WRF-Chem V4.0: 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/

Email: wrfchemhelp.gsd@noaa.gov

Updates in the WRF-Chem 4.0 release

- Potential Vorticity based stratospheric ozone calculation (NOAA/ESRL)
- An updated version of the Model for Simulating Aerosol Interactions and Chemistry scheme (MOSAIC II) (PNNL)
- An updated gas phase chemistry scheme Model for Ozone and Related Tracers (MOZART) version T1 from (NCAR/ACOM)
- A new heterogeneous gas chemistry (based on the Regional Atmospheric Chemistry Mechanism) option coupled with the ISORROPIA II aerosol thermodynamic model (Hong Kong Polytechnic University)
- A Henry's Law Constant table to use the same constants across different chemistry parameterizations, e.g. dry/wet deposition schemes (NCAR)
- An integrated reaction rate diagnostics option (NCAR)
- Diagnostics for WRF-Chem aerosol-radiation feedback in the radiation driver (Universities of Cambridge and Manchester)
- A number of minor bug fixes and enhancements;

Parameterization of O_3 boundary conditions according to Potential Vorticity (PV)

Courtesy of Stu McKeen (NOAA/ESRL)

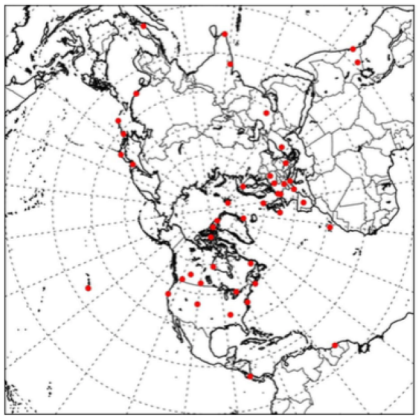
$$PV = \frac{1}{\rho}\left[\nabla\times\vec{v} + Coriolis\right]\cdot\nabla\theta$$

1 PV unit = 10^{-6}·°K·m^2/kg-s

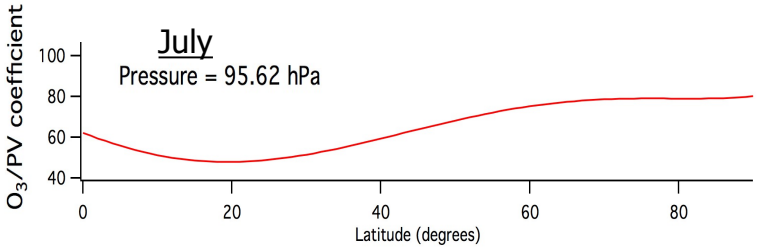
Danielsen (1968): $\boldsymbol{O_3 \propto PV}$ In stratospheric folds and cut-off lows

Literature values: O_3/PV from 35 to 130 ppbv/PVU

Xing et al. (ACP, 2016) – A global climatology of O_3/PV ratios:



- 21 years of data (1990-2010)
- WRF with NCEP reanalysis nudging
- 44 O_3 sonde locations from WOUDC
- Latitude, Month, Pressure dependent



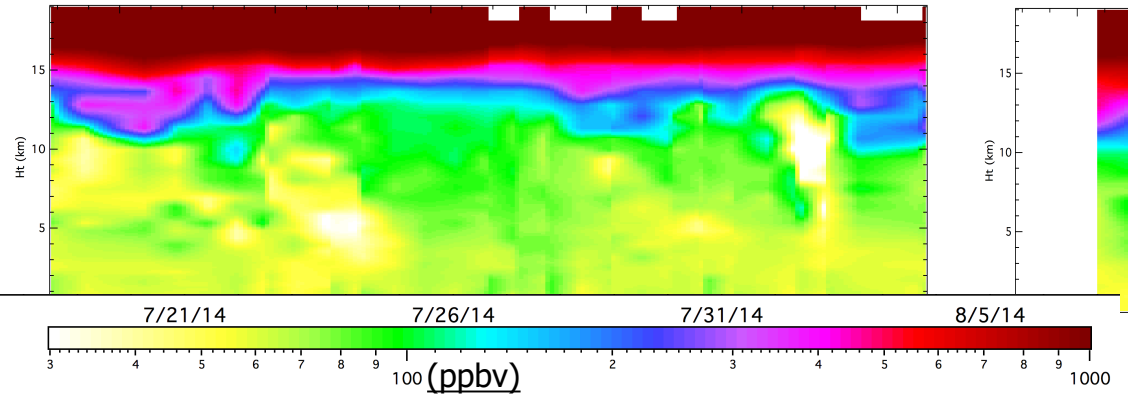
WRF-Chem Stratospheric Tracers:

1) IC/BC O_3 above 500 mb from O_3/PV
2) O_3/PV = 100 – upper limit

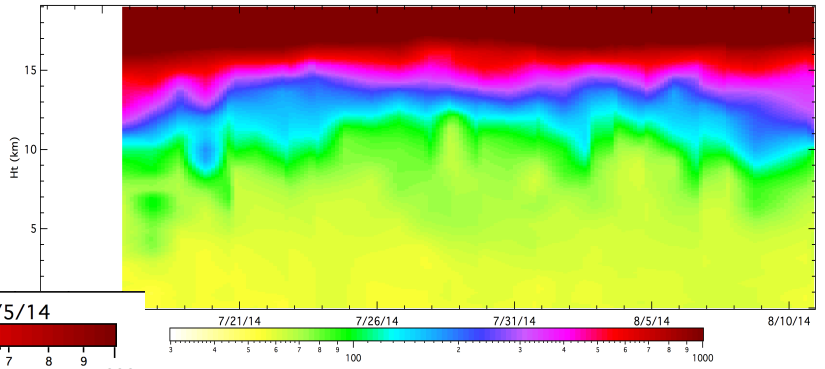
Courtesy of Stu McKeen (NOAA/ESRL)

Penn State Platteville O_3 comparisons

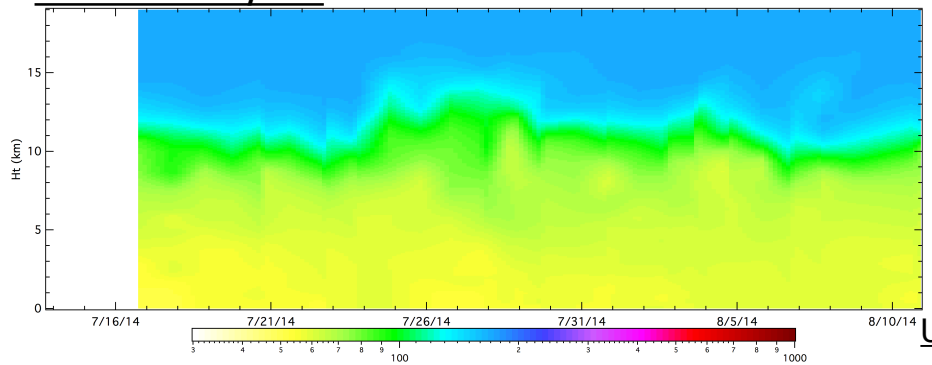
Observations



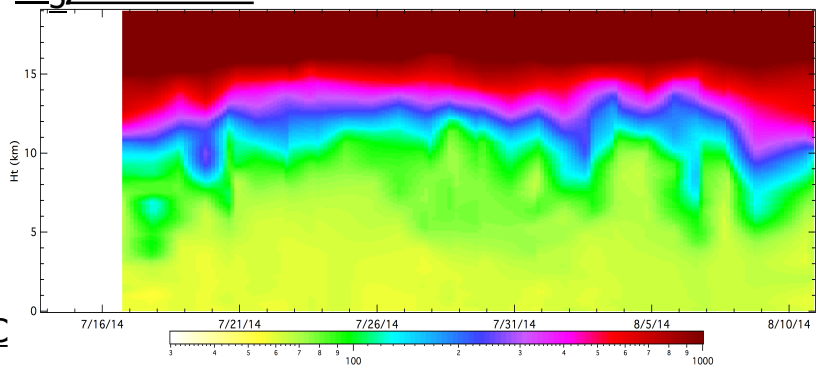
O_3/PV from Xing et al. (2016) used for IC/BC



Default IC/BC



O_3/PV=100



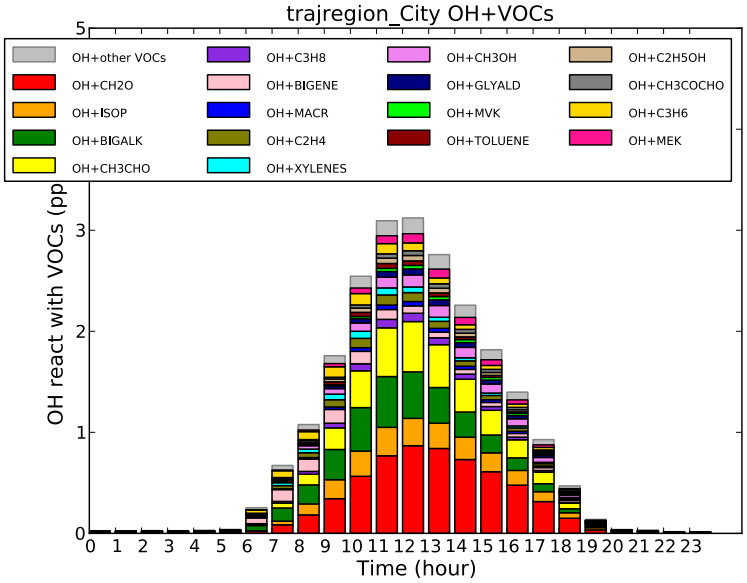
ESRL

New Chemistry and Diagnostics for the MOZART Chemistry Suite

Mary Barth, Gabriele Pfister, Stacy Walters, Louisa Emmons (all at NCAR), Christoph Knote (LMU, Germany)

Check the presentation 2.1 by M. Barth

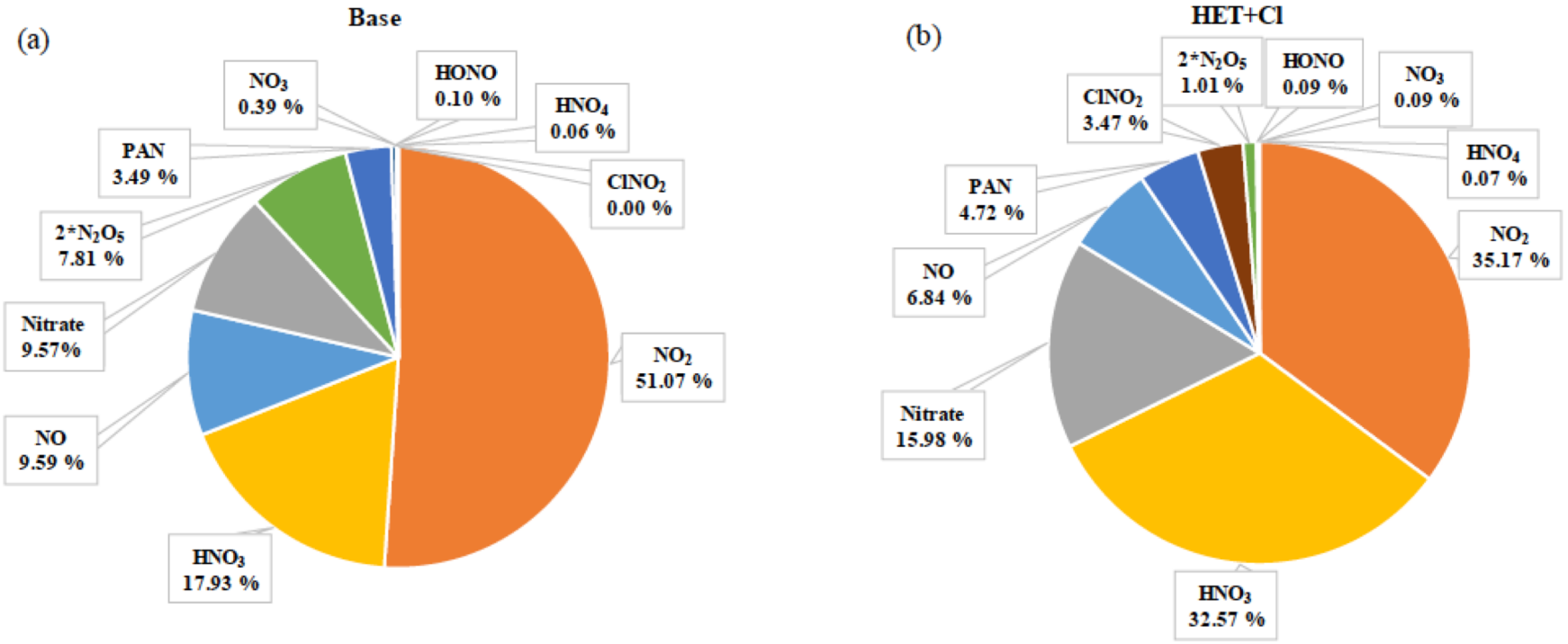
- T1-MOZCART chemistry scheme
  - Expands chemistry from MOZARTv4 (Emmons et al., 2010)
  - Still connected to GOCART aerosols
- Henry's Law coefficients
  - Table of coefficients for KH, K1, K2
  - Used in wet deposition (both subgrid and resolved) and dry deposition schemes
- Integrated rates of reactions
  - Creates new output for analyzing chemistry
- Plan to implement T1-MOZART-MOSAIC in next version



Dominant VOC + OH reactions along a trajectory

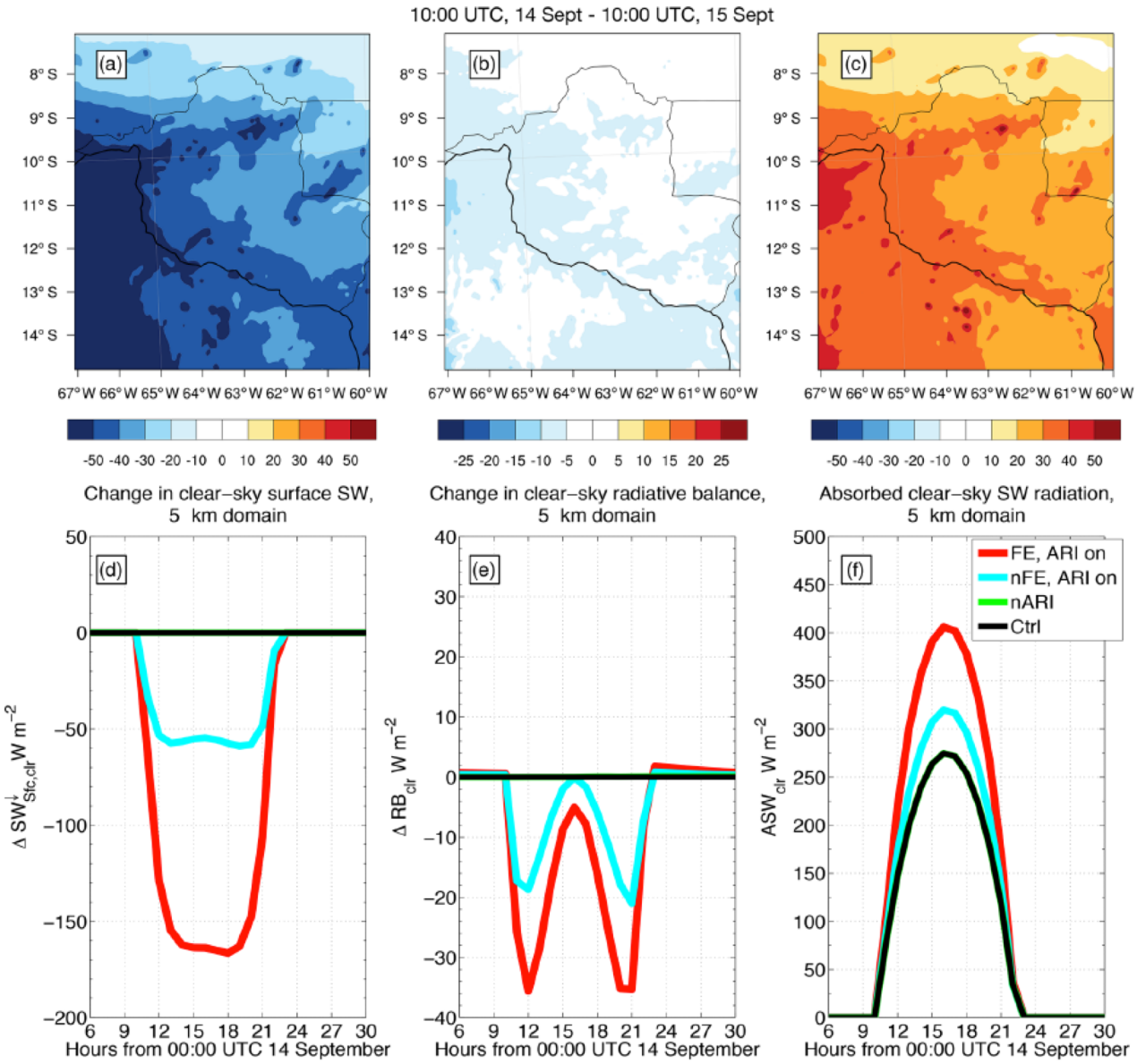
ESRL

A new heterogeneous gas chemistry option (chem_opt=100) in WRF-Chem V4 coupled with the ISORROPIA II aerosol thermodynamic model (The Hong Kong Polytechnic University)



Li et al., *Impacts of heterogeneous uptake of dinitrogen pentoxide and chlorine activation on ozone and reactive nitrogen partitioning: improvement and application of the WRF-Chem model in southern China*, Atmos. Chem. Phys., 16, 14875–14890, 2016.

Diagnostics option for the aerosol-radiation feedback within the radiation driver of WRF-Chem V4 (*clean_atm_diag* namelist option)



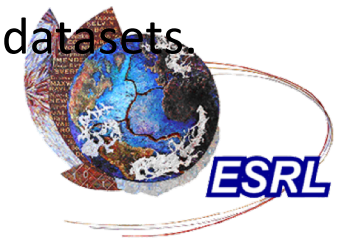
Archer-Nicholls S. et al., ACP, 16, 5573–5594, 2016

Other ongoing WRF-Chem developments

- WRF-Chem/DART (*Mizzi A., NCAR*)
- WRF-Chem adjoint (*Guerrette J.J., NCAR).*
- Tagged ozone mechanism (*see poster P16 by by Lupascu and Butler*)
- RACM2 gas phase chemistry (better suited for SOA simulations)
- Global anthropogenic emission inventory processing for WRF-Chem (S.McKeen NOAA)
- Modeling of fire emissions and plume rise using satellite fire radiative power data by Ahmadov et al. (NOAA, NASA)
- *Some of the new developments will be added to future WRF-Chem releases.*

Updates in anthropogenic emission inventories for WRF-Chem modeling

- The EPA NEI2011 emissions inventory (US domain) is available for using in WRF-Chem modeling. (thanks to S.McKeen from NOAA/ESRL)
- Additionally, the NEI2011 emissions for weekends, updated emissions for the US oil/gas sector can be provided to users.
- The new version of prep_chem source (1.5) includes HTAP2.2 emissions for the entire globe. (*see Janssens-Maenhout et al., ACP 2015*)
- A sample netcdf file with emissions processed for the RADM/RACM gas chemistry mechanisms over the CONUS domain will provided to users.
- Currently there are many emission datasets available for air quality modeling, e.g. developed for specific field campaigns, estimated by inversion studies etc. Check the WRF-Chem publications list to learn more about those emission datasets.



New Anthropogenic Global Emission Inventory

(For use with prep_chem_sources package)

Community Emissions Data System (CEDS)

Rachael Hoesly, Steve Smith et al., 2017, GMDD.

U. Maryland/PNNL's Joint Global Change Research Institute

Based on HTAP-2010

Basis for CMIP modeling projects

Current configuration:

0.5 X 0.5 degree horizontal resolution

Global monthly emissions from 1750 to 2014

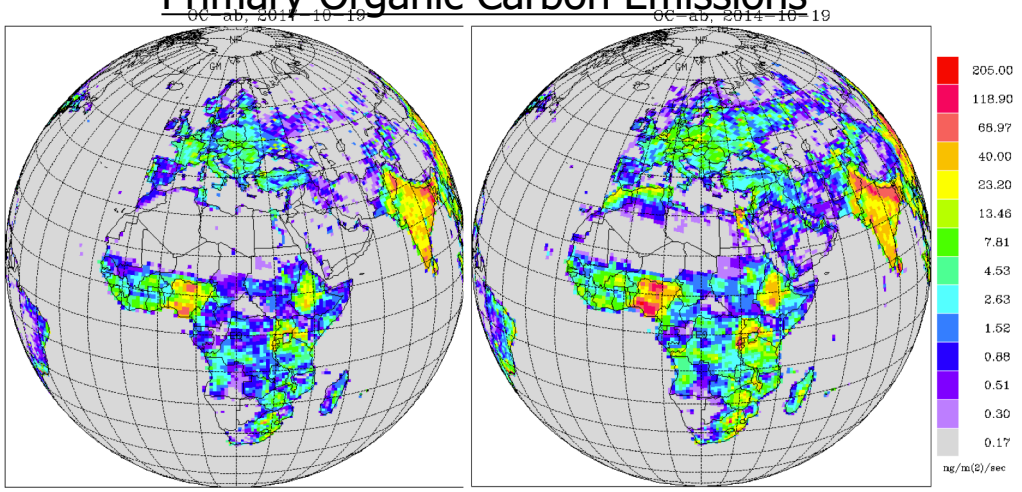
Anthropogenic BC, OC, and other Aerosol

26 VOC species

NOx, SO2, CO, NH3, CO2, CH4

Nine Energy/Use Categories

Primary Organic Carbon Emissions



HTAP-2010 CEDS-2014

Available for WRF-Chem

- GOCART aerosol (currently)
- CEDS (2014) datasets
- Modified prep_chem_sources
- Contact: Stu McKeen

ESRL

A list of recent global inventories

Author	Acronym	Reference or Website	Years	Resolution
Lamarque et al.	ACCMIP	eccad.sedoo.fr	1900-2000	0.5x0.5
Riahi et al.	RCPs	eccad.sedoo.fr	2000-2100	0.5x0.5
Granier et al.	MACCity	eccad.sedoo.fr	2000-2015	0.5x0.5
Maenhout et al.	EDGAR4.2	edgar.jrc.ec.europa.eu	1970-2008	0.1x0.1
Crippa et al.	EDGAR4.3	edgar.jrc.ec.europa.eu	1970, 2010	0.1x0.1
Maenhout et al.	HTAPv2	edgar.jrc.ec.europa.eu	2008, 2010	0.1x0.1
Klimont et al.	ECLIPSE v4, v5	iiasa.ac.at	1990-2030	0.5x0.5
Schultz et al.	RETRO	juelich ftp	1960-2000	0.5x0.5
Bond et al.	Bond	Hiwater.org	1850-2000	country
Junker&Liousse	J&L	eccad.sedoo.fr	1860-2003	1x1
Huang Y. et al.	PKU	inventory.pku.edu.cn	1960-2009	0.1x0.1
Smith et al.	PNNL	sedac.ciesin.columbia.edu	1850-2005	1x1
Blue: inventories providing just a few species				

All the data are publicly available. Most available at: eccad.sedoo.fr, the database of the **Global Emissions InitiAtive (GEIA)**

WRF-Chem Developments by PNNL (Not in Public Version) Fast J. et al.

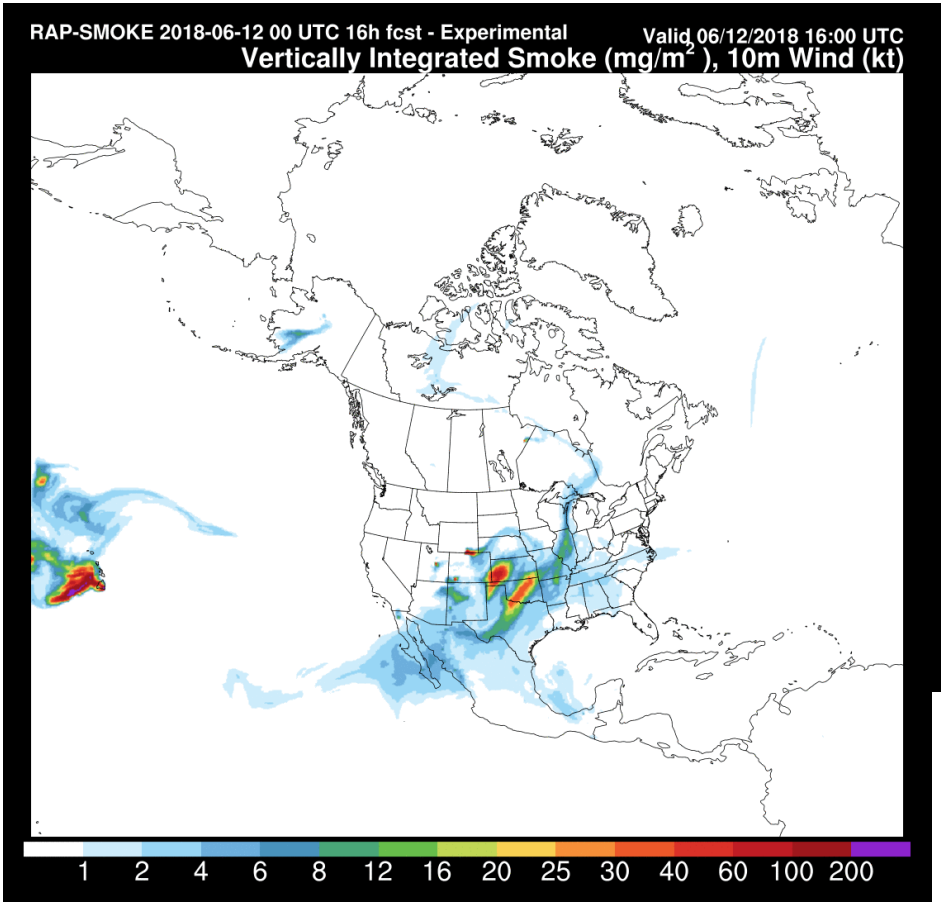
Not currently planned for upcoming releases:

- **Secondary Activation:** Permitting activation above cloud base, shown to be significant for deep convection (Yang et al. JGR 2015)
- **Ice-Borne Aerosols** (Yang et al., JGR 2015)
- **Explicit Nucleation and Ultrafine Particles:** 20-size bin version of MOSAIC, 1 nm – 10 μm (Lupascu et al., ACP 2015)
- **Secondary Organic Aerosol:** Isoprene epoxydiol (IEPOX) and other explicit biogenic chemistry (Shrivastava et al., in preparation)
- **Cloud-Aerosol Interactions with Spectral Bin Microphysics:** Coupling of MOSAIC aerosol model with spectral bin microphysics for cloud-resolving scales (Gao et al. JAMES, 2016)

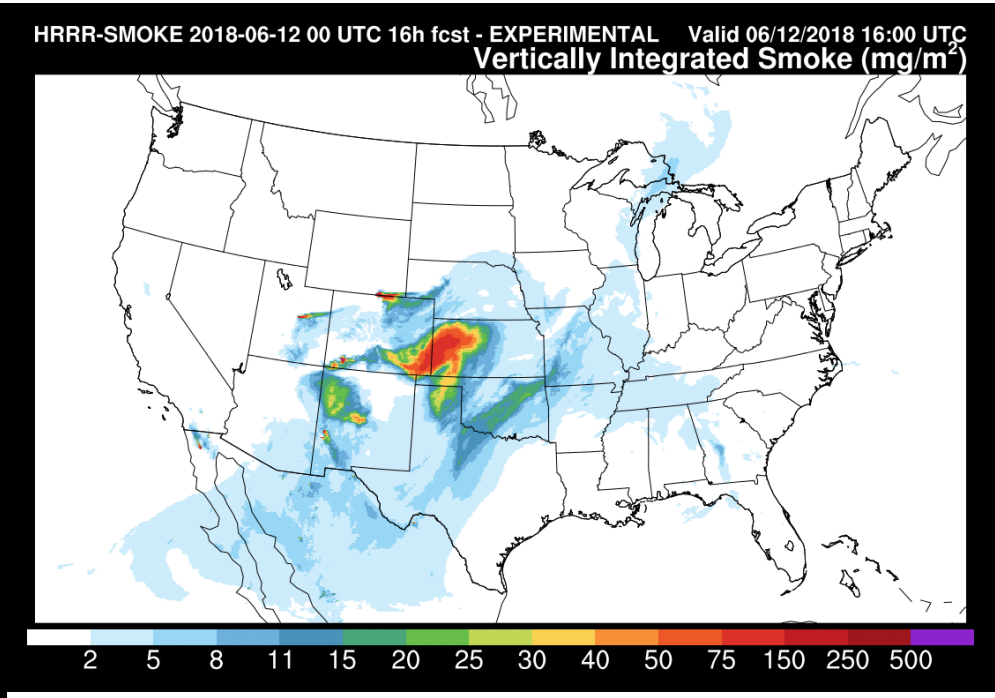
(available upon request)

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

Check the presentations 4.2 and 8.2 by James E. and Alexander C. (NOAA/ESRL)



RAP-Smoke (13.5 km resolution)



HRRR-Smoke (3 km resolution)

Both models are running in real time to produce experimental smoke forecasts, daily 00, 06, 12 and 18UTC, for next 48 (RAP-Smoke) and 36 hours (HRRR-Smoke)

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

Few important notes

- 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.
- We recommend all the users signing up to the new WRF-Chem discussions email group (forum)
- Also, please send us info on your peer reviewed WRF-Chem publications

WRF-Chem info on the WEB:

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

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