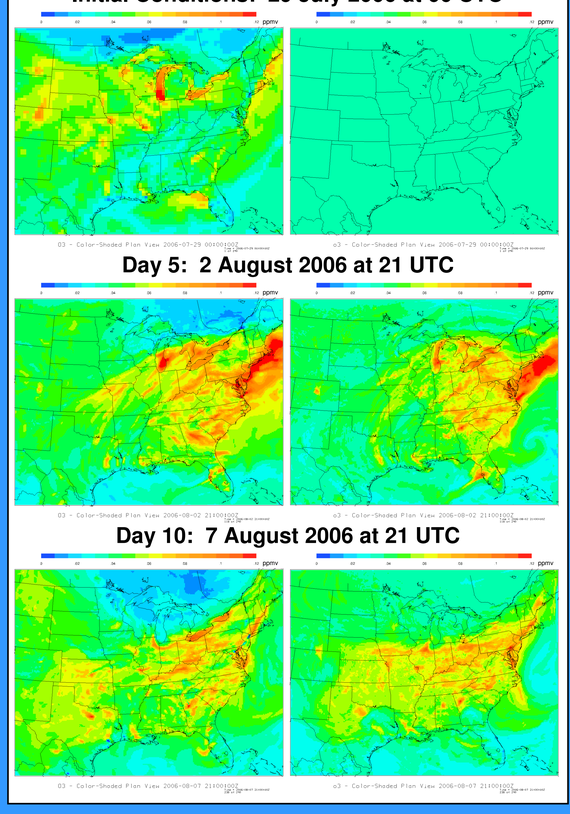
NCSU developed the original program that converts CMAQ-ready emissions to the binary emissions data needed by WRF/Chem's convert_emiss program. The emissions conversion program was modified from CB4 to CB05 speciation, and now converts emissions units from CMAQ's moles s^{-1} to WRF/Chem's moles km^{-2} h^{-1} for gas species and from grams s^{-1} to µgrams m^{-2} s^{-1} for aerosols. Emissions used here are based on 2005.

10-day Test of CB05_KPP in WRF/Chem

29 July – 7 Aug. 2006, qualitative CMAQ comparison

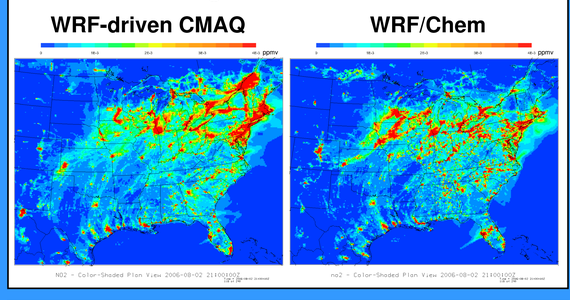
Run Specification Similarities: WRF-ARW met., CB05, same emissions, same E. US 12 km grid with 34 layers.
Run Specification Differences: CMAQ included aerosols with ICs/BCs from larger 36 km parent domain and global chemical model; WRF/Chem CB05 gas-phase only with idealized ICs/BCs, different WRF physics.

Surface Ozone Comparison



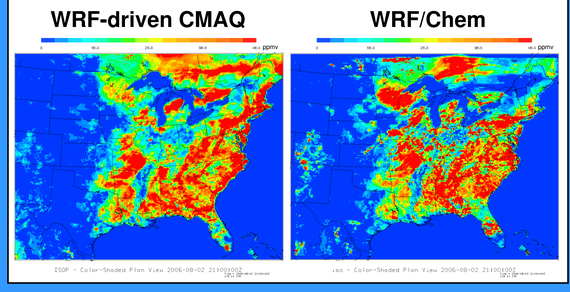
Surface Nitrogen Dioxide Comparison

2 August 2006 at 21 UTC



Surface Isoprene Comparison

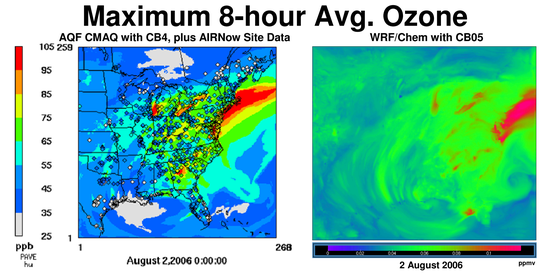
2 August 2006 at 21 UTC



Discussion

Though both models used the same 34-layer configuration (surface - 100 hPa) with 12 km horizontal grid spacing and meteorological BCs driven by NWS North American Mesoscale model forecasts, the WRF-ARW that drove CMAQ used data assimilation and nudging, plus different physics options than used in WRF/Chem (such as Pleim-Xiu vs. Monin-Obukhov surface layer, Pleim-Xiu vs. Noah land surface model, ACM2 vs. YSU boundary layer, and Kain-Fritsch vs. Grell-Devenyi cumulus parameterization). These option differences resulted in different dynamics, and along with different chemical ICs/BCs, help explain the surface mixing ratio differences seen between the two models.

Maximum 8-hour Avg. Ozone



This is a rough preliminary look at max. 8-h averaged O_3 from WRF/Chem for a selected day. The Air Quality Forecast (AQF) version of CMAQ from 2006, also gas-phase only (but CB4), was driven by meteorology from WRF-NMM. Max8h O_3 obs. from AIRNow are shown. (Note: Similar domains, but different color scales.)

Future Plans

The plan is to migrate the CB05_KPP changes to WRF/Chem V3.0, then rerun with the same physics options as used in the WRF-ARW that drives CMAQ, thus allowing a better chemistry model comparison. Statistical evaluation of WRF/Chem results against observations will also be conducted.

References

Byun, D., and K. L. Schere, 2006: Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. *Appl. Mech. Rev.*, **59**, 51-77.

Damian, V., A. Sandu, M. Damian, F. Potra, and G.R. Carmichael, 2002: The Kinetic PreProcessor KPP -- A software environment for solving chemical kinetics. *Computers and Chemical Engineering*, **26**, 1567-1579.

Grell, G. A., S. E. Peckham, R. Schmitz, S. A. McKeen, G. Frost, W. C. Skamarock, and B. Eder, 2005: Fully coupled "online" chemistry within the WRF model. *Atmos. Environ.*, **39**, 6957-6975.

Salzmann, M., and M. G. Lawrence, 2006: Automatic coding of chemistry solvers in WRF-Chem using KPP. Presentation 6.4 at the 7th WRF Users' Workshop.

Sandu, A., and R. Sander, 2006: Technical Note: Simulating chemical systems in Fortran90 and Matlab with the kinetic preprocessor KPP-2.1. *Atmos. Chem. Phys.*, **6**, 187-195.

Sarwar, G., D. Luecken, G. Yarwood, G. Z. Whitten, and W. P. L. Carter, 2008: Impact of an updated carbon bond mechanism on predictions from the CMAQ modeling system: Preliminary assessment. *J. Appl. Meteor. Clim.*, **47**, 3-14.

Yarwood, G., S. Rao, M. Yocke, and G. Whitten, 2005: Updates to the carbon bond chemical mechanism: CB05. Final report to the U.S. EPA, RT-0400675. [Available online at http://www.camx.com.]

Acknowledgements

Shawn Roselle, Robert Gilliam, and Rohit Mathur of the NOAA/OAR/ARL/Atmospheric Sciences Modeling Division.

Shaocai Yu of Science and Technology Corporation.

Golam Sarwar of the U.S. Environmental Protection Agency.

Disclaimer