WRF-Chem V3.9: A summary of status and updates

Ravan Ahmadov (NOAA, Earth System Research Laboratory)

With contributions from:
G. Grell, K.Wong, L.Zhang, M.Bela, S. A. McKeen (**NOAA/ESRL**), S.E. Peckham, S. Jones (**CRREL**), J. Fast, R. Easter, W. Gustafson, B. Singh, C. Zhao (**PNNL**), A. Hodzic, M. Barth, G. Pfister, S. Wolters, S. Madronich (**NCAR**), S. Freitas (**NASA**), P. Tuccella **(Laboratorie de Météorologie Dynamique),** Y. Zhang, K. Wang **(NCSU),** Martina Klose **(University of Cologne),** D.Lowe (**University of Manchester**) and *many more national and international collaborators*

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

Email: wrfchemhelp.gsd@noaa.gov

Haagen-Smit Prize 2016 awarded to the WRF-Chem paper

1238 citations (Google Scholar)

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Atmospheric Environment 39 (2005) 6957–6975

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www.elsevier.com/locate/atmosenv

Fully coupled "online" chemistry within the WRF model

Georg A. Grell[a,*], Steven E. Peckham[a], Rainer Schmitz[c], Stuart A. McKeen[b], Gregory Frost[b], William C. Skamarock[d], Brian Eder[e]

The Executive Editors and the Publisher of Atmospheric Environment take great pleasure in announcing the 2016 "Haagen-Smit Prize", designed to recognize *outstanding papers published in Atmospheric Environment*. The Prize is named in honor of Prof. Arie Jan Haagen-Smit, a pioneer in the field of air pollution and one of the first editors of the International Journal of Air Pollution, a predecessor to Atmospheric Environment.

Updates in WRF-Chem 3.9 (released in April, 2017)

- A new photolysis scheme – new photolysis fluxes, quantum yields and cross-sections;
- A new trajectory option that monitors meteorological and chemical properties along air trajectories;
- Updates to the MOZART gas scavenging: works with the Thompson, Morrison and WSM6 microphysics schemes and allows specifying the ice retention fraction for each gas;
- Modified dust scheme for the MADE and MOSAIC chemistry options;
- Bug fixes for the CB05* and RACM_SOA_VBS_AQCHEM chemistry options;
- A bug fix (tuning factor for dust emissions) in the gocart dust option (dust_opt=1);
- Mapping of wildfire emissions (size distributions) when using the mosaic sectional 8-bin aerosols scheme (emissions module for the MOSAIC options);
- Packaging numerous 3D arrays used to diagnose secondary organic aerosol production, chemical species in the CuP scheme, and photolysis rates in registry.chem in order to reduce the memory footprint of WRF-Chem;
- A number of minor bug fixes and enhancements;

Updates in anthropogenic emission inventories for WRF-Chem3.8 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.

ESRL

Photolysis in WRF-Chem

- Several radiative transfer options:
  - phot_opt = 1 : TUV (140 λs, delta-Eddington)
  - phot_opt = 2 : Fast-J (17 λs, 8-str Feautrier)
  - phot_opt = 3 : F-TUV (17 λs, correction factor, delta-Eddington)

  New option in WRF-Chem v3.9:

  ⇒ phot_opt = 4: updated TUV (140 λs, delta-Eddington)

  ⇒ only works with MOZART_MOSAIC_4BIN_KPP, MOZART_MOSAIC_4BIN_AQ_KPP, and MOZCART_KPP chemical options

- Limitations & advantages
  - Cross section and quantum yield data are hard-coded and not up to date in older schemes;

  ⇒ updated database to the latest TUV model (V5.3, Oct. 2016)

  - Difficult to add new reactions (typically available ~ 20)

  ⇒ 109 reactions relevant for tropo & strato chemistry (e.g. halogens)

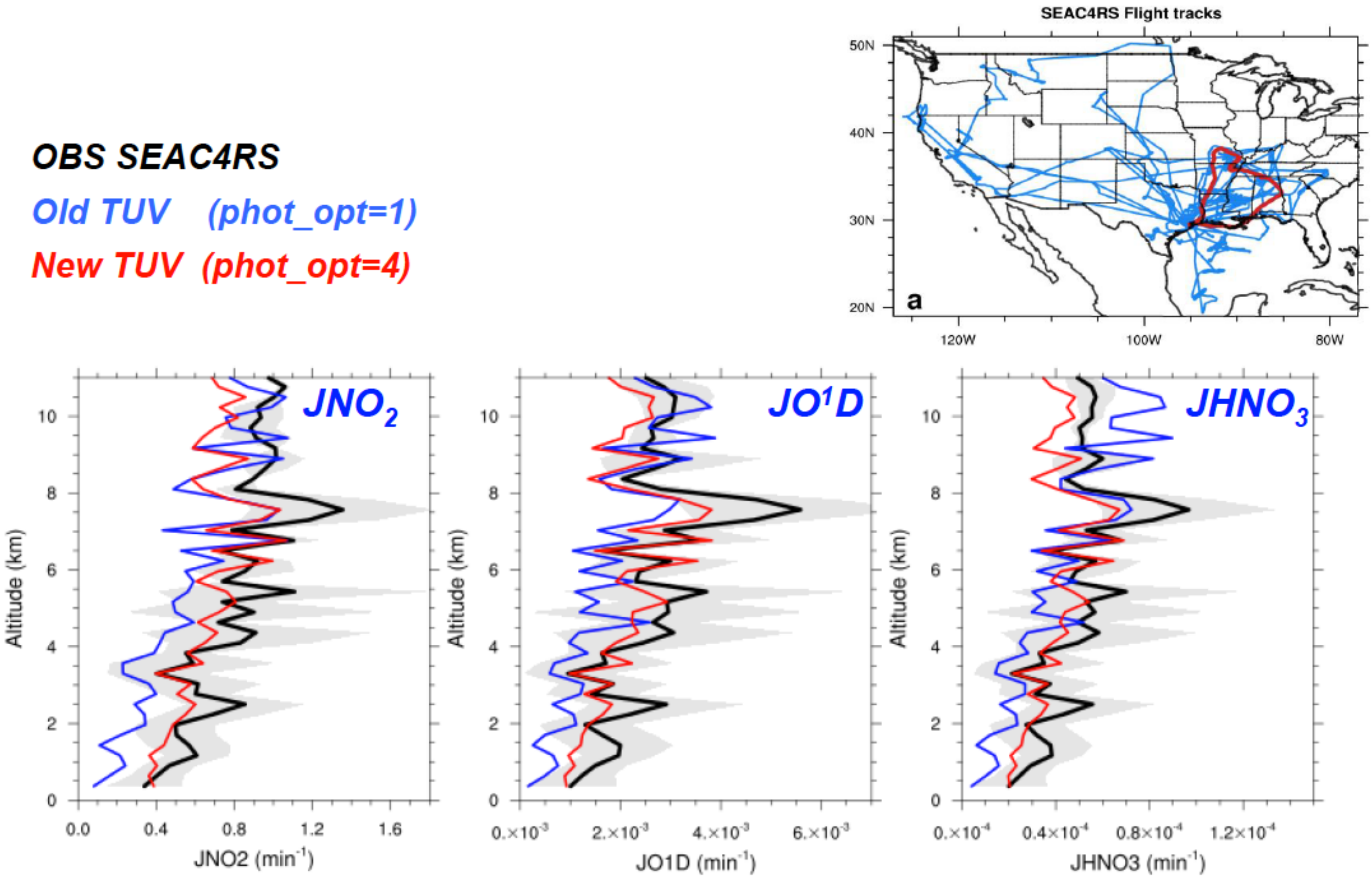
Madronich and Hodzic, WRF-Chem tutorial, 2017

Comparison with the 2013 SEAC^{4}RS flights

OBS SEAC4RS

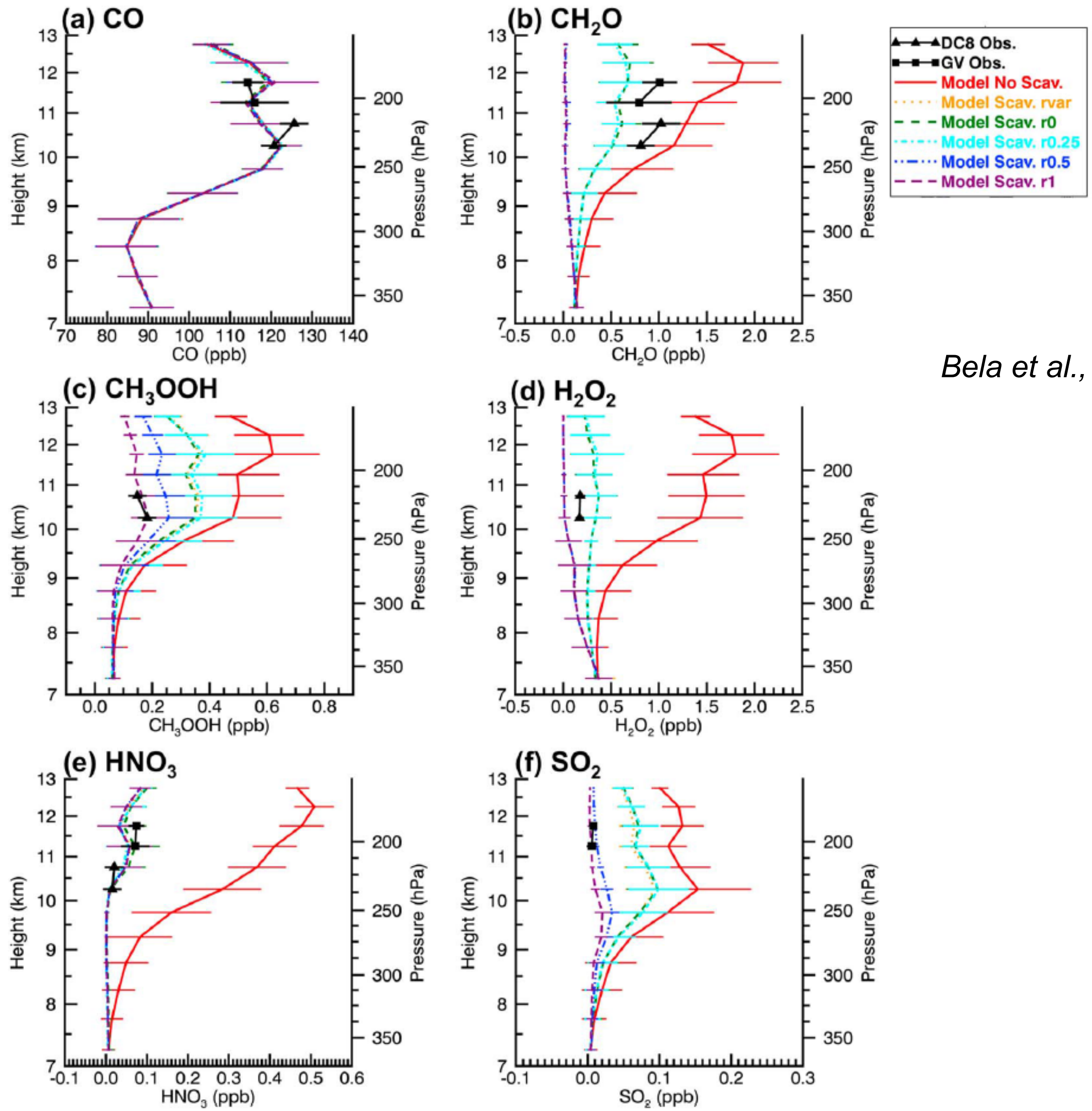
Old TUV (phot_opt=1)

New TUV (phot_opt=4)



Madronich and Hodzic, WRF-Chem tutorial, 2017

Wet removal for the MOZART based chemistry options in WRF-Chem3.9



Bela et al., JGR, 2016

Figure 4. Mean outflow chemical profiles from the Oklahoma 29–30 May 2012 storm as observed by the DC-8 (black triangles and solid lines) and GV (black squares and solid lines) aircraft and mean profiles within the aircraft outflow sampling latitude-longitude region and vertical extent of anvil cloud as simulated by WRF-Chem without (solid red) and with wet removal (Rvar = dot orange; R0 = dash green; R0.25 = dash-dotted cyan; R0.5 = dash dot dot dot blue; and R1 = long dash purple), for (a) CO, (b) CH_2O, (c) CH_3OOH, (d) H_2O_2, (e) HNO_3, and (f) SO_2. The error bars indicate one

Coupling Aerosols and Parameterized Convection For "Large" Dx

J.Fast (PNNL)

Cloud-aerosol interactions are a source of uncertainty in climate simulations, but most convective parameterizations lack these processes

New KF-CuP Chemistry package

- cu_opt=10 (KF+CuP), chem_opt=203 (SAPRC+MOSAIC)
- Modified Kain-Fritsch (deep convection) coupled with Cumulus Potential (CuP) (shallow convection) – both cloud types affect radiation

Berg et al., GMD, 2015

- Aerosol activation
- Transport
- Aqueous chemistry
- Wet removal

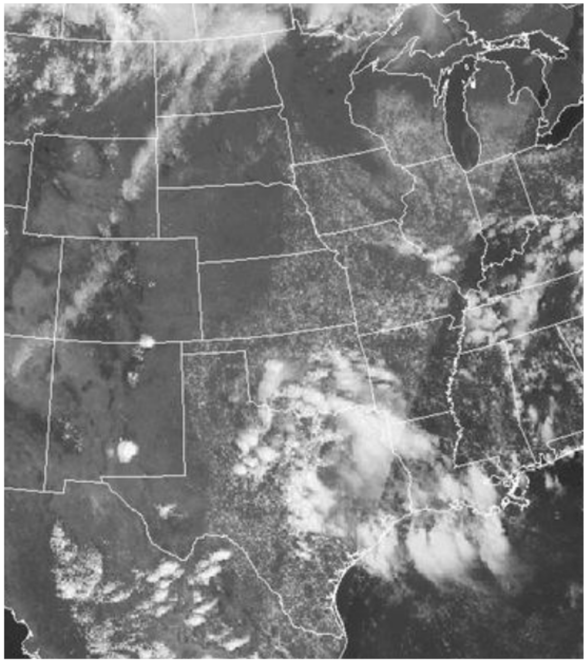
] **in parameterized clouds**

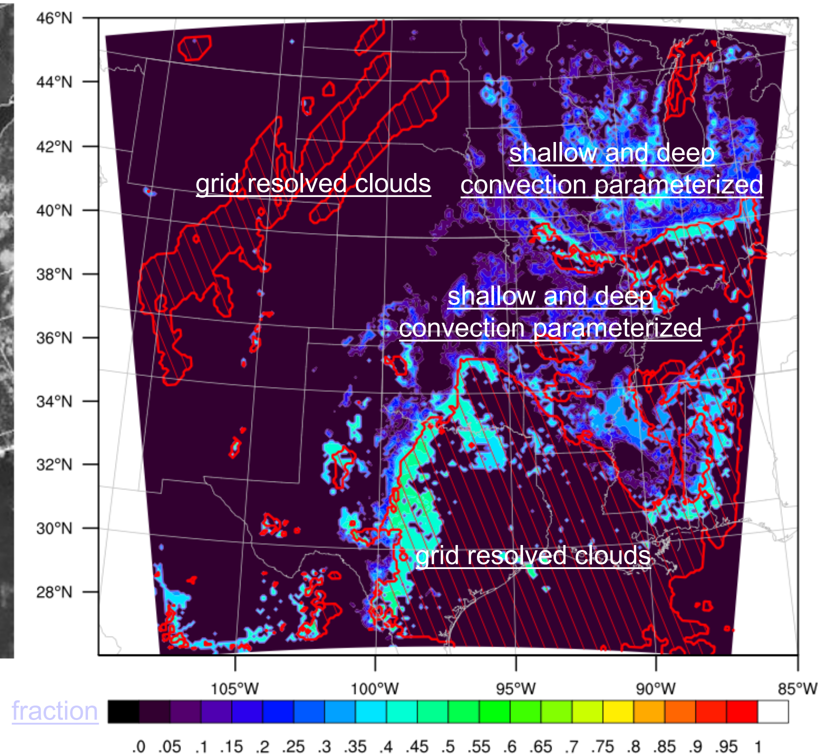
Studies using KF-CuP:
Fast et al., JGR, 2016
Raut et al., ACPD, 2017
Marelle et al., GMDD, 2017
Thomas et al., GRL, 2017

Not Included Yet:

- Feedbacks to radiation, precipitation, etc.

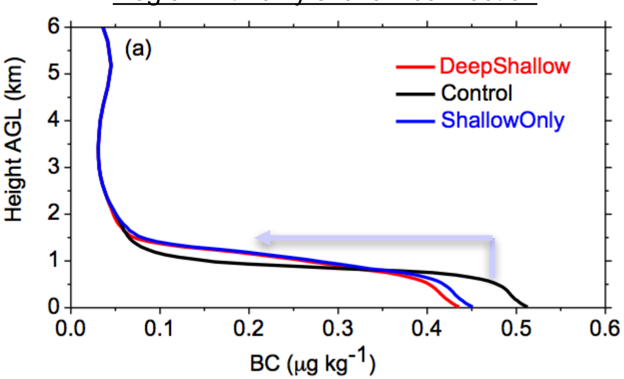
Coupling Aerosols and Parameterized Convection For "Large" Δx
J.Fast (PNNL)



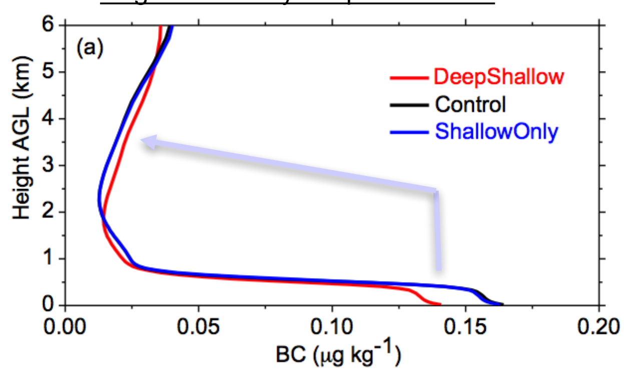


Simulated cloud distribution from KF-CuP qualitatively similar to observed

Region with only shallow convection



Region with only deep convection



(secondary aerosols differnent because of aqueous chemistry)

WRF-Chem Developments by PNNL (Not in Public Version)

Possible inclusion for next release:

- **MOSAIC-2:** Same as MOSAIC, but a large restructuring of the code with more modern Fortran coding to be Open-MP compliant.
- **Updated MEGAN:** Newer version of MEGAN coupled with CLM (Zhao et al. GMD, 2016)

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)

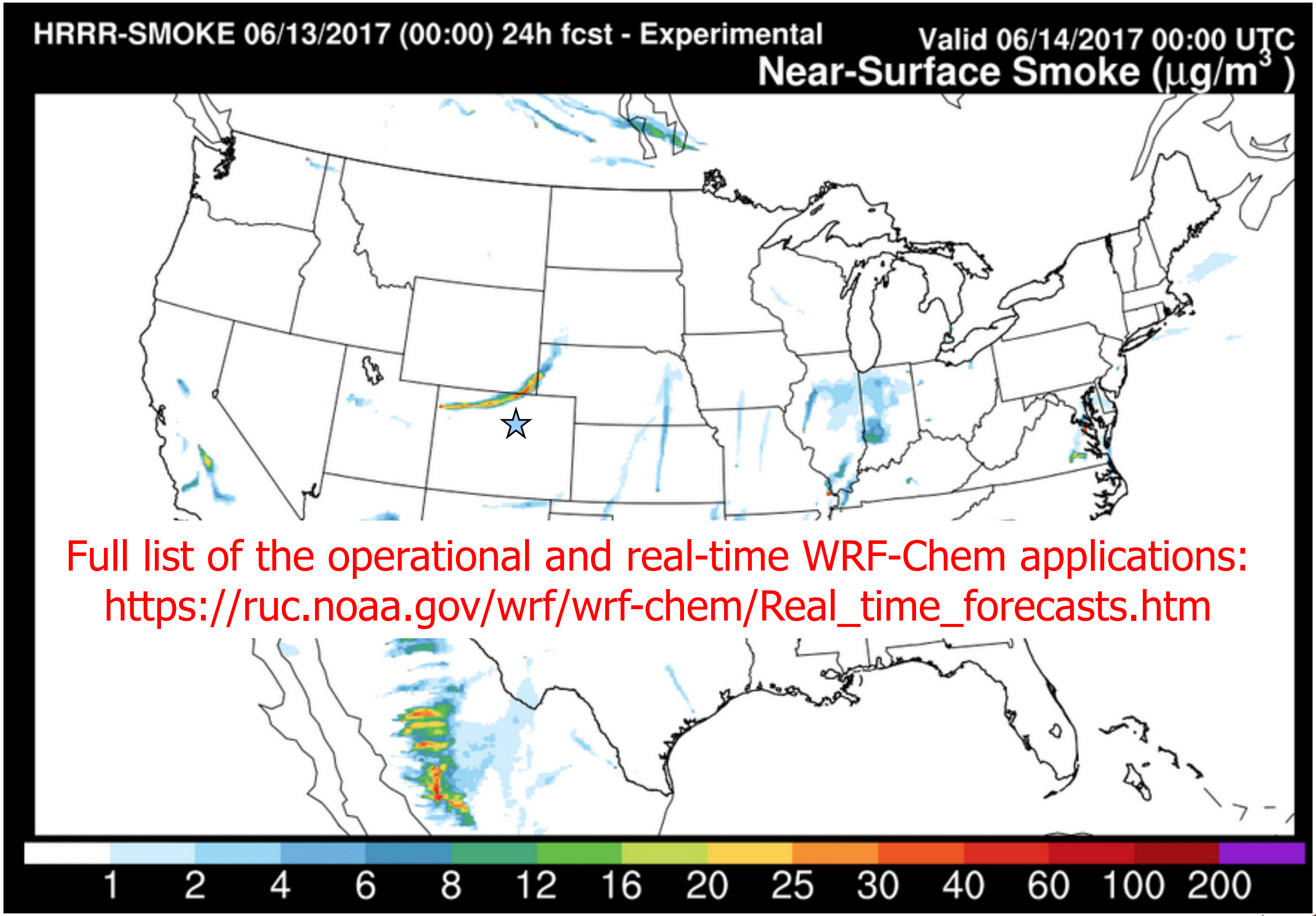
(available upon request)

Other ongoing WRF-Chem developments

- WRF-Chem/DART (*talk by Mizzi Arthur 7A.6*)
- WRF-Chem adjoint (*talk by Guerrette J.J 7B.2).*
- A new chemistry option with heterogeneous chemistry (*talk by Zhang Li 7A.3*)
- Updates to the MOZART gas chemistry for regional air quality application by Pfister G., Knote C. et al. (NCAR, Univ. of Munich)
- Representing the effects of stratosphere–troposphere ozone exchange using a potential vorticity-based parameterization by McKeen et al. (NOAA)
- Tagged ozone mechanism by Lupascu et al. (IASS, Germany)
- Diagnostics for direct and semi-direct aerosol effects by Archer-Nicholls (Univ. of Manchester)
- 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.*

ESRL

Fire smoke forecast for today 6pm
(https://rapidrefresh.noaa.gov/hrrr/HRRRsmoke/)



Full list of the operational and real-time WRF-Chem applications:
https://ruc.noaa.gov/wrf/wrf-chem/Real_time_forecasts.htm

WRF-Chem model on the 3km resolution CONUS domain, run at NOAA/ESRL
No chemistry, primary emissions of aerosols by fires
VIIRS satellite fire detection data are used.

- ***Chemistry session is Thursday morning***
- ***Posters are Wednesday afternoon***
- ***Publication list online:***

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

Please use this list to find papers to read and cite. Please send us your publications too!

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

WRF-Chem forum:

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

WRF-Chem help desk: wrfchemhelp.gsd@noaa.gov

Thank you!