Implementation of the CB05 Chemical Mechanism into WRF/Chem

Jerold A. Herwehe¹, Ying Pan², and Yang Zhang²

¹NOAA/OAR/ARL/Atmospheric Sciences Modeling Division, Research Triangle Park, North Carolina
²North 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 biogenic, toxic, 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 since 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. WRF/Chem is connected to WRF/Chem by the KPP-generated module (KWC) which generates the necessary interface routines between N weather and the KPP-generated modules based on the WRF/Chem registry and the KPP input files (Salzman and Lawrence, 2006).

Approach

Three major steps are required to add a new chemical mechanism into WRF/Chem using the KPP: 1) create the necessary KPP input file 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 an optional package “cb05_kpp” in WRF/Chem. Descriptions of the main cb05_kpp files and subroutine chem/KPP/mechanisms/cb05 follow:

- cb05_def -- Used to define special reaction rates if the characteristic implied by CMAQ V4.6 for idealized initial conditions (ICs) and boundary conditions (BCs) with interpolation to the WRF/Chem vertical grid. BCs includes boundary-specific (i.e., differing) south-east-north-west profile values, also the same as used for CB05 in CMAQ V4.6.
- cb05_dep Simple -- Used to convert CB05 IC/BC specification routines and read all CB05-specified 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 emissions program. The conversion program was modified from CB4 to CB05 specification, and now converts emissions units from CMAQ’s moles s⁻¹ to WRF/Chem’s moles km⁻²h⁻¹ for gas species and from grams s⁻¹ to grams m⁻² s⁻¹ for aerosols. Emissions used here are based on 2005.

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 Pielke-Xu vs. Monin-Obukhov surface layer, Pielke-Xu vs. Noah land surface model, ACM2 vs. YSU boundary layer, and Kain-Fritsch vs. Grell-Devenyi cumulus parameterization). These different physics resulted in different dynamics, and along with different chemical ICs/BCs, help explain the surface mixing ratio differences seen between the two models.

References


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.

Acknowledgements

Shawn Roselle, Robert Gilliam, and Rohit Mathur of the NOAA/OAR/ARL/Atmospheric Sciences Modeling Division, Shaoqian Yu of Science and Technology Corporation, and Dolf Sarwar of the U.S. Environmental Protection Agency.

Disclaimer

The research presented here was funded under the Memorandum of Understanding program for the U.S. Environmental Protection Agency’s Atmospheric Chemistry and Climate Research Program, and it does not necessarily reflect the views of the U.S. Government.