WRF-Chem v4.2: A summary of status, updates, and applications

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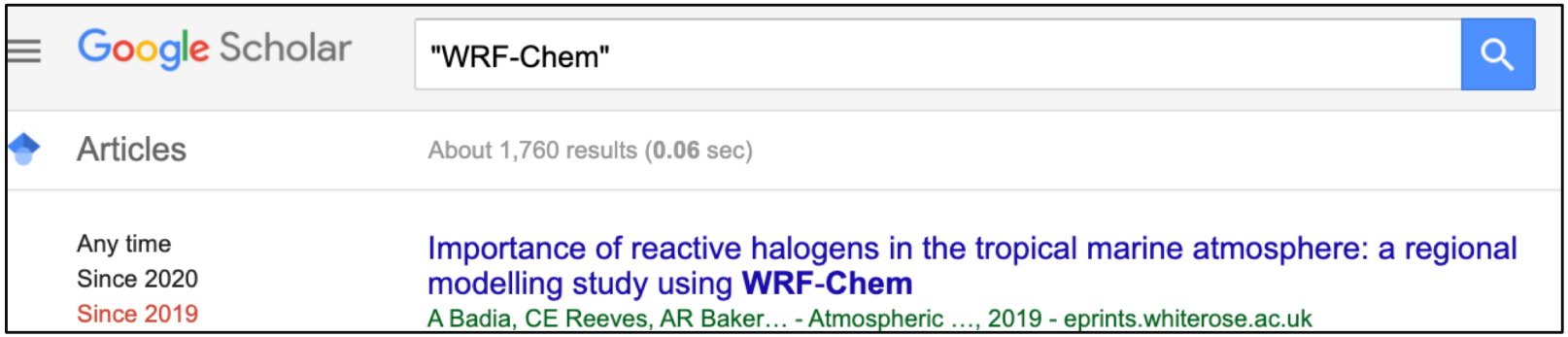
WRF-Chem web site: https://ruc.noaa.gov/wrf/wrf-chem/

General Updates

- WRF-Chem remains one of the most widely used and cited chemistry modeling system in the world → +1700 publications 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 FV3-Chem development (running globally real-time with GOCART dust), but WRF-Chem is still actively used for research

- NCAR will maintain oversight of MOZART-related input data and pre-processors

- 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)

New Tools and Updates

- New ‘convert emiss’ tool (CSL, S. Mckeen)
  - Converts NEI-2011 or prep_chem_src generated binary emissions into two 12-hour emission files
  - To be delivered to the community within 1-2 months.
- 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. Availability expected mid to late summer. (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)

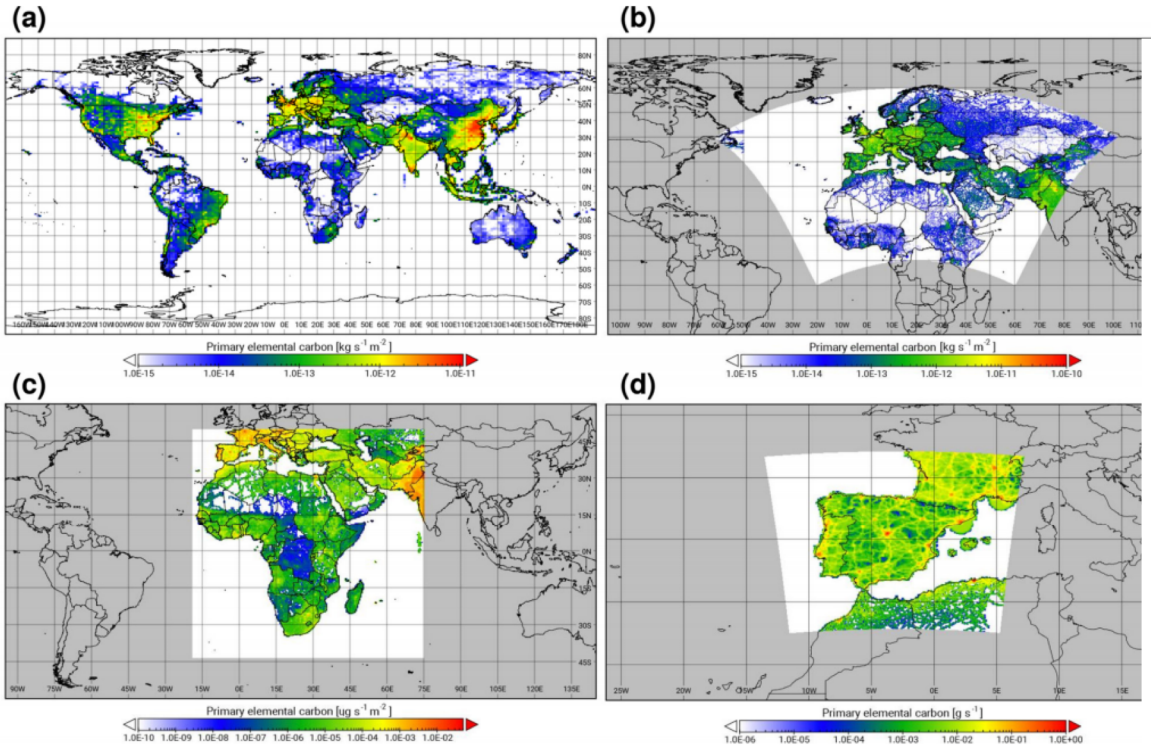


Figure 3. Examples of the HTAPv2.2 black carbon transport emissions regridded onto a 1°×1.4° global regular lat–long dom 0.1°×0.1° rotated lat–long domain **(b)**, 50 km×50 km Mercator grid **(c)** and 4 km×4 km Lambert conformal conic grid **(d)**. All maps are displayed in an equirectangular projection.

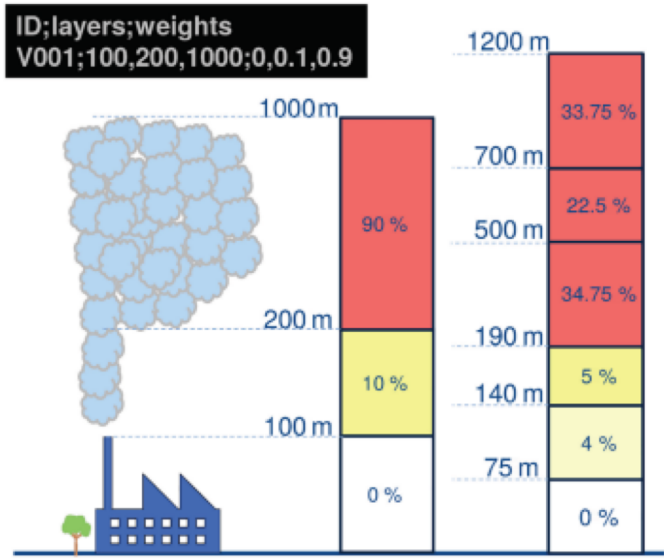
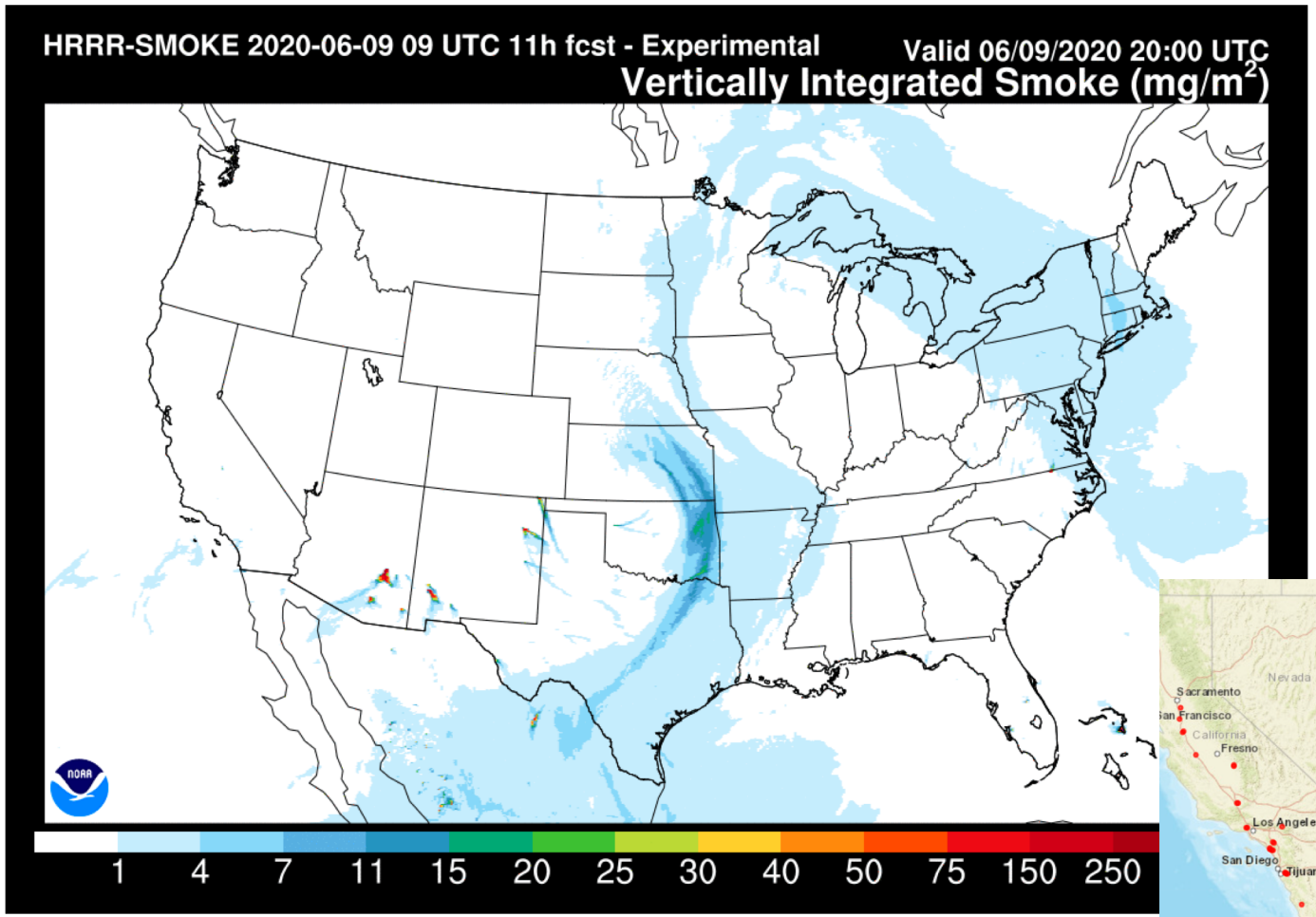


Figure 4. Schematic representation of the e tribution process implemented within HERM

Guevara et al., GMD, 2019

HRRR-SMOKE is (almost) operational

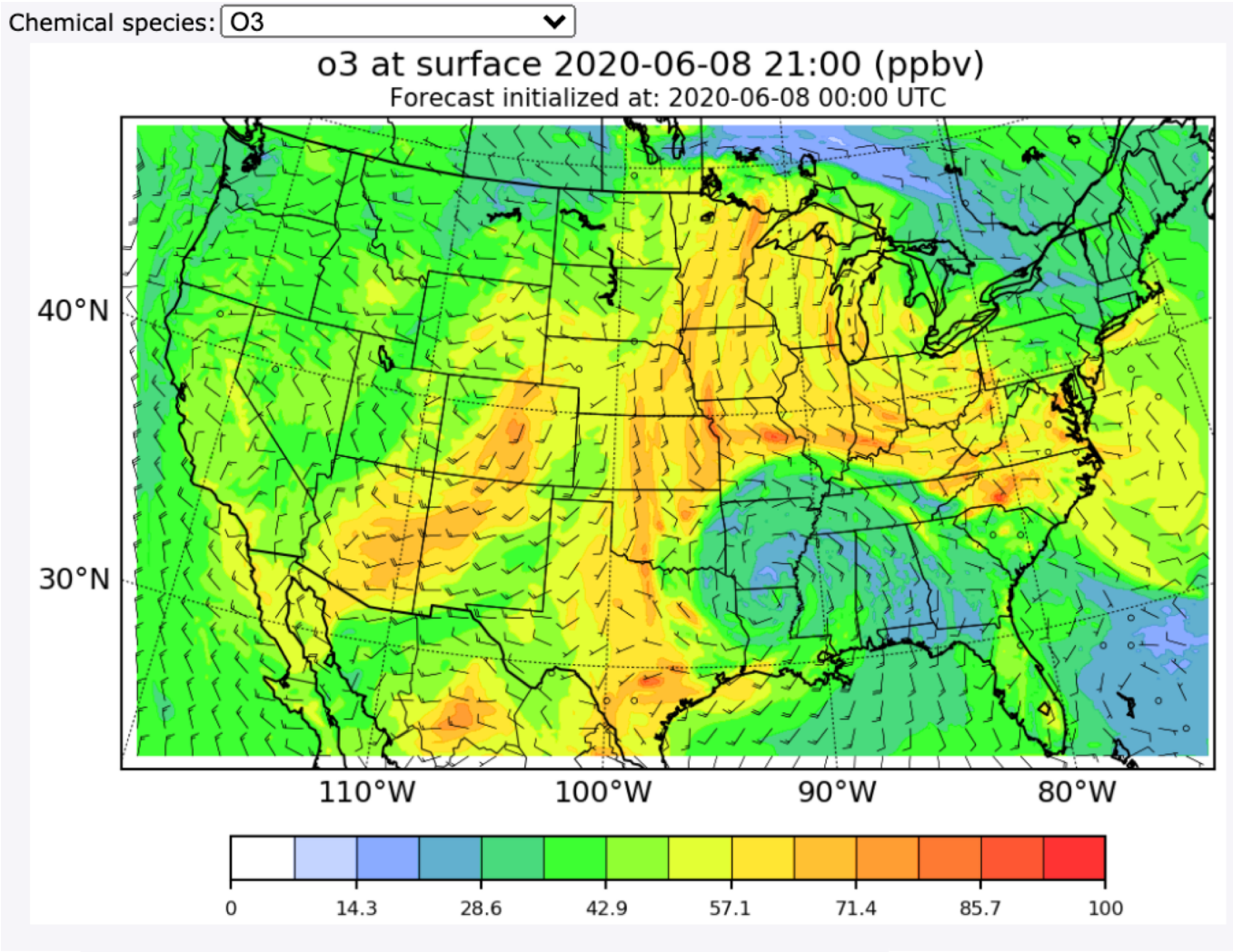
Smoke forecasting using High Resolution Rapid Refresh model (based on WRF and WRF-Chem)



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

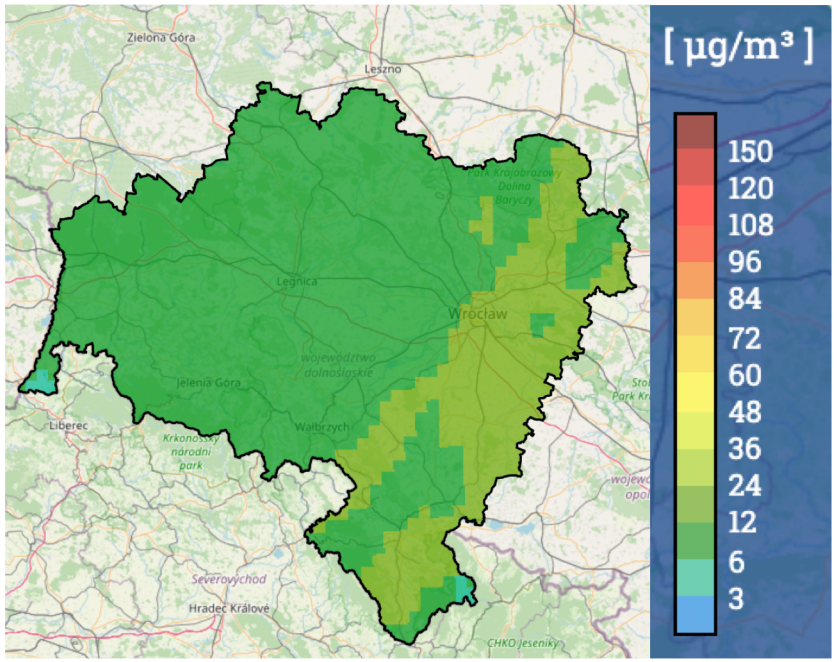
Table 2: Hourly WRF-Chem output description.

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

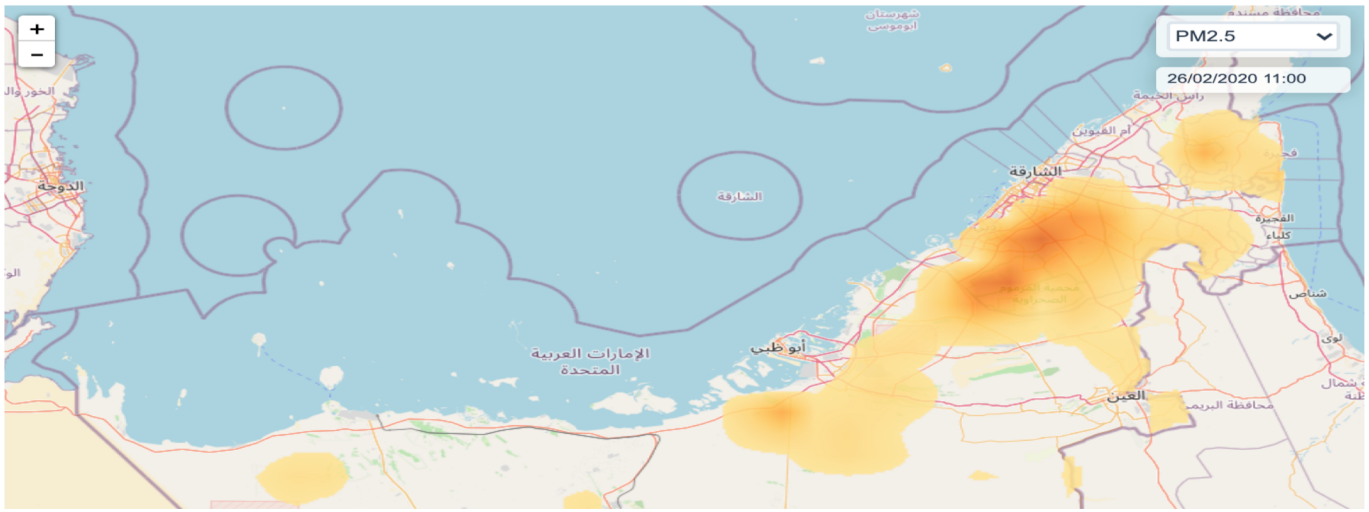
Other WRF-Chem forecasts

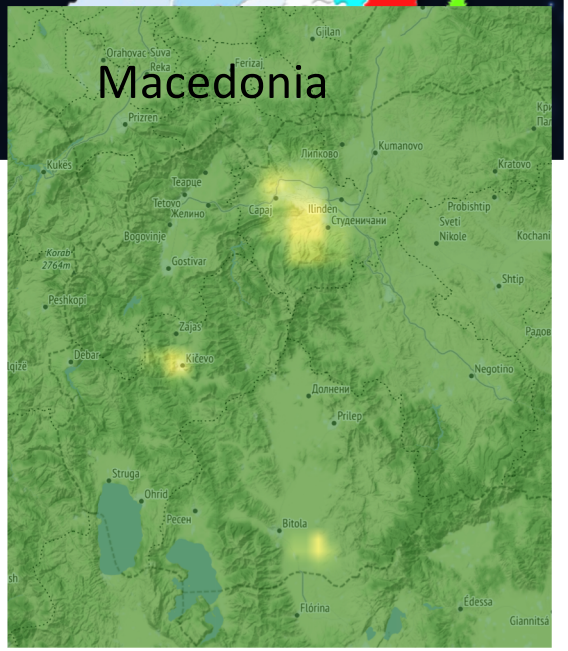
Wroclaw University, Poland



UAE Air Quality Forecast

3-day Forecast over the UAE

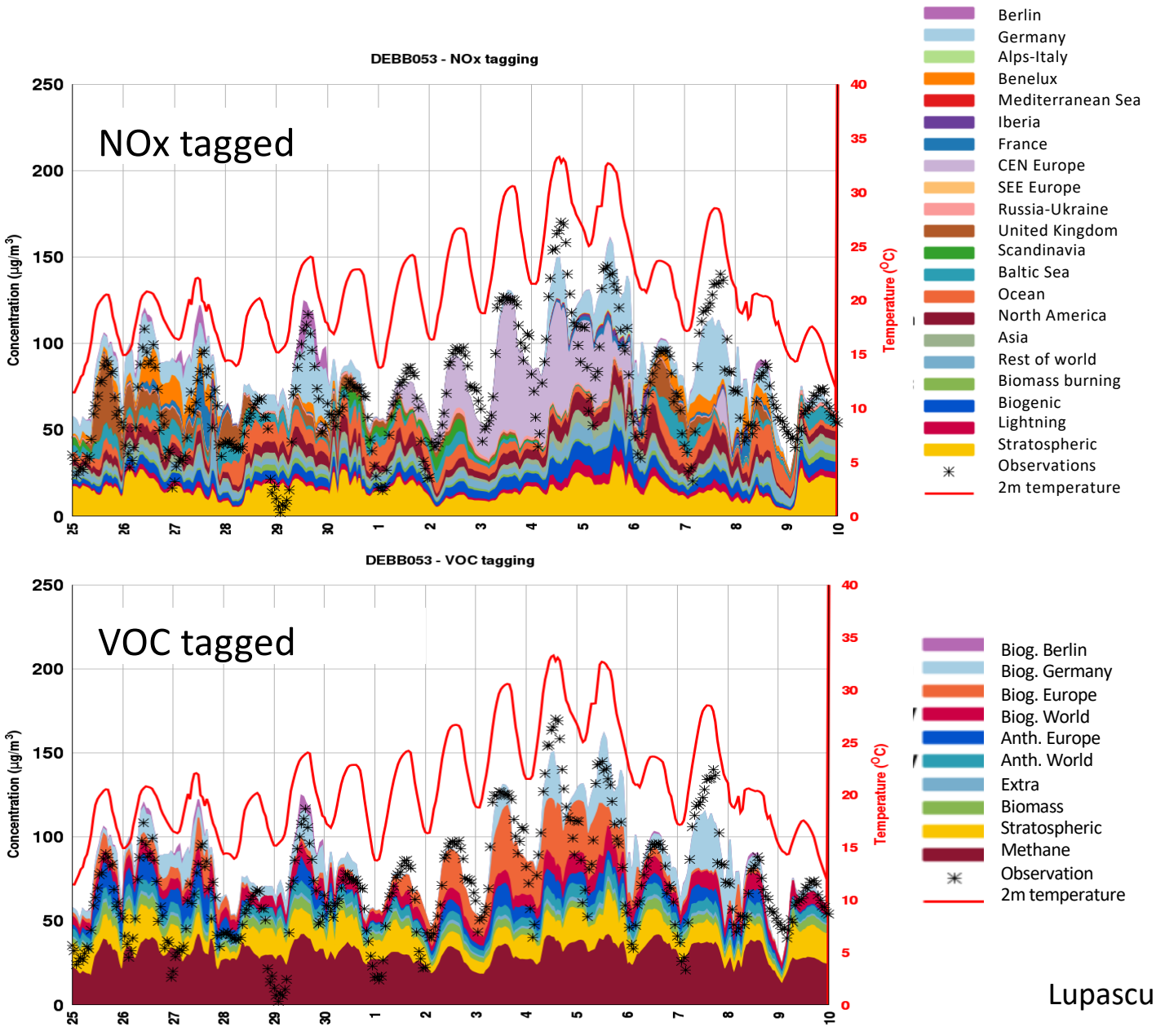




Bug Fixes & Enhancements

- Crimech
  - Fixed double-counting of NO_2 emissions (A. Hilboll, U. Bremen)
  - Fixed alpha/beta pinene emission assignment in MEGAN (D. Lowe (Manchester) & S. Archer-Nicholls (Cambridge)
- GOCART (A. Ukhov)(Ukhov et al. Geosci. Model Dev. Discuss., 2020.)
  - Removed 0.25 tuning factor for SS emissions (now 4x larger)
  - Fixed GOCART dust and SS bins for $PM_{2.5}$ and PM_{10} calculations
  - Fixed AOD calculation to include dust < 0.46 µm
  - Fixed dust gravitational flux to conserve mass
  - mass redistribution between GOCART dust/sea salt and MOZAIC bin
- Bug fix to conserve mass for fire emissions when the plume rise is used (R. Ahmadov, CIRES)
- Multiple fixes/additions to lighting (X. Zhang)

Tagged ozone mechanism: developed by A. Lupascu and T. Butler at IASS – (Not in official release, 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) *in preparation*

New mechanism based on MOZART-4 with halogen chemistry (Br, I, and Cl), including heterogeneous recycling reactions involving sea-salt and other particles, reactions of Br and Cl with VOCs, along with oceanic emissions of halocarbons, VOCs and inorganic iodine – (A. Badia Morages) (**Not in official release,** contact Alba.Badia@uab.cat **if interested)**

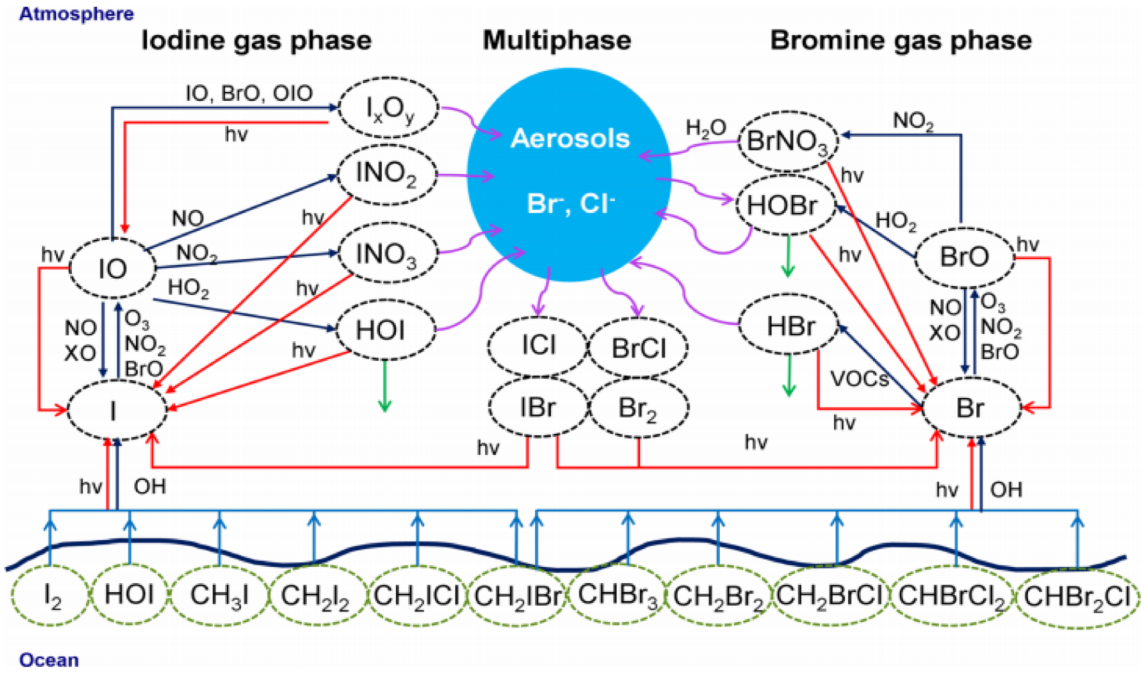
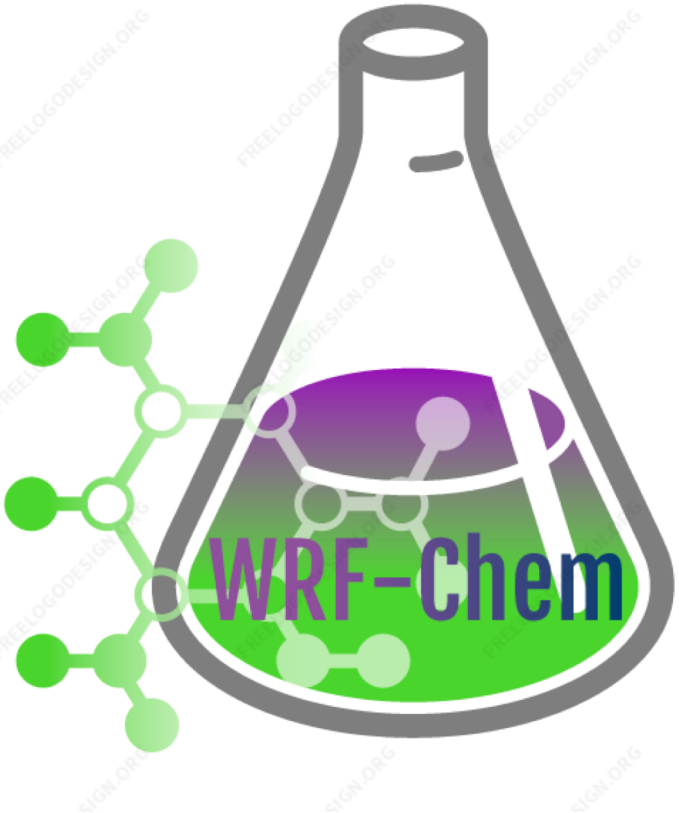


Figure 4. Schematic representation of the implemented iodine and bromine chemistry in WRF-Chem. Chlorine chemistry has been included into the model; since our results are mainly focused on reactive bromine and iodine, we decided not to include chlorine chemistry in this figure. Red lines represent photolytic reactions, dark blue lines gas-phase pathways, light blue lines fluxes, green lines deposition and purple curved lines heterogeneous pathways.

Mechanisms (under development)

- 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)
- Reduced hydrocarbon mechanism (cheap, carbon-bond) – coupled to MADE/VBS_SOA aerosols



Coming soon… (pull requests in wait or soon to be submitted)

- New CLM-MEGAN v2.1 interface (currently v2.0 and BEIS are the other options for online biogenic emissions) – (B. Gaudet)
- Gas 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)
- pH diagnostics for mozart_mosaic_4bin_aq chemistry option (S. Walters)
- Lightning Data Assimilation – (X. Zhang and Y. Li)
- WRF-Chem-PAH model (Mu et al., ACP, 2017)
- Aerosol Water Chemistry module to simulate the heterogeneous reactions in aerosol water – (Y. Cheng, H. Su, & W. Tao, MPI)

New *insider* 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

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 – NEW regression testing available with KPP!

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