WRF-Chem v4.4: updates, applications, and future plans

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WRF/MPAS User Workshop - June 7, 2022

WRF-Chem web site: https://ruc.noaa.gov/wrf/wrf-chem/

General Updates

- WRF-Chem remains one of the most widely used and cited chemistry modeling system in the world → +2500 citations in the last 1.5 years

- WRF-Chem code management is back in the hands of NOAA ESRL (Global Systems Laboratory – Earth Prediction Advancement Division)
- NOAA priority is development with FV3 dynamical core, but WRF-Chem is still actively used for research (e.g., the RAP-Chem experimental forecast model)
- NCAR maintains oversight of MOZART-related code, input data, and pre-processors and has oversight on overall WRF development
- As with WRF, at any time users may submit pull requests for bug fixes, enhancements, or new developments to the WRF Github (https://github.com/wrf-model/WRF) – Get your hard work out there!

Bug Fixes & Enhancements (since v4.3)

- In WRF Chem, remove photolysis rates from the default history stream (these photolysis rates are not used by most modules).
- Output photolysis rates for NO2 and O1D are included in history stream by default
- An indexing bug that incorrectly enhanced vertical mixing at the surface layer in the WRF Chem dry_dep_driver.F file is fixed.
- Minor bug fix for aerosol optics Mie extrapolation cases
- Modifications address an issue in which HONO, TERP and CO2 were not automatically pulled into the RACM mechanisms, even though they were in the anthropogenic emissions file.
- An issue is corrected related to inconsistent data units for gas species (chem_cv_options).

Bug Fixes & Enhancements (since v4.3)

- Fixed bug that caused memory mapping error when MOZART chemistry option is used in conjuction with cu_physics = 3 and conv_tr_wetscav = 1 (for post v4.3)
- Code cleanup of GOCART dust emissions with MOSAIC
- Subgrid boundary layer clouds from the MYNN PBL scheme are now allowed to be accounted for in photolysis, using “phot_opt=4” (TUV). This feature is activated by setting the &chem namelist option “phot_blcld=.true.” “icloud_bl=1” must also be set.
- ISORROPIA in chem_opts = 100,108,109 is now controlled by a logical namelist option do_isorropia

Bug introduced in v4.4

- A bug prevents users from compiling the model. To remedy this, users will need to compile the model by issuing the compile command twice.

Users can alternately compile by modifying the following file:

- */chem/depend.chem (L232)*

FROM:

module_mosaic_addemiss.o: module_data_mosaic_asect.o module_data_sorgam.o

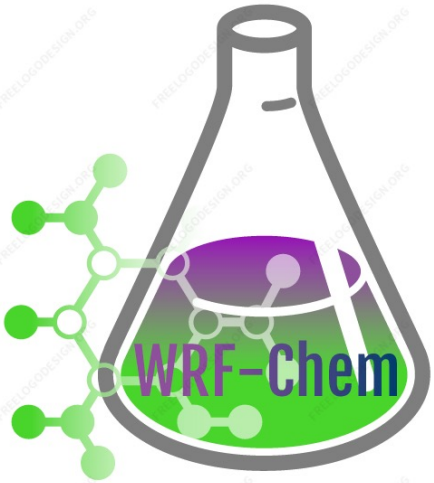
TO:

module_mosaic_addemiss.o: module_data_mosaic_asect.o module_data_sorgam.o ***module_gocart_dust.o***

This issue will be addressed in the next minor release. We apologize for the inconvenience this has caused.

In the pipeline

- Regional Atmospheric Chemistry Mechanism, version 2 (RACM2) – will be coupled to MADE/VBS_SOA (Ahmadov et al., 2012) – (B. Stockwell, E. Saunders, W. Goliff)
- Global Atmospheric Chemistry Mechanism (GACM)
- Adding AFWA dust scheme to MOSAIC aerosols (A. Ukhov)
- Addition of heterogeneous reactions of nitrogen, sulphur, and halogen species (chem_opt = 100, RACM_SOA_VBS_HET)
- Update of the CH4 biogenic fluxes in WRF-GHG (modifications to wetland, soil uptake and termite emissions) – M. Galkowski
- Lightning data assimilation – X. Zhang
- Add ice nucleation in Milbrandt-Yau microphysics scheme on MOSAIC aerosols + take into account the acidity to inhibate ice nucleation -- Available on Zenodo, published here : https://gmd.copernicus.org/articles/13/5737/2020/gmd-13-5737-2020.html



Even more in the pipeline

- New gas-phase mechanism (carbon-bond, computationally inexpensive) coupled to a new version of MADE-VBS-SOA
- Ability to ingest GFS ozone, which can be appended to the chem array or only used for photolysis/radiation
- Inline chemical mixing with MYNN
- Coupling of additional mechanisms to the full TUV photolysis module (currently only available for MOZART mechanisms)
- New dust emission algorithm (FENGSHA)
- New Fire Radiative Power (FRP) based plume-rise algorithm
- Pollen emission (online)

All of these new developments are currently running and being tested in the real-time RAP-Chem experimental forecast model

WRF-Chem Pollen

- Daily primary pollen emissions potentials (Zhang and Steiner 2022), based on the PECM model (Wozniak and Steiner, 2017)
  - Modified online by precipitation, wind speed, sunlight
- Coupled to the MADE-SORGAM aerosol scheme w/ cloud-borne species (Subba et al. *in prep*)
- In RAP-Chem, 2 species, primary pollen (PM10) and sub-pollen particles (SPP, PM2.5).
  - SPP form from the rupture of primary pollen particles due to humidity and lightning

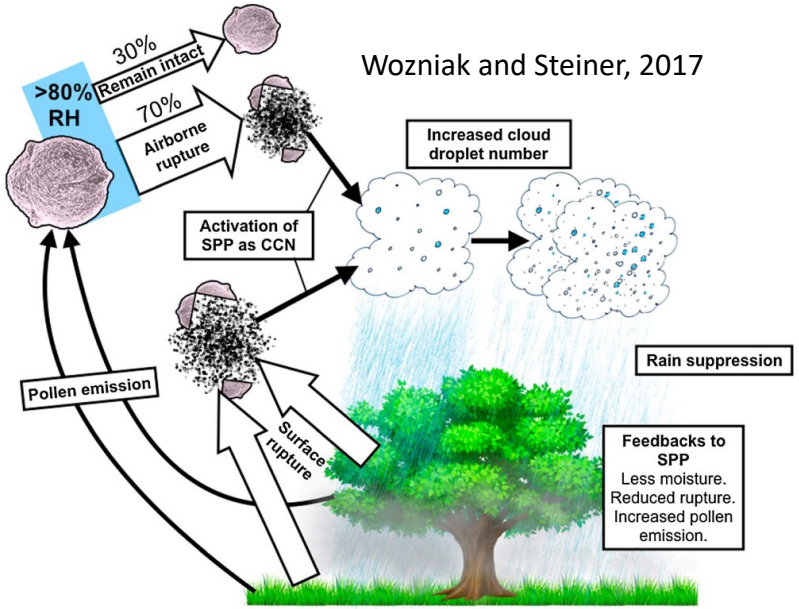
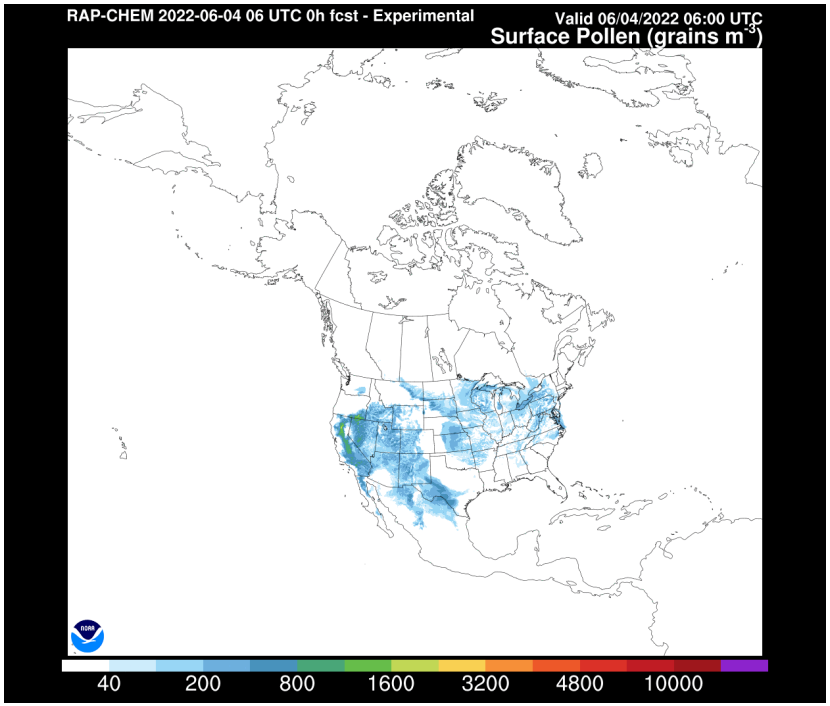
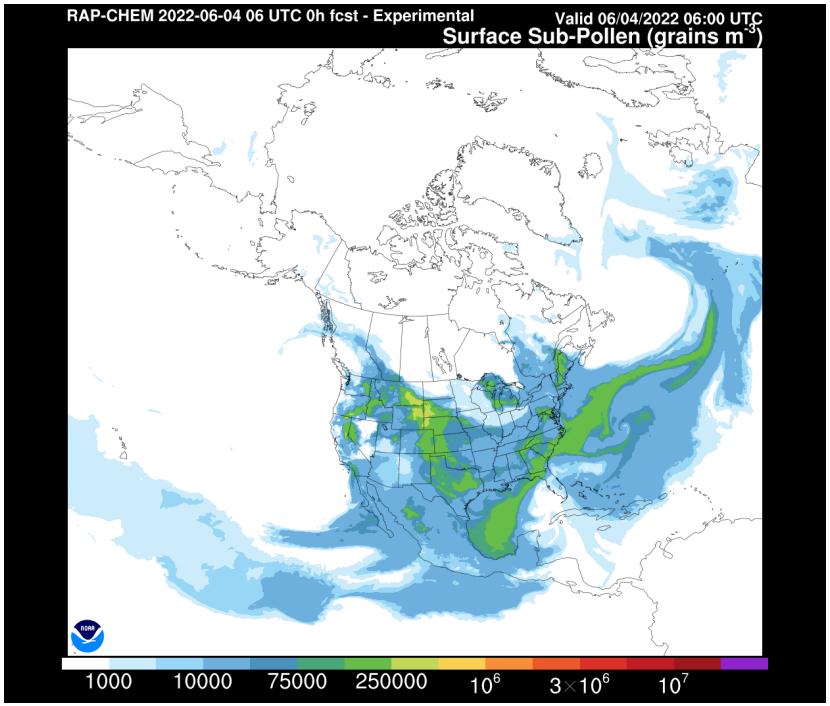


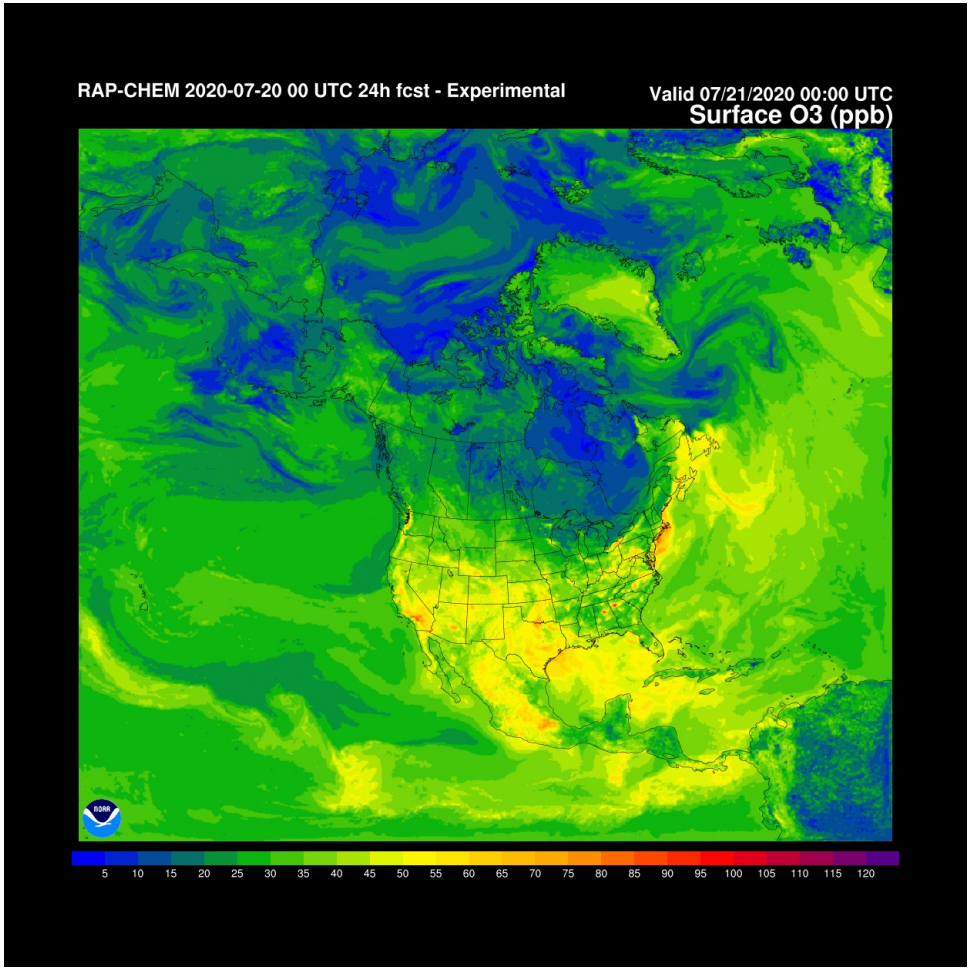
Figure 1. Conceptual diagram of pollen emissions, rupture, SPP production, and impact on precipitation processes. CCN = cloud condensation nuclei; RH = relative humidity; SPP = subpollen particle.





Experimental RAP-Chem air quality forecasts

- The **Rapid Refresh** is the continental-scale NOAA **hourly-updated** assimilation / modeling system operational at NCEP
- Forecasts **initialized at 06Z and 18Z** with a lead time of **36 hours**
- Uses the **operational RAP** IC/BCs
- **Chemical mechanism**: simplified carbon-bond mechanism coupled to VBS-SOA (85 species vs. to 200+ in CMAQ NAQFC)
- **Online emissions:** dust (FENGSHA), sea salt, biogenics (BEIS), and wildfires + FRP based plumerise (gases and aerosols)
- **Photolysis:** full TUV + aerosol direct effects
- **Radiation:** RRTMG + aerosol direct effects
  - Chemistry and land surface arrays are cycled daily (accounts for radiative fdb)
- **Chemical vertical mixing:** MYNN
- **Uses GFS total ozone for photolysis**
- **RAQMS chemical LBCs**

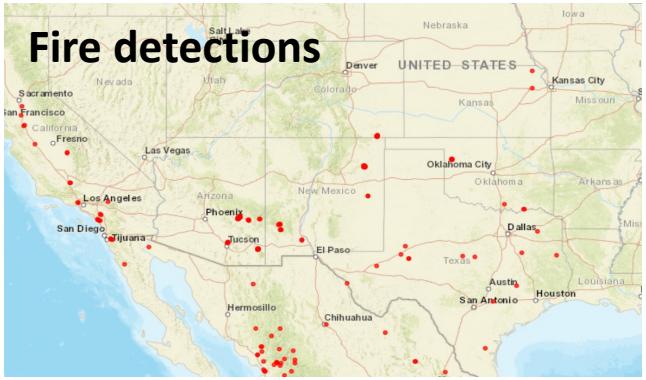


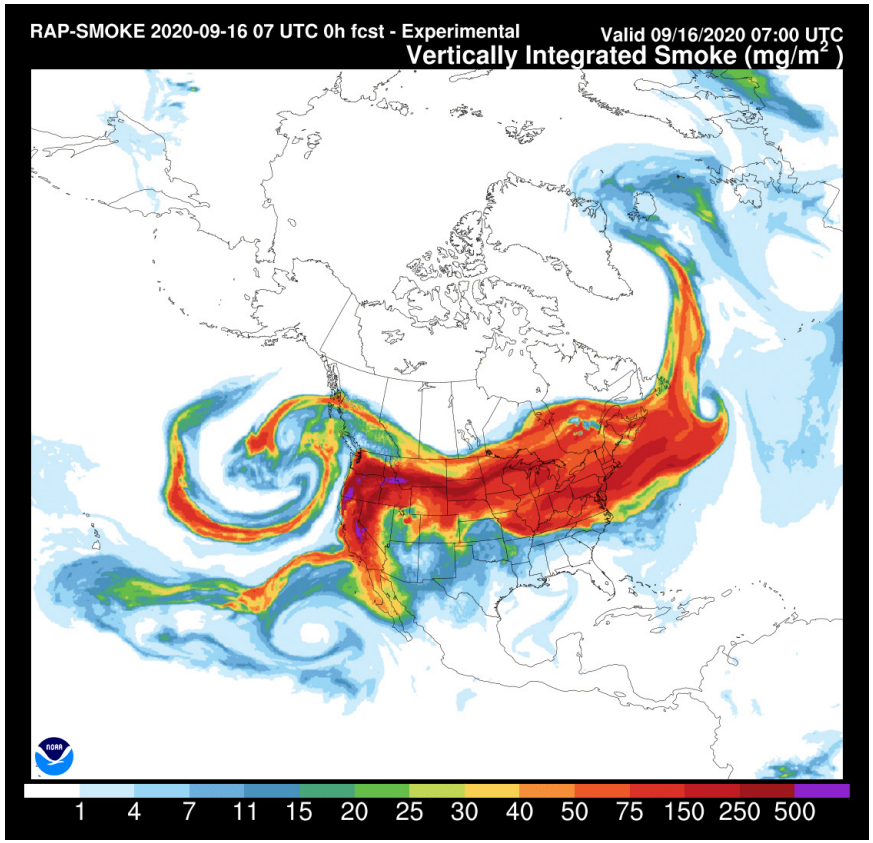
RAP-Chem forecasts use **WRF-Chem chemistry packages**

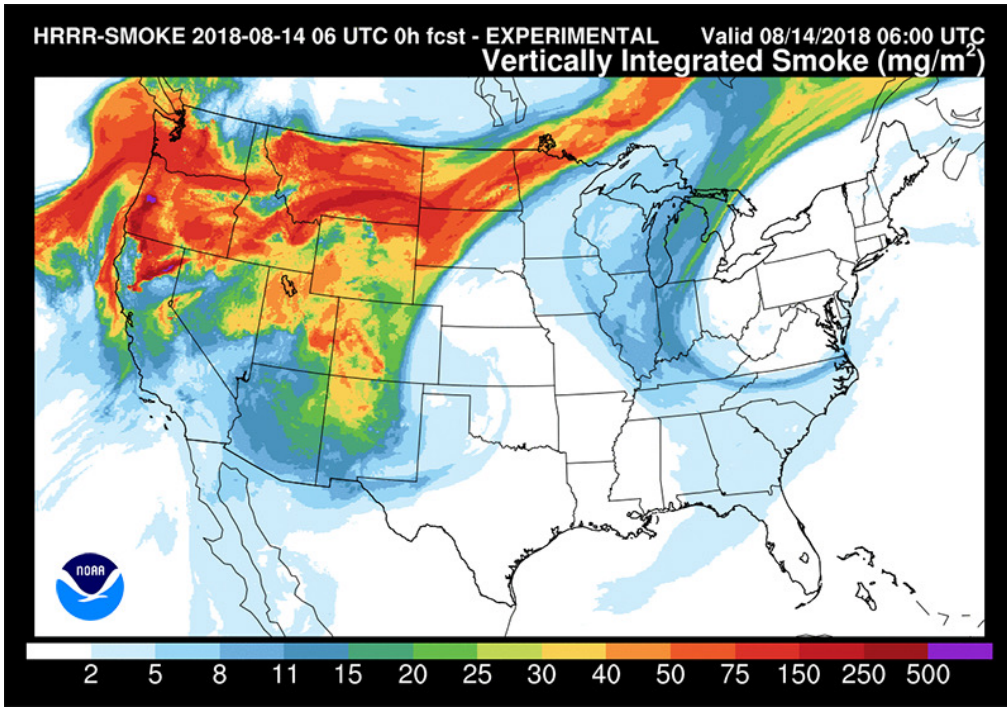
- **Plots** of key weather/chemistry species (https://rapidrefresh.noaa.gov/RAPchem/)

RAP-SMOKE has replaced HYSPLIT at NCEP!

Smoke forecasting using Rapid-Refresh and High Resolution Rapid Refresh model (based on WRF and WRF-Chem)



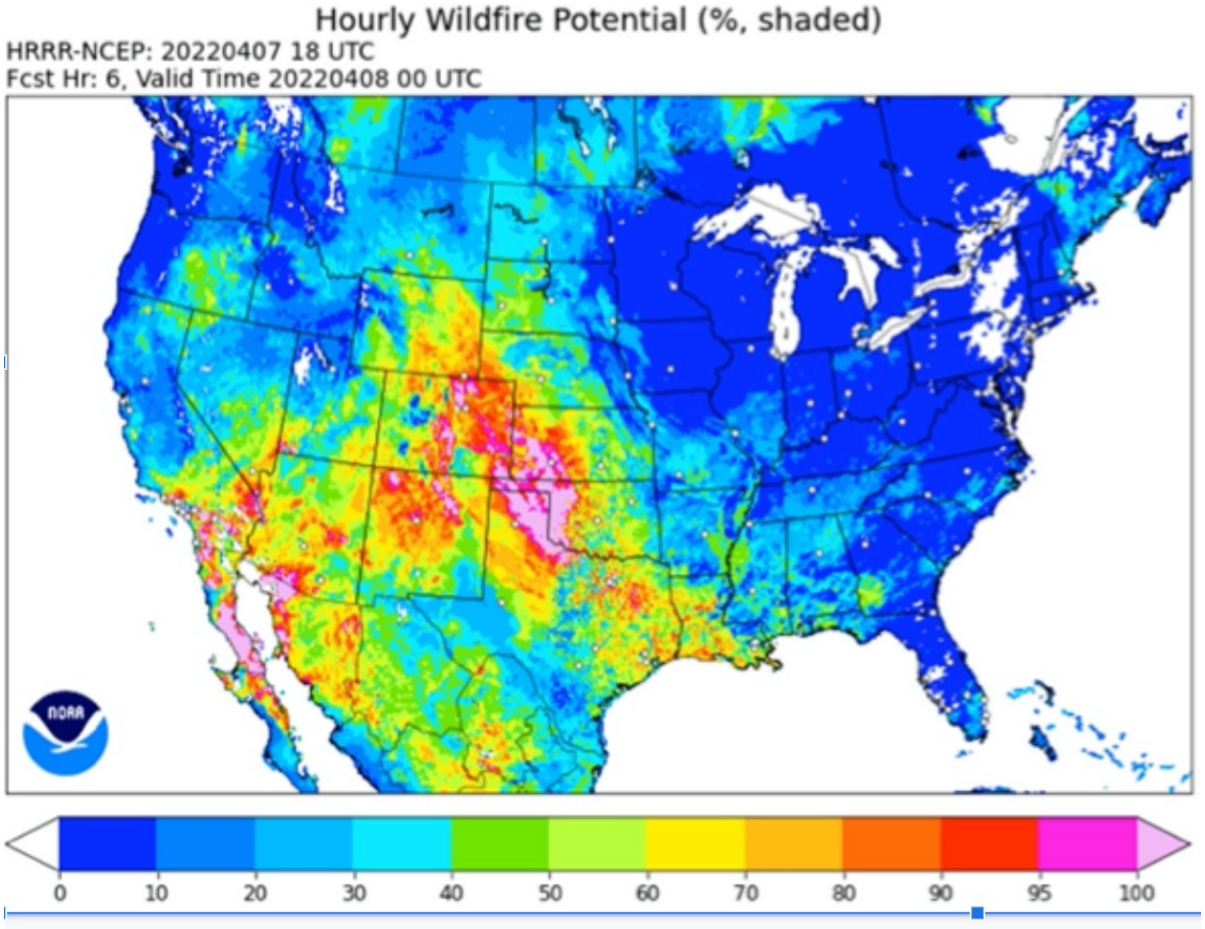




https://rapidrefresh.noaa.gov/RAPsmoke/

https://rapidrefresh.noaa.gov/hrrr/HRRRsmoke/

Hourly Wildfire Potential (HWP) diagnostic product for use in the HRRR-Smoke model



https://rapidrefresh.noaa.gov/hrrr/HRRRsmoke/

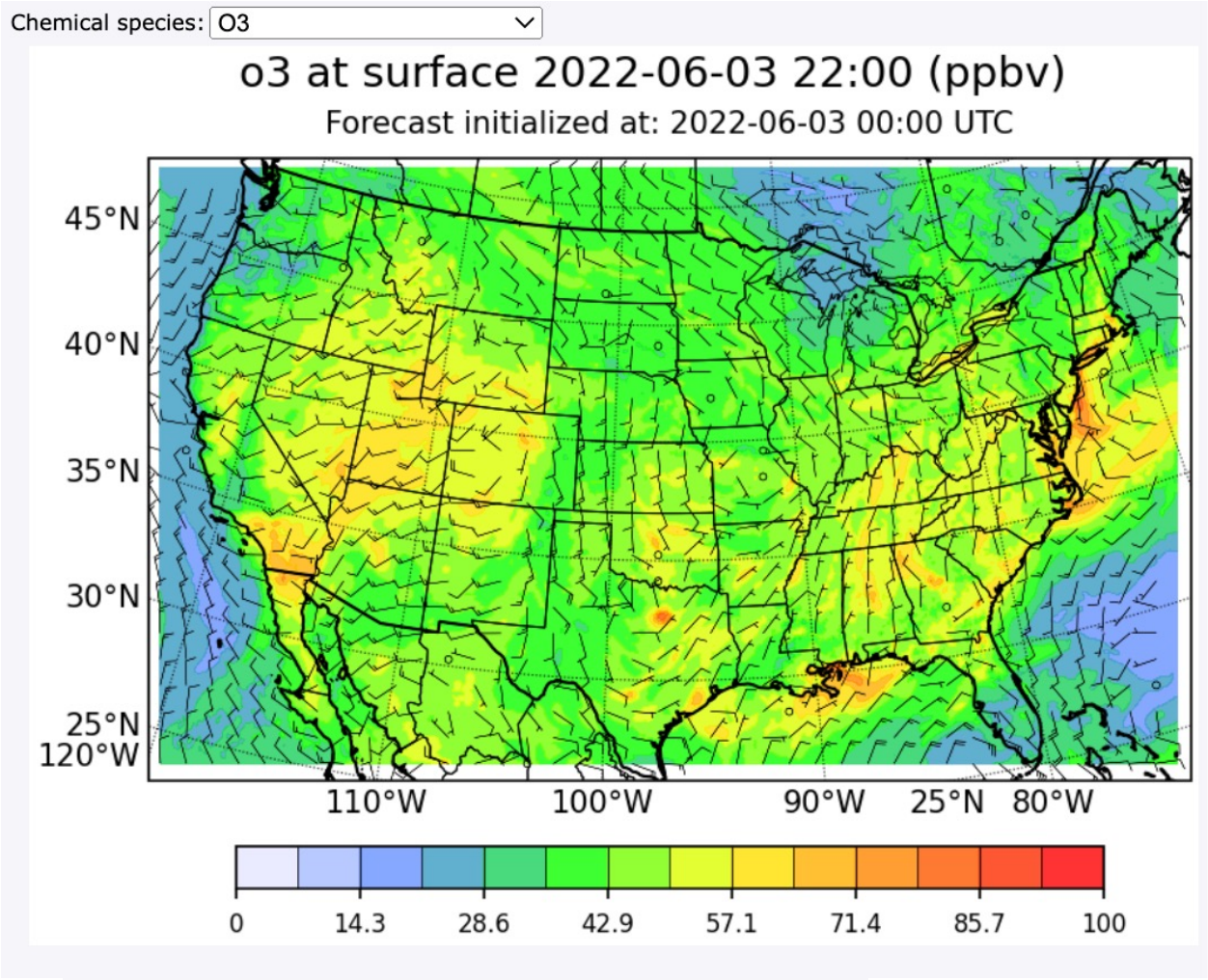
HRRR-Chem (hopefully) coming soon……

The capability to simulate fire weather depends on capturing mesoscale phenomena. Convection allowing models (i.e., HRRR-Smoke) with 3 km grid spacing are capable of representing deep convective storms and their outflows, as well as terrain-induced circulations

Hourly Wildfire Potential (HWP) is a new diagnostic product based on hourly air temperature, humidity, wind gust potential and soil moisture model output.

HWP is provided in real time along with other NWP products from HRRR-Smoke

Other WRF-Chem forecasts



NCAR FIREX-AQ and AQ-WATCH forecasts, 12km, initialized once per day with hourly AQ output available for download (FIREX)

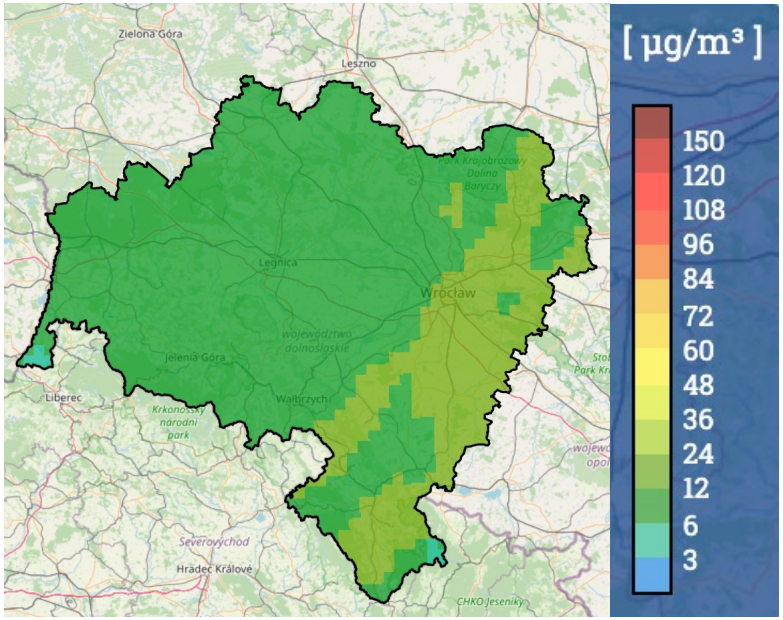
Table 2: Hourly WRF-Chem output description.

Variable Type	Dimension	Variable Names
Air Quality	2-D	o3_sfc, no_sfc, no2_sfc, so2_sfc , ho_sfc, ho2_sfc , co_sfc, hcho_sfc, c2h4_sfc, ch3oh_sfc, ch3cho_sfc, isopr_sfc, tol_sfc, ch4_sfc, acet_sfc, c2h6_sfc, c3h8_sfc, c3h6_sfc, bigene_sfc, bigalk_sfc, pan_sfc, ald_sfc, pm10_sfc, pm2_5_dry_sfc, BC1_sfc, BC2_sfc, OC1_sfc, OC2_sfc, DUST_1_sfc, DUST_2_sfc, DUST_3_sfc, DUST_4_sfc, DUST_5_sfc, SEAS_1_sfc, SEAS_2_sfc, SEAS_3_sfc, SEAS_4_sfc
	3-D	O3, co, co_anth, co_fire, co_chem, co_bdry, co_bdry_fire

https://www.acom.ucar.edu/firex-aq/forecast.shtml

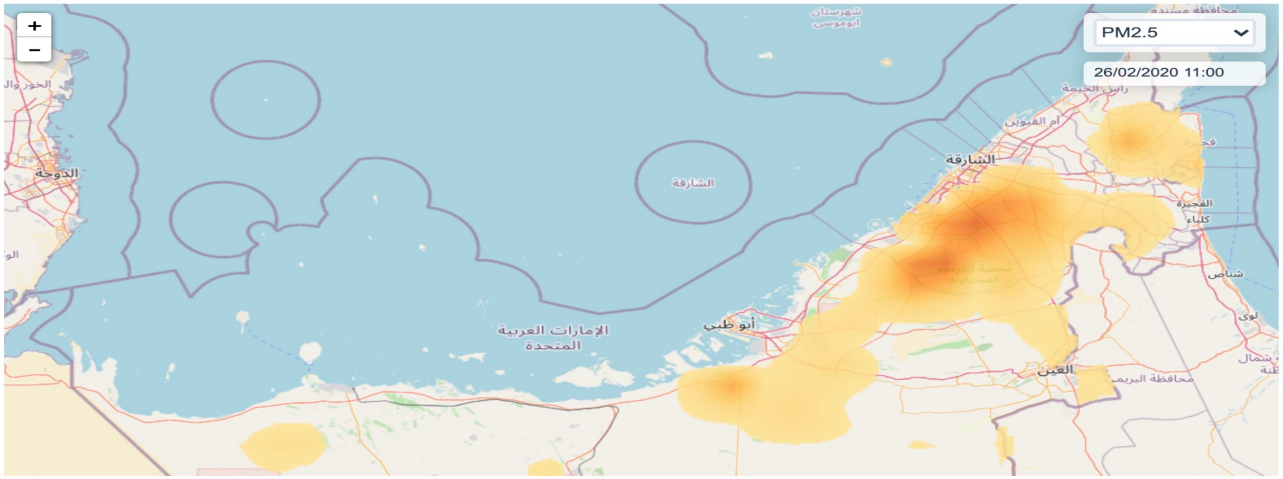
Other WRF-Chem forecasts

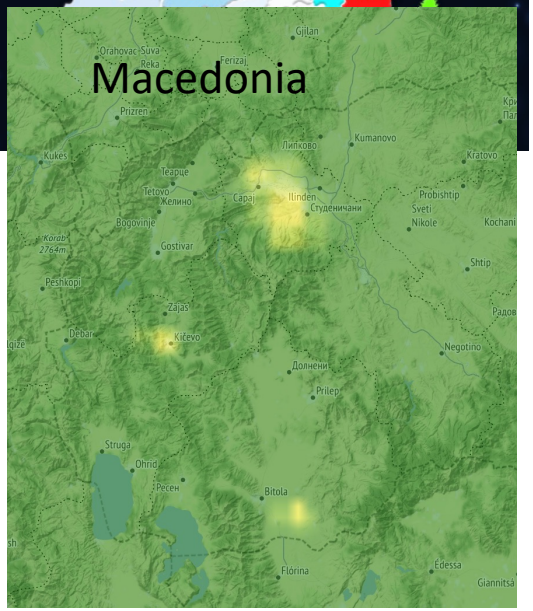
Wroclaw University, Poland



UAE Air Quality Forecast

3-day Forecast over the UAE





Updates to WRF-Chem tools

- **EPA_ANTHRO_EMISS** - Allows the use of SMOKE (CMAS/EPA) processed emissions in WRF-Chem
  - A bug fix has been made which corrects for an error in the mapping and specifically affected the results when mapping to higher resolutions. Thanks to a user for providing this fix
- **FINN v.2.5 (NCAR):** Work has continued over the past year to improve Version 2 of the Fire INventory from NCAR (FINN2) and emissions files for version 2.5 for 2002-2020 are available. This version will be documented in an upcoming publication (Wiedinmyer et al., 2022). FINNv2.5 addresses issues we identified with grassland fire emissions in FINNv2.4.
- February 2022: Thanks to Caterina Mogno (University of Edinburgh, UK) the recently released **EDGARv5.0 emission inventory is now available in MOZART speciation** for use with anthro_emiss. See this link for more information and to download the data set. .
- Update November 2021: Thanks to a WRF-Chem user, **revised mozbc code for use with the new WRF hybrid coordinate** is available in the User Forum.
- **MERRA2BC Interpolator** (Ukhov and Stenchikov, 2020)
  - Constructs initial and boundary conditions for chemical species and aerosols using MERRA-2 reanalysis (available via github, username: ***saneku***)
- **HERMES**: A stand-alone multi-scale emission modeling framework
  - Currently can process EDGAR, CEDS, ECLIPSE, HTAP, GFAS, EMEP, TNO_MACC-iii, Carn et al (Volcanoes), and Wiedinnmyer et al (trash burning)

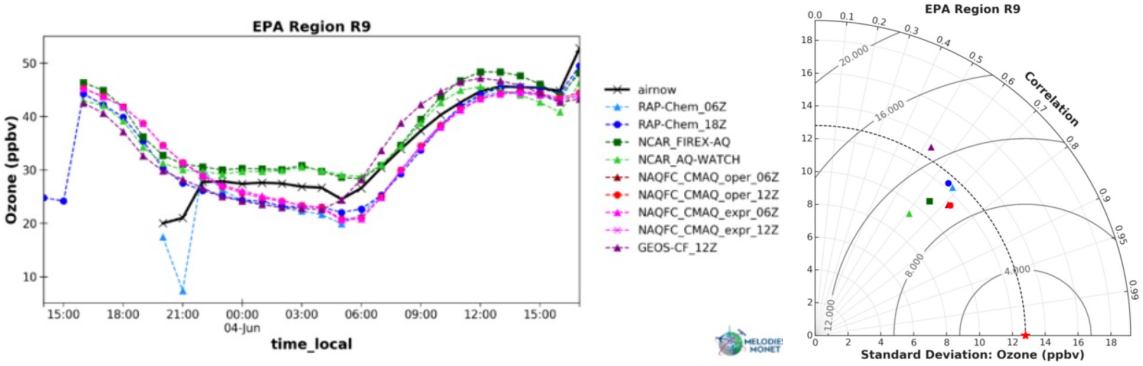
WRF/WRF-Chem install tool

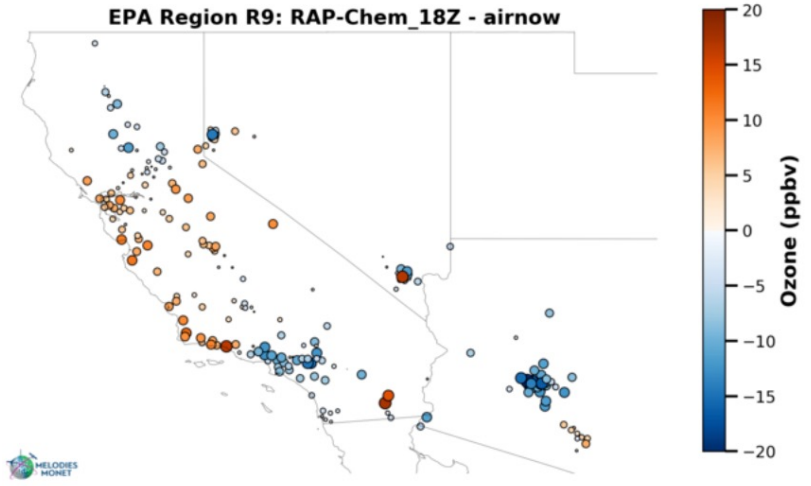
- Four different versions of WRF install scripts
  - WRF 4.4
  - WRF CHEM w/KPP 4.4
  - WRF Hydro Standalone 5.2
  - WRF Hydro Coupled 5.2
- Linux Debian 32/64bit (Ubuntu tested), MacOS, & windows Linux sub-system
- Limits user inputs to a minimum
- Installs all libraries required for using WRF
- Includes pre and post processor tools
  - UPP 4.1
  - ARWpost
  - OpenGrads
  - NCL
  - WRF Python
  - RIP4 (future update)
  - WRFPLUS 4DVAR
  - WRFDA 4DVAR
  - OBSGRID
  - Miniconda3
  - Model Evaluation Tools & Model Evaluation Tools Plus
  - All the WRF Chem Tools and data needed to compile
  - WRF Hydro pre processors
- Currently has issues with Ubuntu 22.04 due to GNU compiler change. Stable on Ubuntu 20.04.4 (Update will fix it)
- Not maintained by NCAR/UCAR or GSL, community code

Developed by Will Hatheway, Meteorologist
https://github.com/whatheway
https://www.linkedin.com/in/williamhatheway/

(coming soon) MELODIES-MONET: WRF-Chem model evaluation tool

- Conceived to be a modular framework to compare multi-scale model results and observations of atmospheric chemistry.
- It is a component of the MUlti-scal Infrastructure for Chemistry and Aerosols (MUSICA) and is funded by NSF EarthCube.
- Capable of quickly comparing observations to model output from WRF and others (e.g., CMAQ, FV3-based)
- Currently, mostly limited to comparisons with EPA AirNOW surface sites, but plans to include satellite, aircraft, and other obs are underway.
- Looking for testers!





https://github.com/NOAA-CSL/MELODIES-MONET

https://melodies-monet.readthedocs.io/

Development worksheet: email access request to: jordan.schnell@noaa.gov

A simple way for the community to facilitate collaboration and to share planned or recent updates that may or may not be submitted and/or implemented into the official version

A	B	C	D
WRF-Chem list of proposed and ongoing model development			
Contact: Jordan Schnell (jordan.schnell@noaa.gov) | Ravan Ahmadov (ravan.ahmadov@noaa.gov)			
This sheet is an attempt to coordinate WRF-Chem model development across labs and collaborators - Please distribute to other developers.			
At minimum, please provide your name, email, and a short description of the development, though additional details are encouraged, including version, modified routines, intended effects, etc.			
Type (bug fix, addition, enhancement)	**Short description of proposed change**	**Status (e.g, planned, ongoing, submitted to GitHub)**	**Notes/Comments**
bug fix	bug fix in the fire plume rise code (mass conservation issue)	submitted	I informed the community about this bug
bug fix	bug fix in volcanic ash emission and deposition	planned	
enhancement	unification of dust emission fluxes in dust_opt=GOCART_SIMPLE, GOCART_AFWA	planned	
enhancement	accumulation of dust emission and deposition fluxes (dust_opt=GOCART_SIMPLE, GOCART_AFWA, GC	planned	
enhancement	Extension of the volcanic emission pre-processor	ongoing	
addition	NOx tagging mechanism (chem_opt=113, package mozart_tag_kpp)	ongoing	
addition	VOC tagging mechanism (chem_opt=115, package mozart_tag_voc_kpp)	under development	
addition	Addition of heterogeneous reactions of nitrogen, sulphur, and halogen species (chem_opt = 100, RACM_	planned	
addition	Addition of halogen chemistry: Br and I, as well as Cl chemistry, including heterogeneous recycling reactions involving sea-salt aerosol and other particles, reactions of Br and Cl with VOCs, along with oceanic emissions of haloc		
addition	Additon of Br, Cl, and Hg chemisry and volcanic emissions	under development	
addition	New dust source (EROD) treatment for dust_opt 1, 3, & 4 (GOCART, AFWA, and UoC)	ongoing - intended publication in early 2021	This alternate treatment incorporates terrain attributes and physi
bug fix	bugfix of CH4 soil uptake in WRF-GHG module (nighttime sinkholes)	planned	
enhancement	update of the CH4 biogenic fluxes in WRF-GHG (modifications to wetland, soil uptake and termite emissic	planned	
addition	Support reading lightning data directly (lightning_option=16)	planned	Some bug fixes of lightning have been submitted to GitHub
addition	lightning data assimilation (lad_opt=1)	planned	This module has been finished by Yunyao Li before. I will merge this with my new lightning_option=16
enhancement	TSLIST: add ozone field to vertical profile output files	submitted	https://github.com/wrf-model/WRF/pull/1107
enhancement	Add Arctic bromine and chlorine chemistry + emissions source descriptions/recycling on the ground and a	planned	

Few important notes

- WRF-Chem User Guide has been updated to v4.4
- Check out WRF-Chem references to know who is working on what, what should be cited, and maybe where to get additional help if needed.
- Sign up to the WRF-Chem discussions email group
  https://list.woc.noaa.gov/cgi-bin/mailman/listinfo/wrf-chem-discussions
- Use the WRF/MPAS forum for WRF-Chem related questions
  http://forum.mmm.ucar.edu/
- Please send us your peer-reviewed WRF-Chem publications
- As with WRF, at any time users may submit pull requests for bug fixes, enhancements, or new developments to the WRF Github
- Memory is becoming an issue for users on small systems, array packaging will be a priority for the next release

The future of WRF-Chem

- NOAA ESRL will continue to support and maintain the WRF-Chem code, though most major effort is focusing on the development of FV3-Chem
- Some schemes currently in WRF-Chem will also be put into FV3-Chem through CCPP.
- NCAR continues to use WRF-Chem for research, though most of their major effort is focusing on MUSICA (Multi-scale infrastructure for chemistry and aerosols
- That said, have no fear, WRF-Chem is here to stay!

WRF-Chem info on the WEB:

WRF-Chem web-page: https://ruc.noaa.gov/wrf/wrf-chem/

UPDATED TUTORIALS for v4.0: https://ruc.noaa.gov/wrf/wrf-chem/tutorialexercises.htm

WRF/MPAS FORUM:
https://forum.mmm.ucar.edu

WRF-Chem discussions email list:
https://list.woc.noaa.gov/cgi-bin/mailman/listinfo/wrf-chem-discussions/

FAQ: https://ruc.noaa.gov/wrf/wrf-chem/FAQ.htm

Publications: https://ruc.noaa.gov/wrf/wrf-chem/References/WRF-Chem.references.htm

WRF Github: https://github.com/wrf-model/WRF

Thank you to all the developers who have submitted bug fixes and enhancements to the WRF-Chem code!

Questions?