NCAR WRF/ACD Tracer Forecast

(Field Catalog Name: NCAR/MMM WRF ARW 3km Forecast Products)

Contact: Gabriele Pfister (pfister@ucar.edu)
NCAR/ACD: Arthur Mizzi, Stacy Walters, Mary Barth, Rajesh Kumar
NCAR/MMM: Glen Romine, Wei Wang, Kevin Manning, Craig Schwartz

WRF V3.3.1 Setup:

- 2-domains (15 km and 3 km), 37 levels up to 10mbar
- Lambert projection
- Initialized with GFS 0.5°x 0.5° 00 UTC and 12 UTC forecasts
- Forecast out to 48 hours, available ~12pm and 12am
- YSU boundary layer, Thompson microphysics, RRTMG radiation schemes, Kain Fritsch CU scheme, Noah land surface model, Monin-Obukov surface layer scheme

Tracers with specified lifetime:

- tr1 NO_x like mobile (based on CDPHE 2018 inventory, 2-day lifetime)
- tr2 NO_x like area/point (based on CDPHE 2018 inventory, 2-day lifetime)
- tr3 C_2H_6-like Oil &Gas (based on WRAP 2008 inventory 2-day lifetime)
- tr4 NH_3-like Agri (based on NEI 2011 inventory 2-day lifetime)
- tr5 NO_x lightning (altitude dependent lifetime)
- tr6 non-Colorado NO_x (based on NEI 2011 inventory 2-day lifetime)
- tr17_1 Lateral boundaries (BDY) (set to 1 at later boundaries of inner domain, 2-day lifetime)
- tr17_5 Stratospheric Tracer (STRAT) (set to 1 above tropopause, 2-day lifetime)

Passive/Air mass age tracers:

- tr17_2 BDY
- tr16_6 STRAT
- tr7 NOx area + point (tr1 + tr2)
- tr8 C_2H_6-like Oil & Gas

Caution: we found a problem in the air mass age for tr7 and tr8!

Notes: Tracers are only active in 3km domain, except for STRAT
Tracers are normalized to 1 based on the respective emission strength, except for tr1, tr2, tr7, which are are normalized to the sum of (tr1+tr2).

Graphics available from FRAPPE Field Catalog and the MMM WRF Website:
http://www.wrf-model.org/plots/realtime_3kmconv.php
More information: Field Catalog Report (20140701)
(http://catalog.eol.ucar.edu/frappe/report/wrf_acd/20140701/14/report.WRF_ACD.201407011400.discussion.pdf)

NCAR WRF/STEP Tracer Forecast

(Field Catalog Name: NCAR STEP WRF ARW 3km Forecast Products)

Contact: Gabriele Pfister (pfister@ucar.edu)
NCAR/ACD: Stacy Walters, Mary Barth, Arthur Mizzi
NCAR/RAL: Mei Xu, Jenny Sun, Yubao Liu and the STEP team

WRF RTFDDA with data assimilation 3km forecast is run as part of NCAR's Short-Term Explicit Prediction (STEP) program (www.ral.ucar.edu/projects/step_hydromet/). NSSL mosaic reflectivity data are assimilated in addition to GTS data with observation nudging and hourly cycles. Uses MYJ boundary layer scheme.
0-24h forecasts are launched at 02, 05, 08, 11, 14, 17, 20, 23 UTC.

The tracers in this product are the same tr1-tr5 as in the NCAR WRF/ACD Tracer Forecast products (see above).

Graphics available from FRAPPE Field Catalog and the MMM WRF Website:
http://www.wrf-model.org/plots/realtime_step2.php
Note: Met plots are labeled as 00 UTC, 03 UTC, 06 UTC, etc. so as to conform with the other forecasts run as part of the STEP project. The tracer plots are labeled using the actual initialization time.

More information on the STEP project: http://ral.ucar.edu/projects/step/

NCAR/ACD MOZART-4 Forecast

(Field Catalog Name: Mozart4 Chemical Forecast Products)

Contact: Louisa Emmons (emmons@ucar.edu)

Full chemistry and tracers are run in MOZART for 3-day forecasts. Full chemistry forecasts are at 2 degree horizontal resolution and tracers are at 0.5 degrees. Both are driven by GEOS-5 meteorology and include real-time daily fire emissions from FINN.

The tracers include:
CO-fire: from CO fire emissions with 15-day lifetime
CO-anthro: from Streets-ARCTAS anthropogenic emissions, 15-day lifetime
NO-anthro: from MACCity anthropogenic emissions, 5-day lifetime
NO-lightning: based on model simulated cloud heights, 5-day lifetime
Isoprene and Terpenes: from online MEGAN biogenic emissions, 2-day lifetime
O3-strat: set to O3 climatology in the stratosphere, 10-day lifetime

Full chemistry forecasts: http://www.acd.ucar.edu/acresp/forecast/
Tracer forecasts: in FRAPPE Field Catalog, under Model
Real-time FINN: http://www.acd.ucar.edu/acresp/forecast/fire-emissions.shtml

NCAR/ACD Flexpart

(Field Catalog Name: NCAR FLEXPART 4km Forecast Products)

Contact: Christoph Knote (knote@ucar.edu), Rajesh Kumar (rkumar@ucar.edu)

The Lagrangian particle dispersion model FLEXPART (http://flexpart.eu) is run to estimate the atmospheric dispersion of emitters like power plants and animal feeding operations ("forward" mode), as well as to understand the origin of an air mass sampled by a ground site ("backward" mode).

A Lagrangian particle dispersion model (LPDM) is a "statistical" version of a trajectory model. Imagine a balloon being released from a certain point in time and space, which is then followed along its way through the atmosphere (describing its 'trajectory'). At the resolution of our models, processes like turbulence and convection act stochastically on such a trajectory, hence the path of one balloon through the atmosphere is only one possible outcome. In an LPDM, thousands of parcels (balloons) are released and the effects of stochastic processes are applied at random, creating dispersion amongst the parcels. At certain time intervals of the simulation, the atmosphere is gridded into boxes (the "model resolution") and the number of parcels in each box is determined.

This "parcel concentration" is what is shown in the products in the FRAPPE field catalog. All simulations are based on meteorological input data from the NOAA / NCAR WRF models, which have a horizontal resolution of 4 / 3 km. Consequently, output of FLEXPART is also provided on a 4 / 3 km horizontal grid. In the vertical, 10 layers are (100, 250, 500, 1000, 1500, 2000, 3000, 5000, 7500, 20000 m AGL) used. Runs are conducted at 12 and 18 UTC with a forecast time of 24 hrs.

Products provided:

"Forward"

- pplants_xy - column integrated parcel concentrations after 24h of continuous emissions from the 22 highest emission power plants in Colorado. Plumes are color-coded according to the plant, and opacity of the plume is a measure of the column load. Emissions are scaled according to actual power plant NOx emissions.
- pplants_xz/yz_<lat/lon>E/N - vertical transects at certain lat/lon, showing plume concentrations after 24 hours of continous release and dispersion (see pplants_xy)
- cafo_* - like pplants, but for Animal Feeding operations. Scaled according to animal head count per feeding operation.

"Backward"

- back_<station>_xy - air mass history of air sampled at a station during the given 1 hour period. Map on the left shows regions where airmass was in contact with ground (0-100m), color-coded by the time before the air mass arrived at the station. Opacity is a measure of concentration. The plot on the left shows the integrated amount (arbitrary units) of emissions from several sources picked up during these ground contacts. It hence serves as a measure the pollution load of the airmass sample. The units of this loading are arbitrary, but don't change between runs - hence you can compare each emission source between different runs ("today we have less oil & gas influence than yesterday"). You CANNOT compare amounts of different emission sources between each other ("there's twice as much isoprene as there is mobile"). A 2

day e-folding lifetime is applied to all emissions to account for losses during transport.
- back_<station>_xz/yz - vertical transects at certain lat/lon, showing where and when the air that is sampled has been in the last 24 hours (see back_<station>_xy).

Adding emission sources and stations is easy to do - just drop me an email and I'll add it.

NOAA/ARL NAQFC-β

(Field Catalog Name: TBD)

Contact: Ken Pickering (kenneth.e.pickering@nasa.gov), Pius Lee (pius.lee@noaa.gov)

The National Air Quality Forecasting Capability *β* version (NAQFC-β) modeling system is one of the AQ forecasting systems assisting the DISCOVER-AQ campaigns: Baltimore and Washington (BW) between July 1 and July 29, 2011, San Joaquin Valley (SJV), California between Jan 16 and Feb 6, 2013, Houston/Galveston (HG), Texas between September 4 and September 26, 2013, and Front Range (FR), Colorado between July 16 and August 10, 2014.

The NAQFC-β system is an off-line coupled atmospheric chemical concentration forecasting modeling system using the National Centers for Environmental Predictions (NCEP) North American Meso-scale non-hydrostatic Model (NAM) with the United States (US) Environmental Protection Agency (EPA) Community Multi-scale AQ model (CMAQ). It solves the material continuity equation for the chemical constituents in the troposphere. At the lateral boundaries, a zero-flux divergence outflow condition is imposed. Chemical lateral boundary conditions for inflow are adopted from a species mapping methodology introduced by Tang et al. which uses matching constituent correspondences between the CMAQ chemistry mechanisms with those in the Harvard University GEOS-Chem model. CMAQ utilizes the CB05 chemical mechanism and Aero5 aerosol mechanism in this application. The vertical coordinate consists of 42 unevenly spaced layers.

For the 12 km horizontal grid spacing parent domain, estimation of emission fluxes are similar to that in NAQFC (2005 NEI with mobile sources projected to current year, along with 2012 CEM data for major point sources). Biogenic emissions are from BEIS-3.14. For the 4 km horizontal grid spacing nested domain (as used in the FR campaign) the emission fluxes were estimated based on a separate set of surrogate flux intensity data using a finer spatial distribution than those used in NAQFC. We have chosen to use a hot spot and smoke plume detection product by the NOAA Hazard Mapping System (HMS) which blends multiple satellite retrievals and human analyst products to provide detection and hot-spot counts of wild fires over the Continental United States. The HMS product is used to estimate the next day wild fire emissions. WRAP oil and gas emission data are employed.

NASA GEOS-5
(Field Catalog Name: NASA GEOS5 Chemical Forecast Products)

Contact: Ken Pickering (kenneth.e.pickering@nasa.gov)

The GEOS-5 Forward Processing (FP) Atmospheric Data Assimilation System (GEOS-5 ADAS) uses an analysis developed jointly with NOAA's National Centers for Environmental Prediction (NCEP), which allows the NASA Goddard Global Modeling and Assimilation Office (GMAO) to take advantage of the developments at NCEP and the Joint Center for Satellite Data Assimilation (JCSDA). The GEOS-5 AGCM uses the finite-volume dynamics (Lin, 2004) integrated with various physics packages (e.g, Bacmeister et al., 2006), under the Earth System Modeling Framework (ESMF) including the Catchment Land Surface Model (CLSM) (e.g., Koster et al., 2000). The GSI analysis is a three-dimensional variational (3DVar) analysis applied in grid-point space.

The GEOS-5 ADAS is documented in Rienecker et al. (2008). More recent updates to the model are presented in Molod et al. (2011). The GEOS-5 system actively assimilates roughly $2 \cdot 10^6$ observations for each analysis, including about $7.5 \cdot 10^5$ AIRS radiance observations. The input stream is roughly twice this volume, but because of the large volume, the data are thinned commensurate with the analysis grid to reduce the computational burden. Data are also rejected from the analysis through quality control procedures designed to detect, for example, the presence of cloud.

To minimize the spurious periodic perturbations of the analysis, GEOS-5 Forward Processing uses the Incremental Analysis Update (IAU) technique developed by Bloom et al. (1996). The assimilation is performed at a horizontal resolution of 0.3125-degree longitude by 0.25-degree latitude and at 72 levels, extending to 0.01 hPa. All products are generated at the native resolution of the horizontal grid. The majority of data products are time-averaged, but four instantaneous products are also available. Hourly data intervals are used for two-dimensional products, while 3-hourly intervals are used for three-dimensional products. These may be on the model's native 72-layer vertical grid or at 42 pressure surfaces extending to 0.1 hPa. Documentation about the current access methods for GEOS-5 products can be found on the GMAO products page: http://gmao.gsfc.nasa.gov/products/. Forecasts with the GEOS-5 system are provided on the same grid out to 120 hours.

The GOCART aerosol algorithms are run within the GEOS-5 AGCM and generate mass concentrations of dust, black carbon, organic carbon, sea salt, and sulfate, along with estimates of aerosol optical thickness for each aerosol component. The GEOS-5 system assimilates OMI Total Ozone and MLS ozone on stratospheric layers. Carbon monoxide tracers from fossil fuel combustion and biomass burning are included.

NOAA RAQMS

(Field Catalog Name: CIMSS RAQMS 1x1 Degree Forecast Products)

Contact: R. Bradley Pierce (brad.pierce@noaa.gov)

The Real-time Air Quality Modeling System (RAQMS) is a unified (stratosphere/troposphere), online (meteorological, chemical, and aerosol) modeling system which has been developed for assimilating satellite observations of atmospheric chemical composition and providing real-time predictions of trace gas and aerosol distributions (Pierce et al., 2007, 2009, Verma et al., 2009, McMillan et al., 2010, Dupont et al., 2012, Natarajan et al., 2012). The chemical formulation follows a family approach with partitioning on the basis of photochemical equilibrium approximations. The non-methane hydrocarbon (NMHC) chemical scheme is based on the carbon bond lumped structure approach (Pierce et al., 2007). Photolytic rates are calculated using the Fastj2 method. The RAQMS aerosol model incorporates online aerosol modules from GOCART (Chin et al., 2002). Seven aerosol species (SO4, hydrophobic organic carbon (OC), hydrophilic OC, hydrophobic BC, hydrophilic BC, dust, sea-salt) are transported. RAQMS biomass burning emissions use twice daily ecosystem/severity based emission estimates coupled with Moderate-Resolution Imaging Spectroradiometer (MODIS) Rapid Response fire detections (Al-Saadi et al., 2008). Total direct carbon emissions are calculated as the product of area burned and the ecosystem- and severity-specific carbon consumption estimates. Ecosystem-dependent carbon consumption databases for three classes of fire severity (low, medium, and high) are considered. Fire weather severity is estimated using the U.S. Forest Service Haines Index, which considers atmospheric moisture and thermal stability. Emissions of other species are determined by combining published emission ratios for different ecosystems. RAQMS assimilates near-real-time (NRT) stratospheric ozone profiles from the Microwave Limb Sounder (MLS) and total column ozone from the Ozone Monitoring Instrument (OMI) onboard the NASA Aura satellite. RAQMS also assimilates NRT aerosol optical depth (AOD) from the Moderate Resolution Imaging Spectroradiometer (MODIS) instrument onboard the NASA Terra and Aqua satellites. During the chemical and aerosol assimilation cycle the RAQMS meteorological forecasts are reinitialized from NOAA Global Forecasting System (GFS) analyses at 6 h intervals.

RAQMS FRAPPE configuration:

- 24hr assimilation cycle begun at 12Z each day
- The following satellite retrievals from previous 24hrs are assimilated
  - Terra/Aqua MODIS Aerosol Optical Depth (AOD)
  - Terra/Aqua MODIS fire detection
  - Aura OMI cloud cleared Total Column Ozone
  - Aura MLS stratospheric (<50mb) ozone profiles
- 96hr forecasts saved at 00Z, 06Z, 12Z, 18Z (Current RAQMS forecast cycle is found in yesterday's calendar tab!)
  - CONUS: http://raqms.ssec.wisc.edu/
  - PAC/CONUS: http://raqms-ops.ssec.wisc.edu/index.php
- Verification with AIRNOW surface O3 and PM2.5

- NOx emissions based on INTEX (2006) with 35% reduction over US based on 2010 EPA trends report (testing 50% NOx reduction and 25% VOC reduction based on 2012 EPA trends)