Beltsville PBL Air Quality Modeling – Atmospheric Chemistry
3-D Air Quality Models CMAQ, WRF-Chem and CAM-X
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Objective: Students will examine 3-D air quality models that are commonly used in the United States. These models include the U.S. EPA Community Multiscale Air Quality model (CMAQ), the Weather Research and Forecasting model with Chemistry (WRF-Chem) and the Comprehensive Air Quality Model with eXtensions (CAM-X). Students are referred to the previous units for more detailed discussions of the processes simulated by 3-D air quality models. Here our objective is to inform students about some of the capabilities of available models and we note that there are many training opportunities, tutorials and extensive documentation available online for these models.

Community Multiscale Air Quality Model (CMAQ)

CMAQ is a 3-D air quality model that is capable of providing 3-D pollutant fields and deposition retro-casts and forecasts over the regional scale. CMAQ is well documented at the EPA Community Model and Analysis System (CMAS) Center. https://www.cmascenter.org/cmaq/ (EPA-CMAQ; EPA-CMAQ-About; EPA-CMAQ-Doc; CMAQ-Factsheet; CMAQ-Learn; CMAQ-Pubs). It is a prognostic model that relies on first principles to simulate the emissions, transport, chemistry, deposition, cloud and aerosol processes that affect ozone, particulates, mercury, toxic compounds and acid deposition. CMAQ is a modeling system with a single open-source framework that can be implemented on multi-processor computing platforms. One of the major CMAQ applications is regulatory modeling where CMAQ is used to examine how proposed emission control regulations would affect ozone mixing ratios or particulate matter concentrations and for air quality forecasting. Figure 1 shows an example of ozone measurements and CMAQ simulations across the Continental United States (CONUS) and the overall agreement is very good (EPA-CMAQ-About).

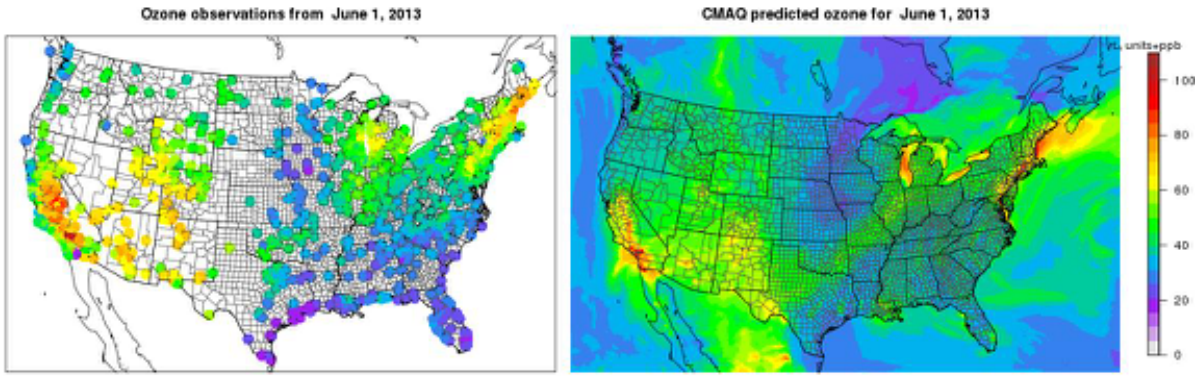

Figure 1. The left plot shows observed 8-hr average ozone mixing ratios across the Continental United States. The right plot shows the CMAQ simulated 8-hr average ozone mixing ratios (EPA-CMAQ-About).

The workshop units on atmospheric chemistry and 3-D Air Quality Models – Processes: Emissions, Transport, Deposition, Cloud / Aerosol Physics – Chemistry: discuss the processes simulated by CMAQ and similar models in more detail. CMAQ requires input from a regional-scale numerical meteorology model; the Weather Research and Forecasting (WRF) model is used to provide meteorological fields. Also, EPA has coupled CMAQ with NCAR MPAS (Model for Prediction Across Scales) both in an off-line and on-line mode. NOAA/NWS has coupled it with North American Mesoscale (NAM) model, FV3-GFS, but in an offline mode. The required meteorology includes temperature, 3-D winds, cloud formation, and precipitation rates.

Figure 2 shows an outline of the CMAQ modeling system. CMAQ has a Meteorology-Chemistry Interface Processor (MCIP) that may be used to more closely couple atmospheric dynamics and chemistry simulations. CMAQ simulations used to be limited to a one-way data flow in that atmospheric chemistry did not affect the meteorological simulations. Now the interaction of meteorology and air quality can be explored with a two-way coupled WRF-CMAQ system. For example, the effects of particles on solar radiation and the resulting influences on the simulated meteorology can be investigated with the two-way coupled WRF-CMAQ system. The Sparse Matrix Operator Kernel Emissions (SMOKE) is used to process emissions data and format it into data files for CMAQ.

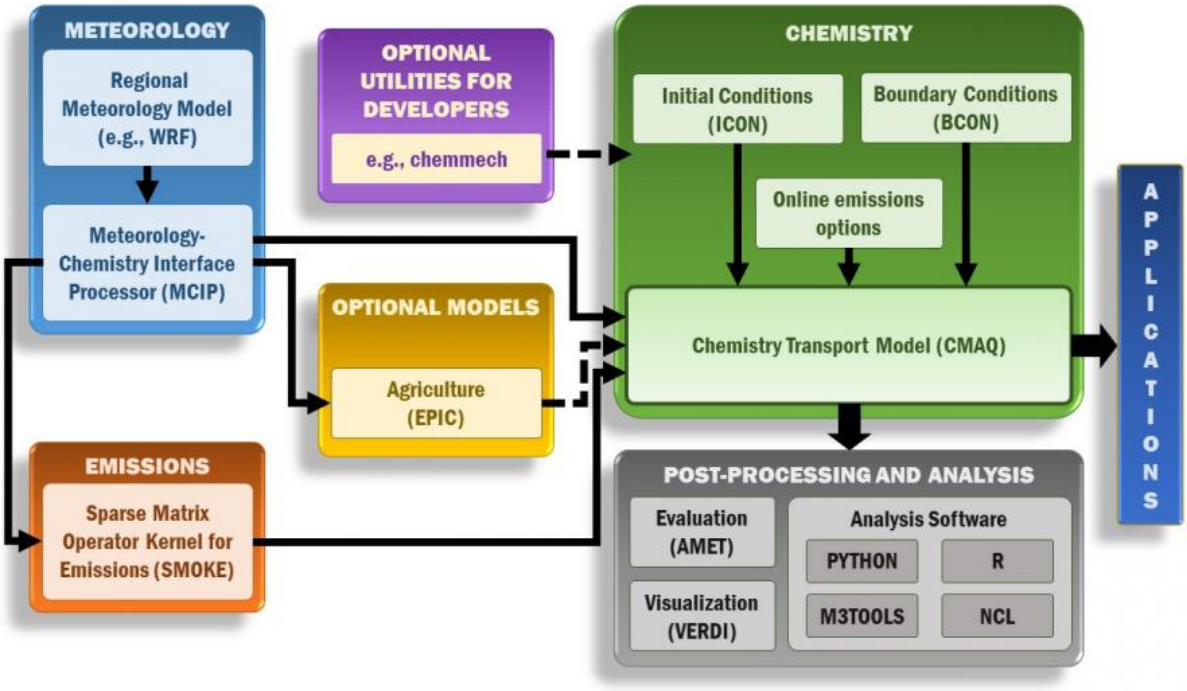

Figure 2. The CMAQ simulated 8-hr average ozone mixing ratios (EPA-CMAQ-About).

Running CMAQ requires setup information (model options, start and stop times, etc.), boundary conditions, 3-D meteorological fields and chemical species emission rates. CMAQ characterizes atmospheric transport, chemical and physical processes as discussed in previous units (Byun and Schere, 2006). CMAQ contains modules for particle microphysics and chemistry which include

organic aerosol, $PM_{2.5}$ trace elements and cloud chemistry. Several gas-phase chemical mechanisms are implemented in CMAQ including Carbon Bond (CB05e51, CB05TUCl, CB05TU, CBO5 and CBO6), Regional Atmospheric Chemistry Mechanism, version 2 (RACM2), SAPRC (SAPRC07tic, SAPRC07T) and modules for marine halogens and chlorine nitrate chemistry (EPA-CMAQ). The marine chemistry is used to represent halogens and dimethyl sulfide which affect ozone depletion, sulfate formation and aerosols. The module M3DRY simulates surface exchange processes. The treatment of PM-aerosol chemistry can be complicated due to the need to simulate both inorganic and secondary organic aerosol formation. The (AERO7) module explicitly tracks 84 particulate species. There is an expanded representation of secondary pollutant formation in clouds (AQCHEM-KMT2). The Surface Tiled Aerosol and Gaseous Exchange (STAGE) model is a deposition module used to estimate land-use specific deposition. Specific Versions of CMAQ include CMAQv4.5, CMAQv4.7, CMAQv5.0, CMAQv5.1, CMAQv5.2 (EPA-CMAQ), CMAQv5.2 and CMAQv5.3 (EPA-CMAQ). CMAQ is used by NOAA's National Weather Service for air quality forecasting across the United States (NOAA's National Air Quality Forecast Capability; NAQFC)).

Useful tools that are available in CMAQ include the Direct-Decoupled Method (DDM) and the Integrated Source-Apportionment Method (ISAM). See the unit 3-D Air Quality Modeling and Data Assimilation for a discussion of DDM. CMAQ-DDM helps users quantify the sensitivity of simulated model outputs to model parameters and emissions. CMAQ-ISAM allows users to estimate the contribution of individual emission sources or groups of sources to air pollution at given sites (EPA-CMAQ). There is an EPA sponsored center, the Community Modeling and Analysis System that is a central point for providing the CMAQ community with support (CMAS-Center; CMAS-CMAQ).

Weather Research and Forecasting Model with Chemistry (WRF-Chem)

WRF-Chem is the Weather Research and Forecasting model with modules added to simulate atmospheric chemistry in-line with the meteorology calculations (WRF-Chem-UCAR; WRF-Chem-User's-Guide A; B; WRF-Chem-NOAA; WRF-Chem-Docs). WRF-Chem can simulate air quality based on the WRF simulated meteorology online. For the online approach, the chemistry is run inside the meteorological model. The advantages of this method allows for interaction of th chemistry with meteorology at very frequent time steps as well as consistency with physical processes between the meteorological and chemistry modules. WRF and WRF-Chem can be used to simulate weather and climate on the hemispheric (with MPAS, CMAQ is run globally), regional and local scales and it can be used to investigate factors that affect global climate change problems such as aerosol direct and indirect forcing. The MPAS grid is shown in Figure 3. The online treatment of meteorology and chemistry was initially intended to allow the air quality module to make use of finer temporal resolution in the meteorology and to allow chemistry (such as aerosol formation) to have some effect on meteorology. However, although innovations such as MCIP for CMAQ allow for exchange between meteorology and chemistry, there is a huge speed advantage in online approaches due to reduced i/o requirements. The WRF model has been

discussed briefly in the unit, 3-D Air Quality Models-processes: emissions, transport, deposition, cloud/aerosol physics-chemistry.

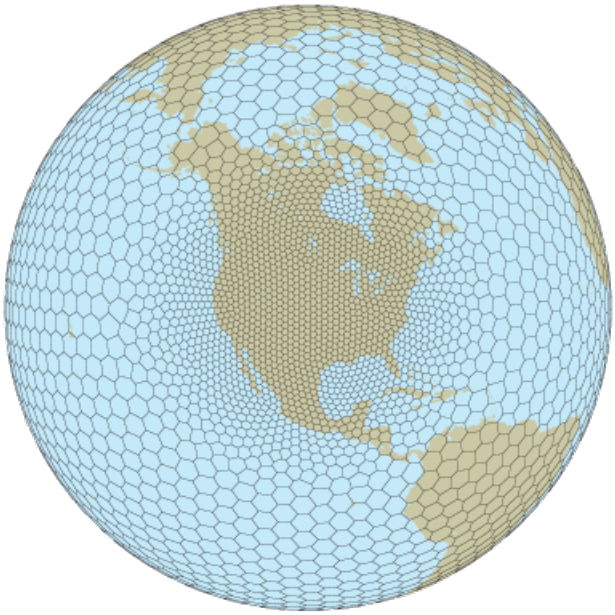

Figure 3. The MPAS grid is shown in Figure 3.

There are several options in the treatment of emissions in WRF-Chem. The user may specify anthropogenic emissions and biogenic emissions may be calculated online by standard biogenic emission modules. The online calculation of biogenic emissions such as isoprene and monoterpenes is important because their emission rates depend strongly on temperature. Volcanic ash aerosol and wildfire emissions may be treated. Photolysis depends upon meteorological conditions such as clouds, aerosols, precipitation etc. and WRF-Chem allows this to be taken into account by three different computational methods (Madronich, Fast-J and F-TUV). There are several choices in gas-phase chemical mechanisms that include the Regional Acid Deposition Model Mechanism, version 2 (RACM2), the Regional Atmospheric Chemistry Mechanism (RACM), Carbon Bond-4 (CB-4) and CBM-Z. There is a Kinetic Pre-Processor, (KPP) that can be used for chemical mechanisms in WRF-Chem.

There are five modules to choose from to treat aerosol chemistry: the Modal Aerosol Dynamics Model for Europe (MADE/SORGAM), the Modal Aerosol Dynamics Model for Europe with the Volatility Basis Set aerosols (MADE/VBS), the Modal Aerosol Module (MAM) with 3 or 7 bining schemes closely coupled to CAM5 physics, the Model for Simulating Aerosol Interactions and Chemistry (MOSAIC - 4 or 8 bins) sectional model aerosol parameterization and a bulk aerosol module from NASA-GOCART. The effects of the aerosol direct effect and indirect effect on atmospheric radiation, photolysis, and microphysics can be in WRF-Chem. It should be noted that some options in WRF will not work properly in WRF-Chem and so it is necessary to be careful when selecting the settings to used.

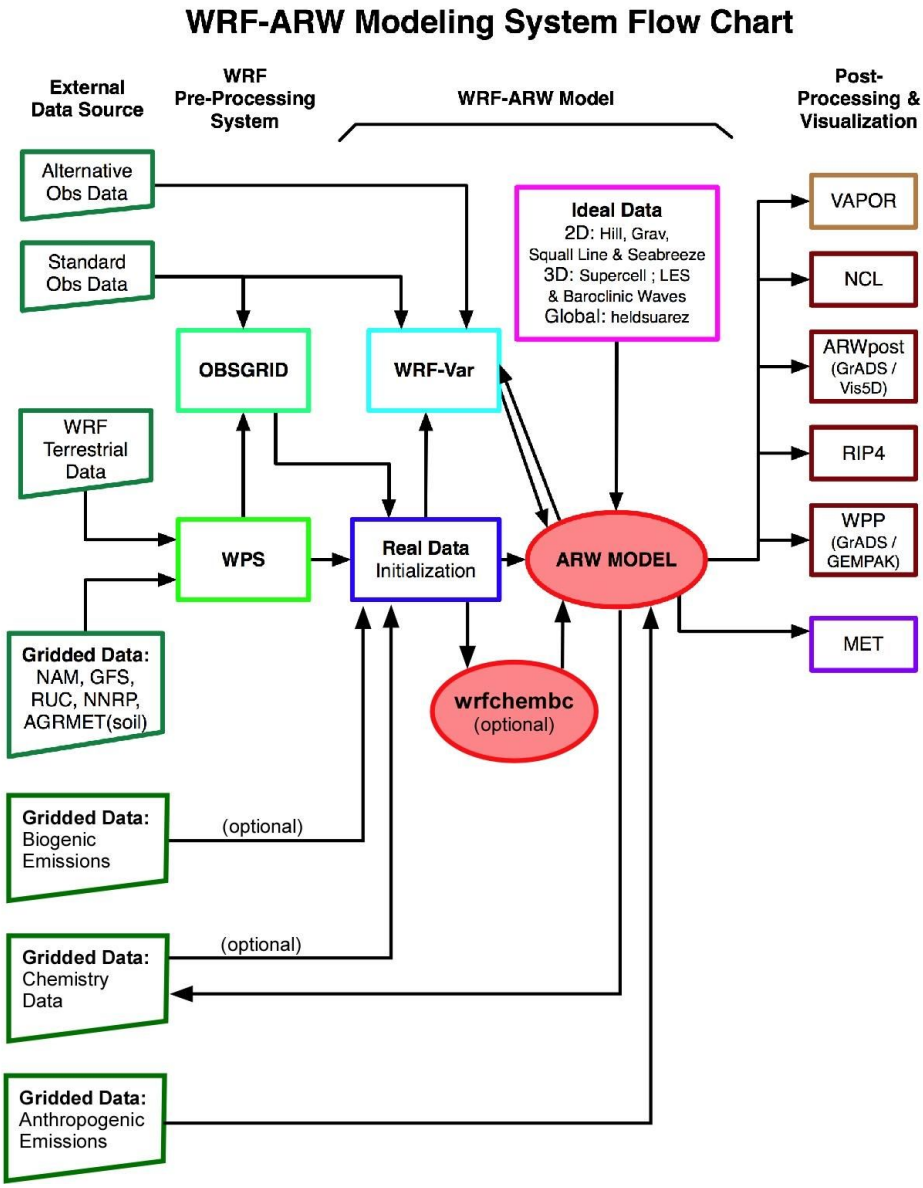

Figure 4. Shows that the structure of the WRF-Chem modeling system. The WRF-Chem modeling system follows the same structure as the WRF model (WRF-Chem Users Guide).

The WRF-Chem system includes the WRF Pre-Processing System (WPS), the WRF-Var data assimilation system, the WRF-Chem solver and post-processing and visualization tools, Figure 4. The WRF-Chem solver is restricted to the ARW core due to the need to conserve mass in an air quality model. The number of required emissions fields, boundary conditions and other inputs illustrate the complexity in running WRF-Chem. It may be necessary to modify WRF-Chem code to solve a particular problem. It would be best if a new user be very familiar with WRF before trying to learn to use WRF-Chem.

Comprehensive Air Quality Model with Extensions (CAMx)

CAMx has capabilities that are similar to CMAQ and WRF-Chem. CAMx can be used to simulate over multiple scales. It can simulate ozone, PM, mercury and toxic compounds. CAMx has DDM and advanced process analyses tools. CAMx can run on multiprocessor systems. See the website, CAMx Home for more information.

Unified Forecast System

This section is quoted from the NOAA-Virtual Lab website and referenced in the References section (see: NOAA-Virtual Lab below). The Unified Forecast System (UFS) is a community-based, coupled comprehensive Earth system modeling system. The UFS numerical applications span local to global domains and predictive time scales from sub-hourly analyses to seasonal predictions. It is designed to support the Weather Enterprise and to be the source system for NOAA's operational numerical weather prediction applications. The various components of the UFS are shown in Figure 5.

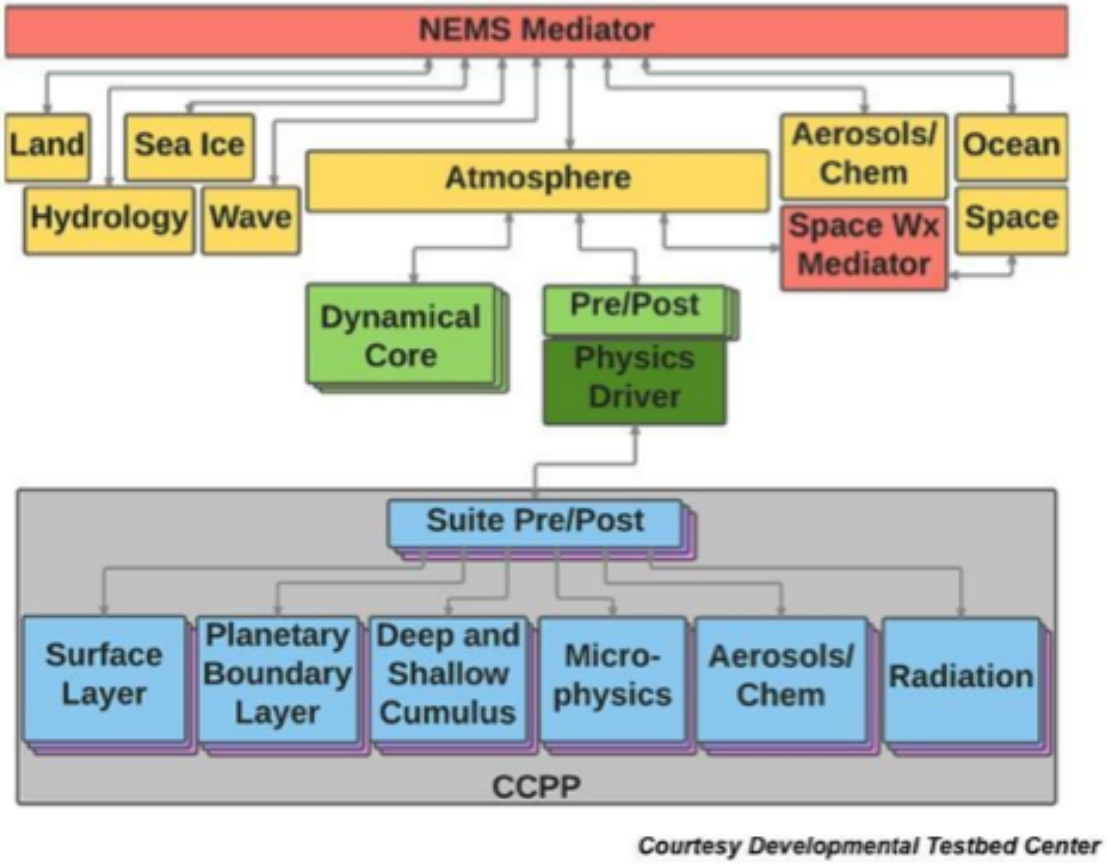

Figure 5. Schematic of a unified atmospheric forecast system with coupling to ocean, ice, wave, air quality process modules.

Goals

- Implement a weather-scale, fully-coupled NWP System
- Extend forecast skill beyond 8 to 10 days
- Improve hurricane track and intensity forecast
- Extend weather forecasting to 30 days

The current operational Global Forecast System (FV3-GFS) was upgraded to run as a Next Generation Global Prediction System (NGGPS) within the NEMS (NOAA Environmental Modeling System) infrastructure in 2019 Unified coupling of ocean, waves and aerosol processes ito the GFS have begun and then UFS will replace the current system by around 2023. During 2014, NOAA initiated the evaluation process for five potential candidate dynamical cores to serve as the foundation for the NGGPS:

- Global Non-hydrostatic Mesoscale Model (NMM & NMM-UJ) - EMC
- Model for Prediction Across Scales (MPAS) - NCAR
- Non-hydrostatic Icosohedral Model (NIM) - ESRL
- Navy Environmental Prediction System Using the NUMA Core (NEPTUNE) - Navy
- Finite Volume Model version3 - (FV3) – GFDL

NOAA chose the Finite Volume on a Cubed Sphere (FV3) dynamic core for its global forecast system implemented in 2019. This core is also used for the NASA and Harvard global atmospheric chemistry models. NWS has coupled CMAQ with the FV3GFS in an offline fashion for implementation in 2022. NOAA with EPA has begun to couple CMAQ CB -VI chemistry for both global and regional applications. The convective allowing model (CAM) run regionally and covering much of North America at 3 km horizontal resolution is under development with targeted operational implementation around 2024.

EPA is coupling CMAQ within the NCAR MPAS model. The model is unique in that it allows variable resolution (stretching) on a hexagonal grid. This is an alternative to a nesting approach where horizontal resolution is gradually increased rather than abruptly.

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. doi:10.1115/1.2128636.

CMAQ Descriptions

EPA-CMAQ, https://www.epa.gov/cmaq
EPA-CMAQ-About, https://www.epa.gov/cmaq/cmaq-models-0
EPA-CMAQ-Doc, https://www.epa.gov/cmaq/cmaq-documentation#user-guide
CMAQ-Factsheet, https://www.epa.gov/cmaq/cmaq-fact-sheet
CMAQ-Download, https://www.epa.gov/cmaq/download-cmaq

CMAQ-Learn, https://www.epa.gov/cmaq/learn-about-cmaq
CMAQ-Pubs, CMAQ Publications (Has some references to chemical mechanisms), https://www.epa.gov/cmaq/how-cite-cmaq

CMAQ Output Examples
CMAQ-Animation, Predicted pollutant concentrations over the US
https://ofmpub.epa.gov/rsig/rsigserver?cmaq_application/public/singlecmaq.html
CMAQ-Output Examples, https://www.epa.gov/cmaq/cmaq-output
NOAA-AQF, https://airquality.weather.gov
NOAA-CMAQ-Output, http://www.emc.ncep.noaa.gov/mmb/aq/cmaq/web/html

CMAS Community Modeling and Analysis System Center
CMAS-Center, A, Community Modeling and Analysis System Center, https://www.cmascenter.org/other/about.cfm
CMAS-Center, B, CMAS-CMAQ, https://www.cmascenter.org/cmaq/

WRF-Chem Descriptions
WRF-Chem-UCAR, https://www2.acom.ucar.edu/wrf-chem
WRF-model-User's-Guide A (http://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V3/contents.html).
WRF-Chem-User's-Guide B, Version 3.9.1.1 https://ruc.noaa.gov/wrf/wrf-chem/Users_guide.pdf
WRF-Chem-NOAA, https://ruc.noaa.gov/wrf/wrf-chem/
WRF-Chem-Docs, https://ruc.noaa.gov/wrf/wrf-chem/model_info.htm

WRF-Chem Output Examples
WRF-Chem-Output, WRF-Chem Detailed Output, https://rapidrefresh.noaa.gov/RAPchem/

CAMx
CAMx Home, http://www.camx.com

NOAA-Virtual Lab, NWS/Environmental Modeling Center
https://vlab.ncep.noaa.gov/web/environmental-modeling-center/unified-forecast-system

Assignments

The NOAA-CMAQ-Output site provides data for ozone and $PM_{2.5}$ from May 1, 2019 to July 6, 2020 while the WRF-Chem-Output site provides data for many other quantities from Jun 27, 2016 to May 02, 2019. The CMAQ and WRF-Chem data overlap for May 1 and 2, 2019. Compare the simulated surface ozone and $PM_{2.5}$ by CMAQ and WRF-Chem during that interval and discuss. For WRF-Chem compare the other simulated quantities for May 1 and 2, 2019 and discuss.

For WRF-Chem, compare the simulated quantities from the WRF-Chem-Output site for a mid-summer day and for a mid-fall day and discuss. How do NO_x and organic compounds appear to affect ozone and $PM_{2.5}$ concentrations across the CONUS region? What may be said about how

the upper air meteorological variables and upper air ozone mixing ratios affect surface ozone and PM_2?

Explore the other CMAQ output examples in the references listed above and discuss.