WRF-Chem v4.3: A summary of status, updates, applications, and future plans

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WRF/MPAS User Workshop - June 8, 2021

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 v4.2)

- Added new species (NH3, CO2, CH4) of fire emissions for RACM mechanisms (M. Bela)
- TUV diagnostics disabled unless debugging (X. Zhang)
- Code cleanup and harmonized diagnostics for dust emissions schemes (A. Ukhov)
- Allow N2O5 hetchem with chem_opt = 202 (L. Conibear)
- Remove optimization flags for KPP compilation (D. Lowe)
- Improper indexing in add aircraft emissions (S. Walters)
- Wet scavenging optional for MP schemes (S. Walters)
- pH diagnostics for mozart_mosaic_4bin_aq chemistry option (S. Walters)

Significant Enhancements

- **Model for Emissions of Gases and Aerosols from Nature (MEGAN) version 2.1** now available (previously was 2.0) – B. Gaudet

PFTs can now be determined from a geographical mapping in the wrfinput file rather than from an internal vegetation type-based table - the code is looking for a variable of name 'PCT_PFT' in the wrfinput file; **it is up to the user to use external software to insert the variable containing the percentages for each CLM PFT**

Option ('***bio_emiss_opt = 4***') to invoke MEGANv2.1

When a user runs the new CLM without selecting bio_emiss_opt = 4, the old CLM method of mapping land use to PFTs is used, in order to reproduce the meteorology of previous versions of the model.

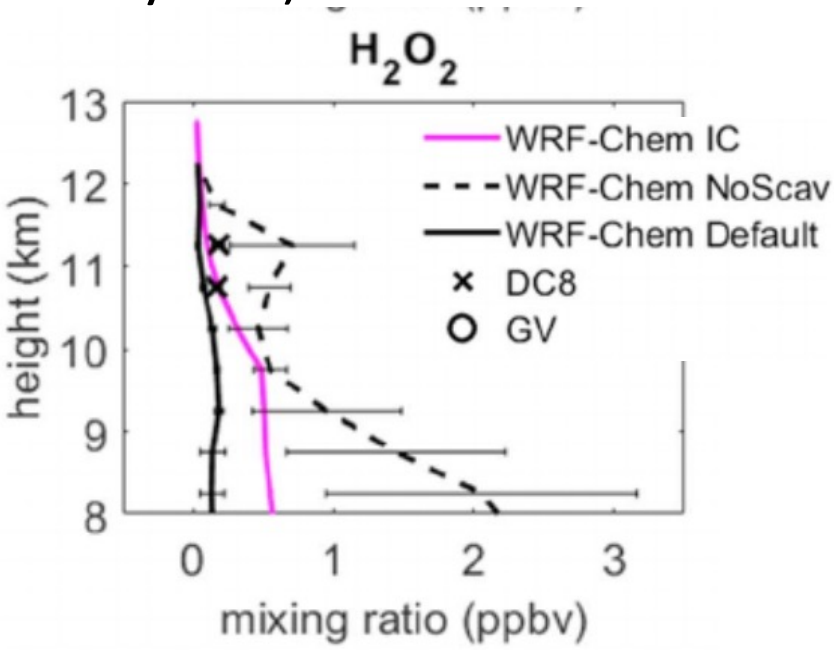
Significant Enhancements

Addition of trace gases and aerosol subgrid-scale convective transport (Grell and Freitas, 2014; Li et al., 2018), subgrid-scale wet scavenging (including the improvements of ice retention factors and the conversion ratio of cloud water to rainwater, Li et al., 2019), and aqueous chemistry to the GF cumulus parameterization. - Y. Li (U. Maryland)

TESTS CONDUCTED:

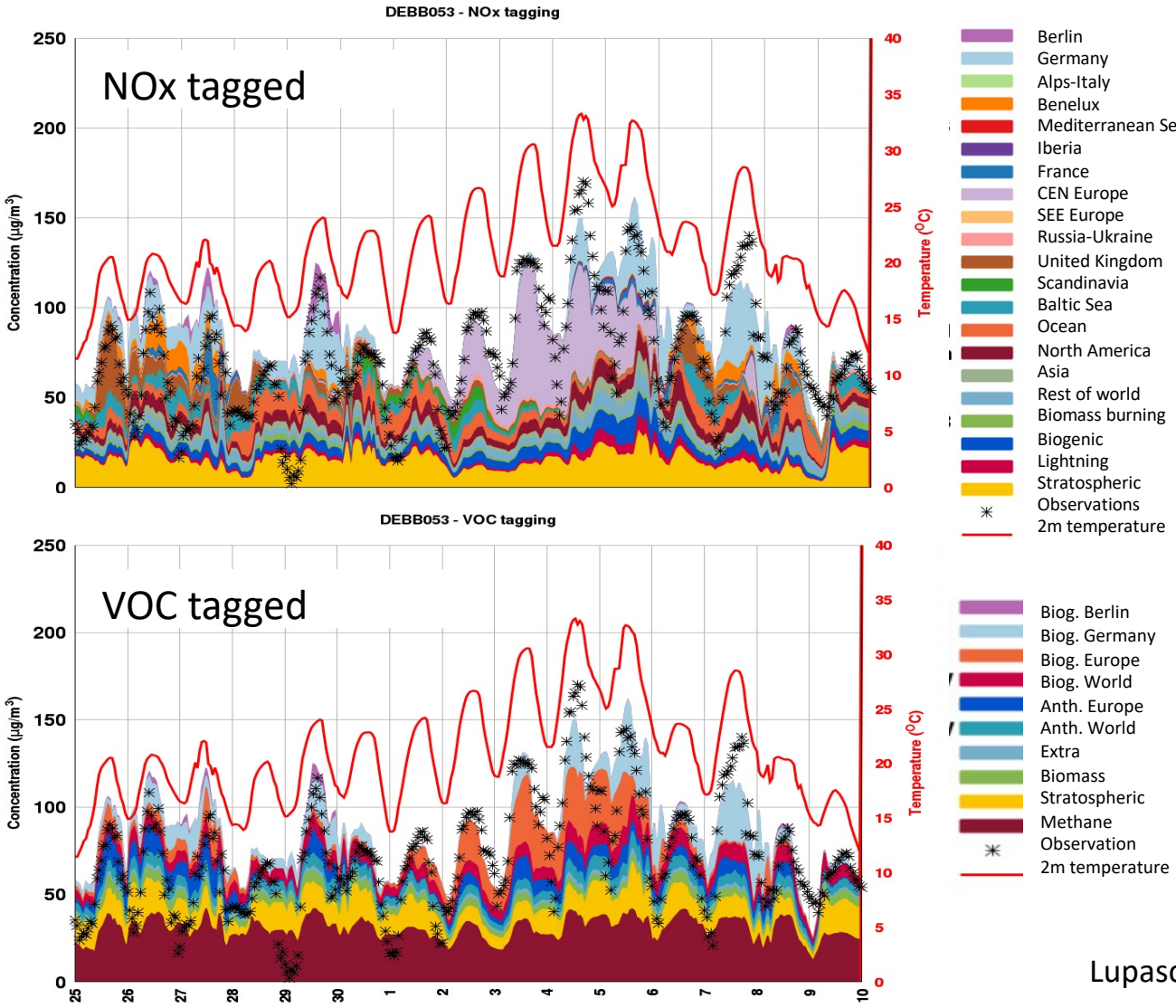
Li, Y., Pickering, K.E., Barth, M.C., Bela, M.M., Cummings, K.A., and Allen, D.J. (2019). Wet Scavenging in WRF-Chem Simulations of Parameterized Convection for a Severe Storm during the DC3 Field Campaign, J. Geophys. Res. Atmos. 124, 7413–7428. https://doi.org/10.1029/2019JD030484.

Li, Y., Pickering, K.E., Barth, M.C., Bela, M.M., Cummings, K.A., and Allen, D.J. (2018). Evaluation of Parameterized Convective Transport of Trace Gases in Simulation of Storms Observed During the DC3 Field Campaign. J. Geophys. Res. Atmos. 123, 11,238-11,261.



In the pipeline

Tagged ozone mechanism: developed by A. Lupascu and T. Butler at IASS – (Not in official release… yet, contact **Aura.Lupascu@iass-potsdam.de if interested)**



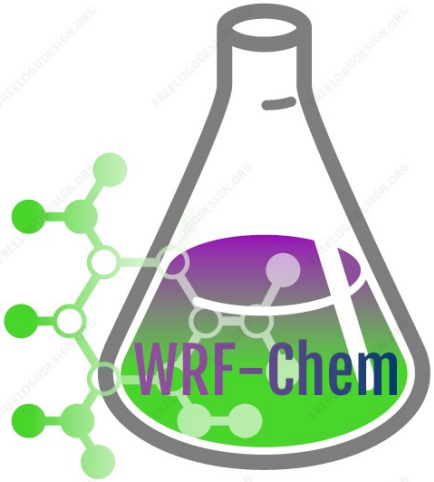
Source attribution of O_3 : Berlin June-July 2015

Slide provided by Aura Lupascu, IASS

Lupascu et al. (2020)

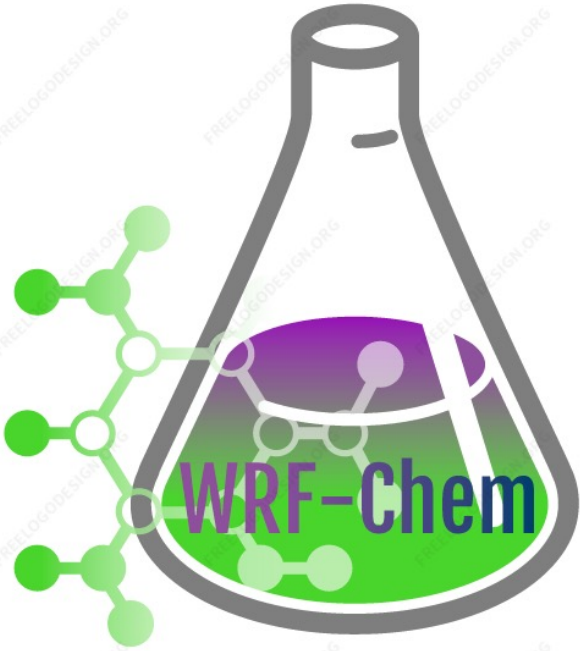
More in the pipeline

- 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 FRP based plume-rise algorithm

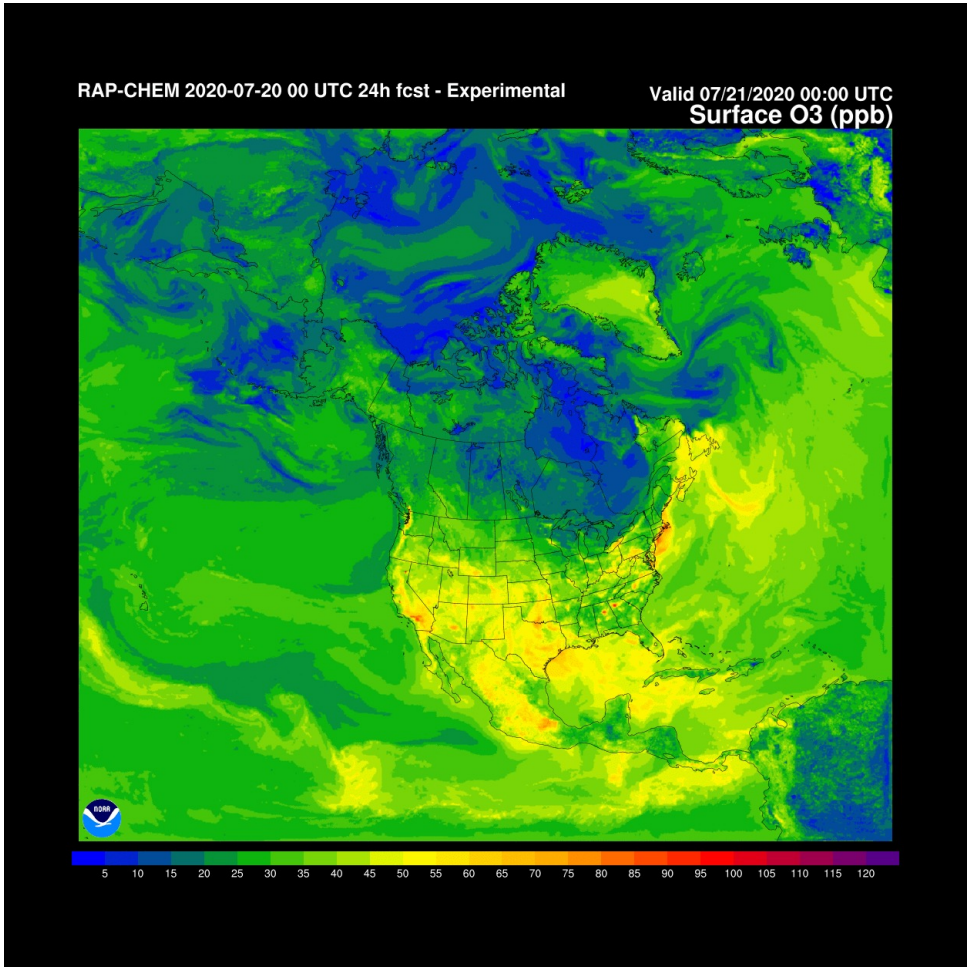


All of these new developments are currently running and being tested in the real-time RAP-Chem experimental forecast model

Experimental RAP-Chem air quality forecasts

- 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), dev. in collab w/ NCAR
- **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 ozone for layers > 15 km**

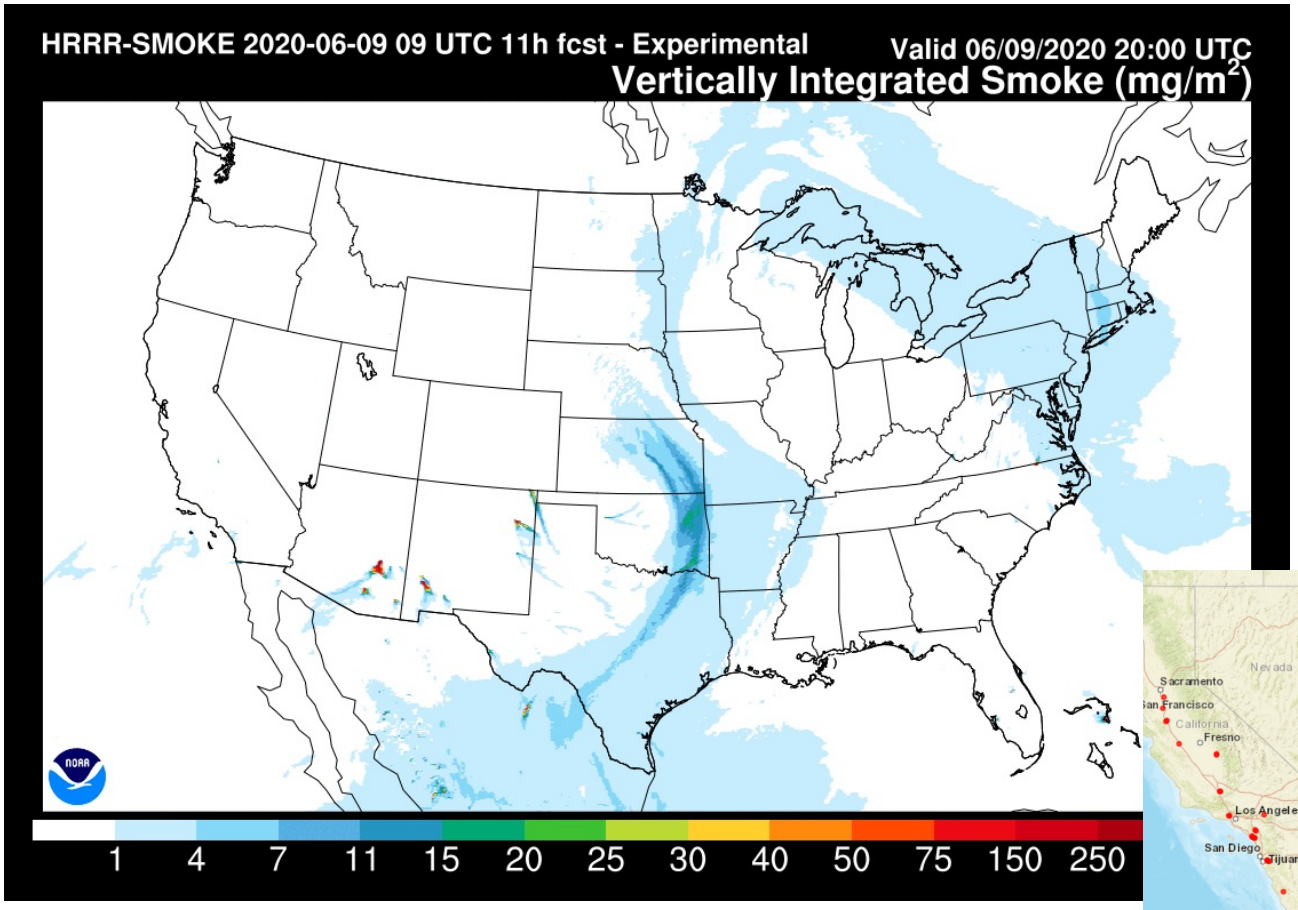


RAP-Chem forecasts use **WRF-Chem chemistry packages**

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

HRRR-SMOKE is operational

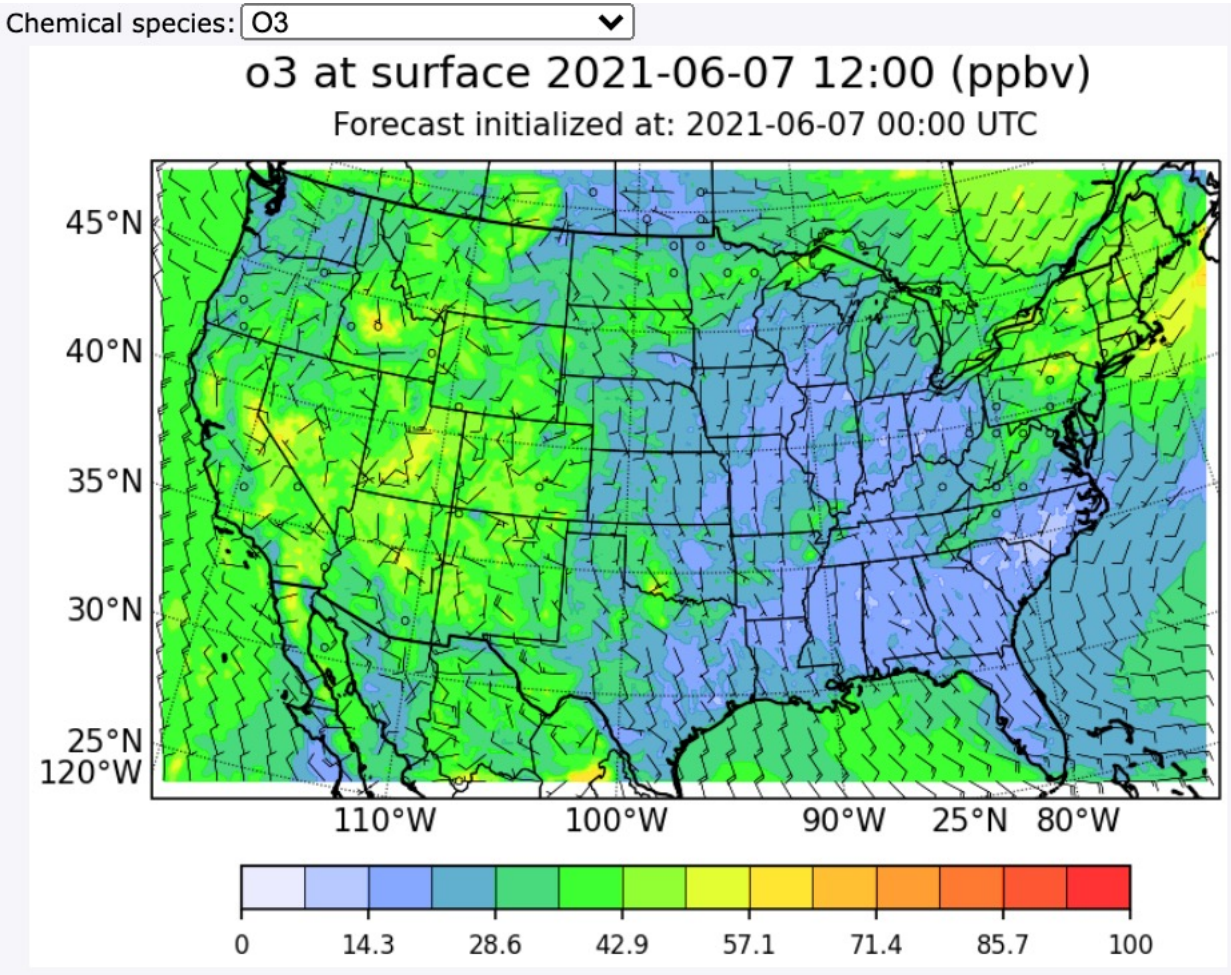
Smoke forecasting using High Resolution Rapid Refresh model (based on WRF and WRF-Chem)



Model running in real time to produce smoke forecasts, daily 00, 06, 12 and 18UTC, for next 36 hours (HRRR-Smoke)

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

Other WRF-Chem forecasts



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

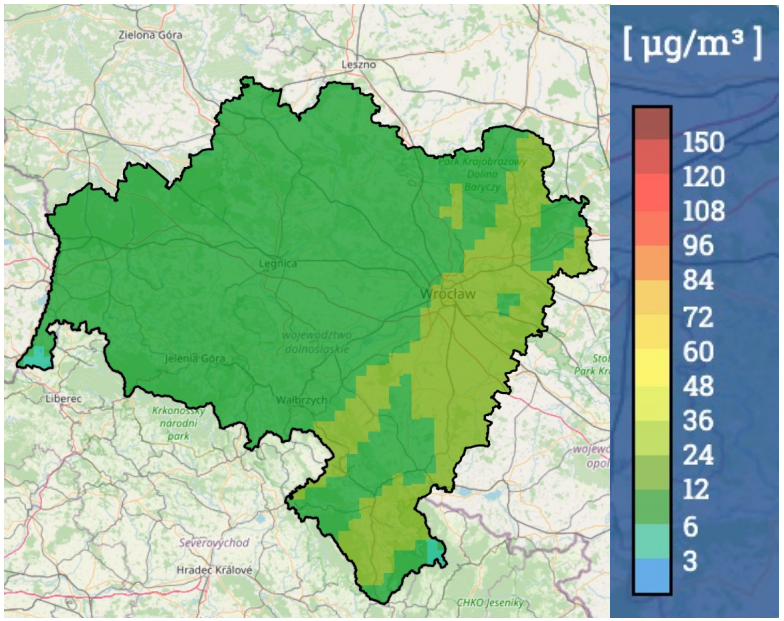
Table 2: Hourly WRF-Chem output description.

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

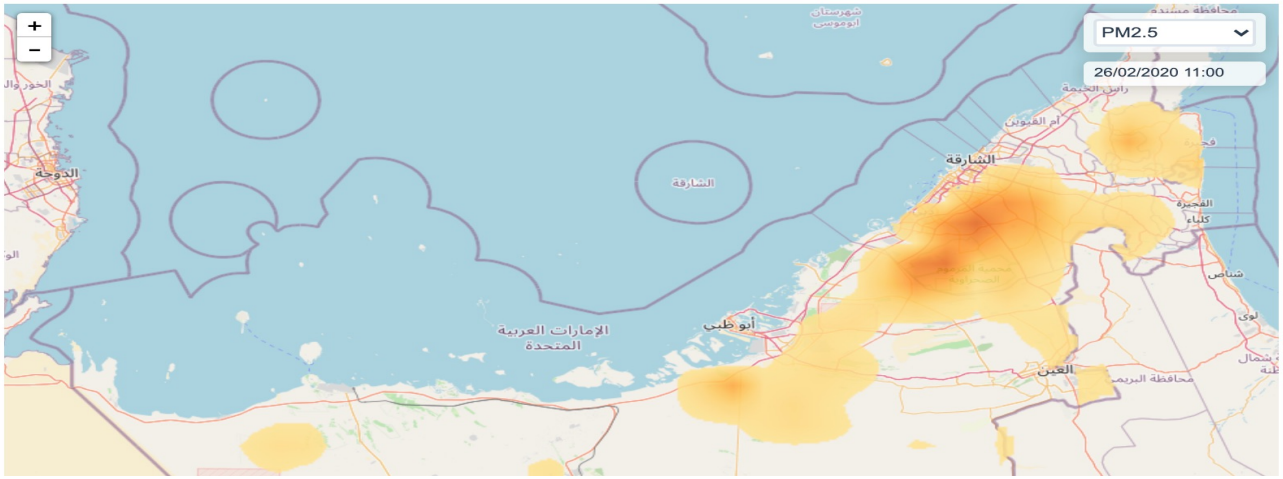
Other WRF-Chem forecasts

Wroclaw University, Poland



UAE Air Quality Forecast

3-day Forecast over the UAE



Updates to WRF-Chem tools

- 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***)
- EPA_ANTHRO_EMISS (available via NCAR)
  - Allows the use of SMOKE (EPA) processed emissions in WRF-Chem
- FINN v.2.2 (NCAR)
  - NCAR/ACOM is currently modifying the fire_emis preprocessing tool to work with the FINNv2.2 data files. (https://www2.acom.ucar.edu/wrf-chem)
- 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)

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 tutorials have been updated to v4.0
- 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 new 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

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 CCCP.
- 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?