

WRF-Chem (V3.7) Summary of status and updates

Georg Grell

S. E. Peckham, R. Ahmadov, S. A. McKeen, (**NOAA/ESRL**), R. Easter, J. D. Fast, W. Gustafson, P.L. Ma, P. Rasch, B. Singh, (**PNNL**), A. Hodzic, M. Barth, G. Pfister, S. Wolters (all **NCAR**), S. Freitas (**CPTEC, Brazil**), P. Tuccella (**Laboratoire de Météorologie Dynamique and University of L'Aquila ITALY**), Yang Zhang and Kai Wang (**NCSU**), Martina Klose (**University of Cologne, Germany**)

+ *many more national and international collaborators*

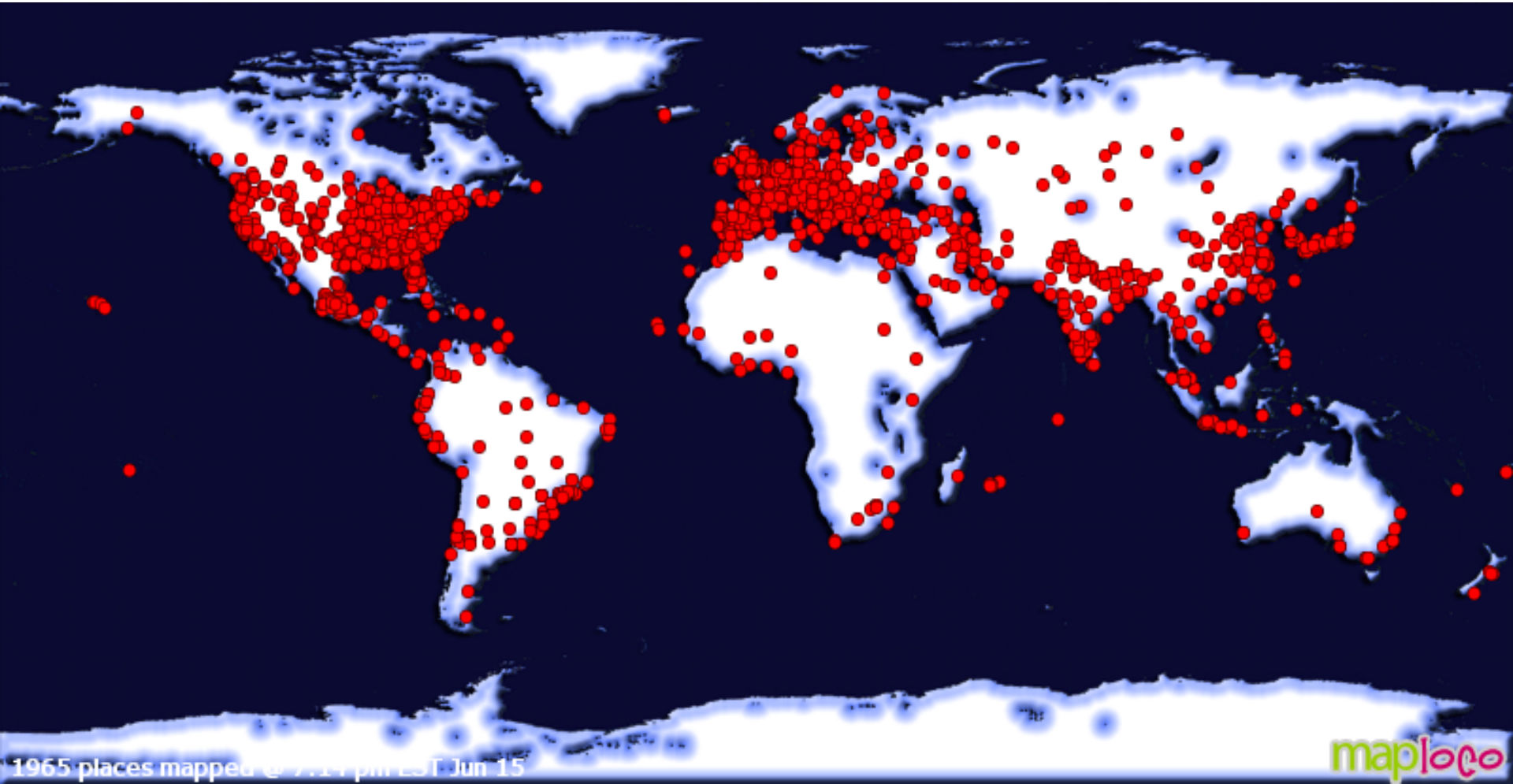
WRF/Chem web site - <http://wrf-model.org/WG11>



Warning

**This talk may contain acronyms
that may be inappropriate for
meteorologists**

Who is looking at WRF-Chem Website?

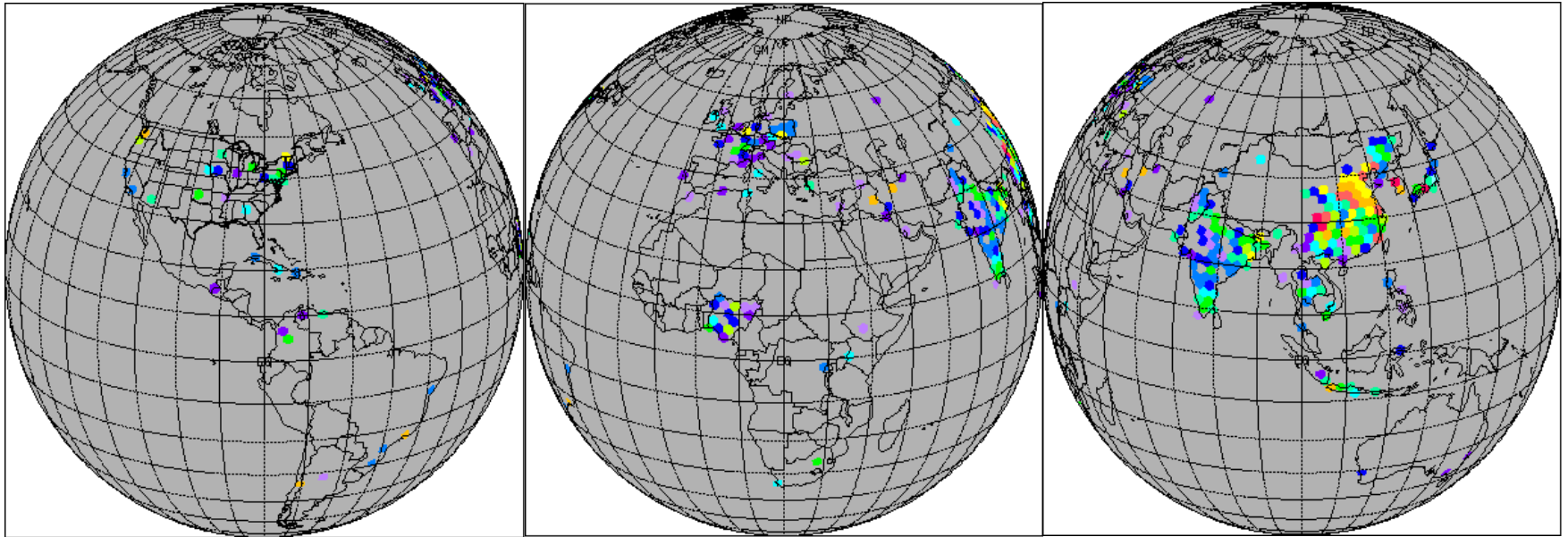


PREP-CHEM-SRC: a preprocessor of trace gas and aerosol emissions

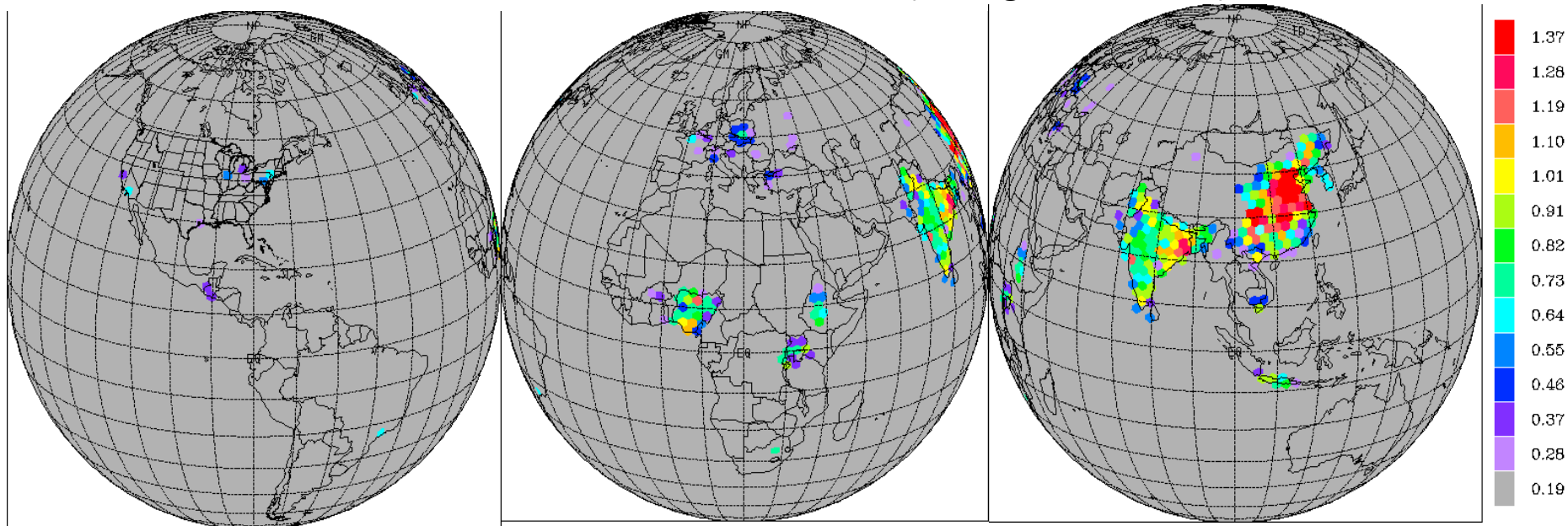
Provides emission fields (anthropogenic biogenic, and biomass burning) on polar-stereo, Lambert-conformal, Mercator, lat-lon, gaussian, icosahedral grids

Prep-chem-src can now use a new higher resolution (0.1x0.1 degree) global emissions data set produced by the Task Force on Hemispheric Transport of Air Pollution (HTAP)

ANTHROPOGENIC GOCART (updated Asian) Black Carbon Emissions (nanogram/m²/sec)



HTAP-2010 Black Carbon Emissions (nanogram/m²/sec)

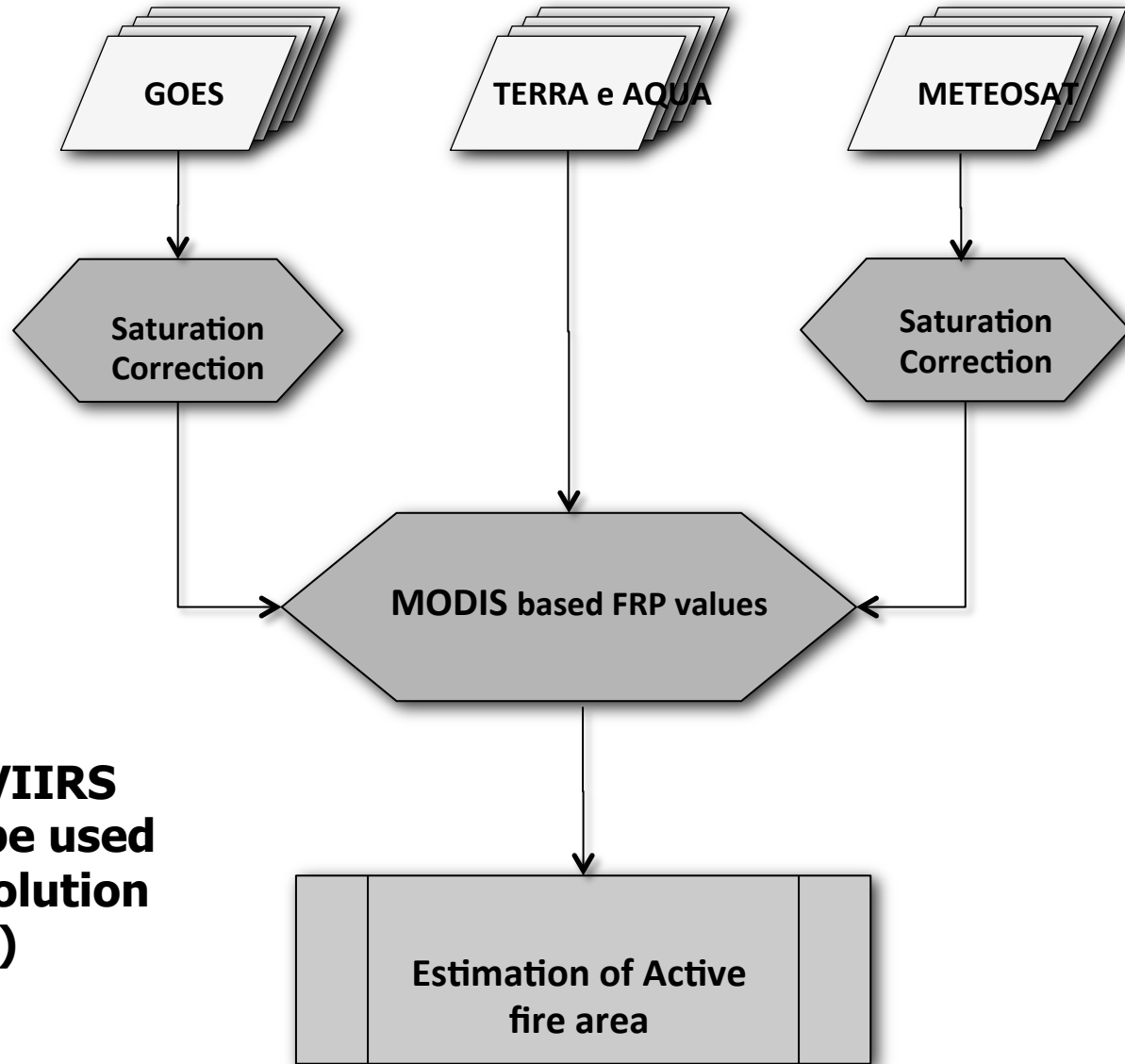


Another new addition coming soon to prep-chem-src: the use of Fire Radiative Power (FRP)

GOES, MODIS and Meteosat (only to East region of Brazil) are processed. Filter of duplicate values in MODIS and low confidence fires.

Correction of sensor characteristics assuming MODIS as reference.

FRP values corrected and filtered.

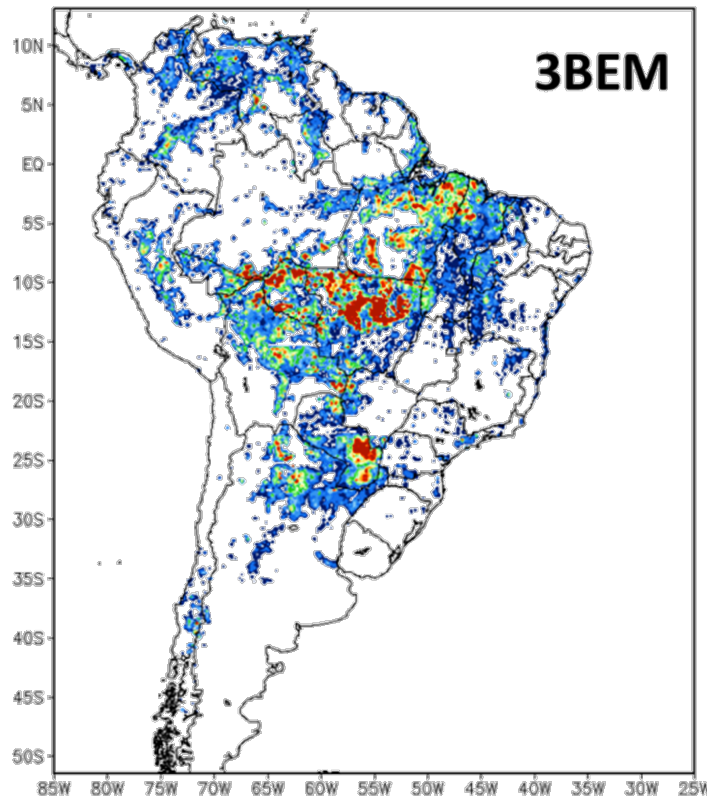


We will also apply this to VIIRS Satellite data, and this will be used in a version of the High Resolution Rapid Refresh (HRRR)

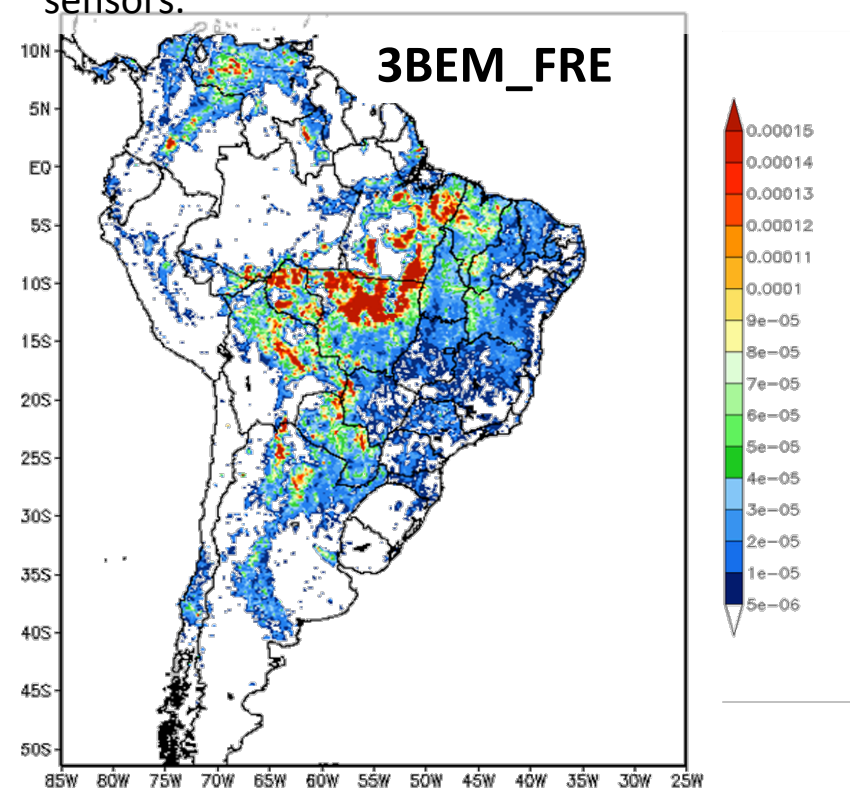
Brazilian Biomass Burning Emission Model

3BEM and 3BEM_FRE

The bottom-up approach: fire size/burnt area, carbon density, emission and combustion factors.



The top-down approach: from FRE Emissions estimate using the Fire Radiative Energy (FRE) from MODIS, GOES and SEVIRI sensors.



Mean Emission of CO (kg.m⁻²) for 2000 to 2011

Dust emission modules from University of Cologne (provided by Martina Klose)

- Selection of University of Cologne (UoC) dust emission modules with **dust_opt = 4** (with GOCART chemistry or dust only mode)
- Choice of emission scheme with namelist option dust_schme
 - dust_schme = 1 Shao (2001)
 - dust_schme = 2 Shao (2004)
 - dust_schme = 3 Shao et al. (2011)
- Currently four dust size bins: 0-2.5, 2.5-5, 5-10, and 10-20 μm diameter; Fifth bin is summation bin.
- From WRF V3.7.1 five size bins: 0-2, 2-3.6, 3.6-6, 6-12, and 12-20 μm (consistent with GOCART and AFWA dust emission modules).
- No additional input data needed.

Dust emission modules from University of Cologne

For a comparison to the AFWA scheme:

1. The Shao-scheme(s) is a physics-based dust emission parameterization with an explicit representation of the dust emission processes of saltation bombardment and aggregate disintegration (the two major emission mechanisms). It therefore directly predicts size-resolved dust fluxes.
2. The AFWA implementation is a combination of the semi-empirical Marticorena and Bergametti (1995) dust emission parameterization with the airborne dust size distributions from Kok (2011). MB95 predicts bulk dust fluxes. Then, the size-resolved fluxes are obtained by distributing the bulk fluxes according to the observed airborne dust size distributions.
3. Both are among the best available for the above mentioned processes (together with the newer Kok-parameterization).

UoC dust emission modules

- Simulation of a dust storm in Australia with Shao (2004) dust emission scheme (dust_opt = 4, dust_schme = 2).

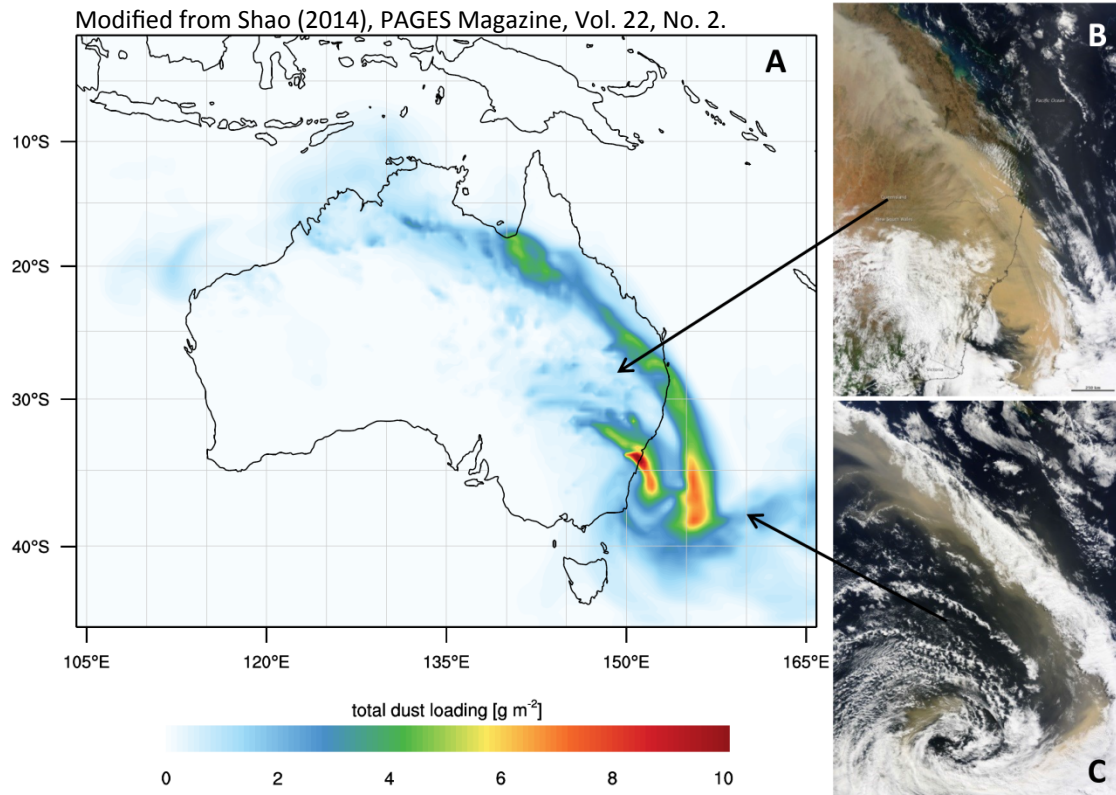


Fig. 1: (A) Dust load on 23 September 2009 modeled with WRF-Chem at 30km horizontal resolution; MODIS satellite images from (B) 23 September 2009 and (C) 24 September 2009.



**Important to note for GOCART or AFWA/GOCART dust schemes,
when using other than GOCART aerosol options:**

Settling is not fully treated –mods will be necessary, otherwise
overprediction will result

As of now they only will work fine and as intended for bulk aerosol
modules, or if used by themselves (without other aerosol modules)

**Another future addition may be CMAQ's FENGSHA module (Tong et al.
2015)**

Current work with convective parameterizations

- Cloud-aerosol interactions are a large source of uncertainty in climate simulations
- Most convective parameterizations lack cloud-aerosol interactions – which makes interpretation of aerosol indirect effect somewhat suspect

2 new developments in WRF-Chem:

1. Scale and aerosol aware Grell Freitas (GF) scheme, cu_physics=3 (talk by Georg Grell on Thursday afternoon, physics section)
2. New development by L. Berg (see also talk by Jerome Fast on Thursday morning) for Kain-Fritsch scheme

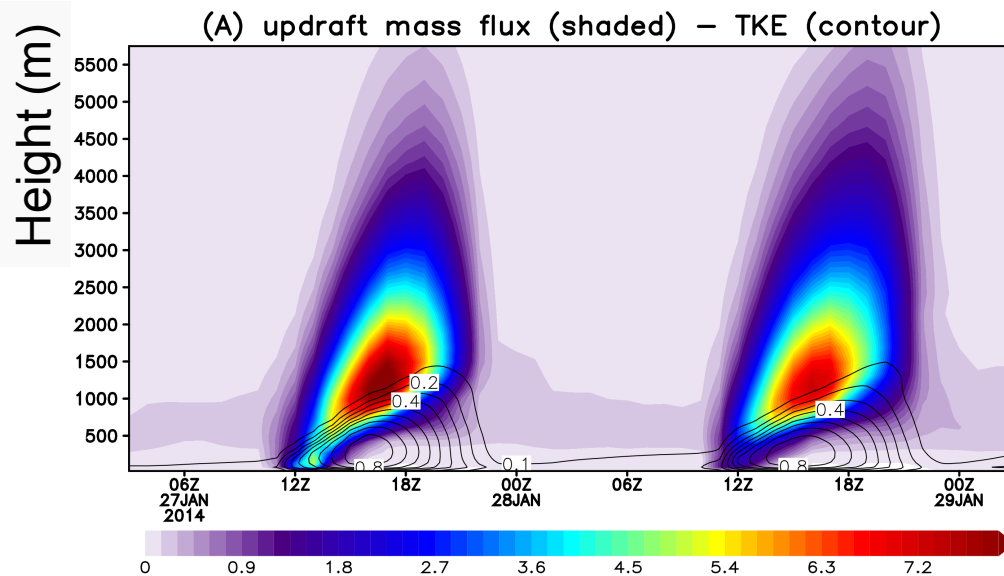
New additions for GF scheme (3.7.1 or 3.8)

- PDF's were implemented for vertical mass flux distribution (this allows easy application of stochastic perturbation of vertical heating and moistening profiles)
- Completely mass conserving
- Refinement of aerosol interactions
- Bechtold approach for diurnal cycle
- Momentum transport
- Scheme is currently being evaluated in MPAS(scale awareness), FIM (aerosol awareness and capability to produce the dreaded "good" height anomaly correlations), HWRF (scale-awareness), WRF (aerosol awareness), and B-RAMS
- Will be operational in Rapid Refresh (RAP) at NCEP and is operational at CPTEx in Brazil

Grell-Freitas-Olson (GFO) Shallow Convection Scheme

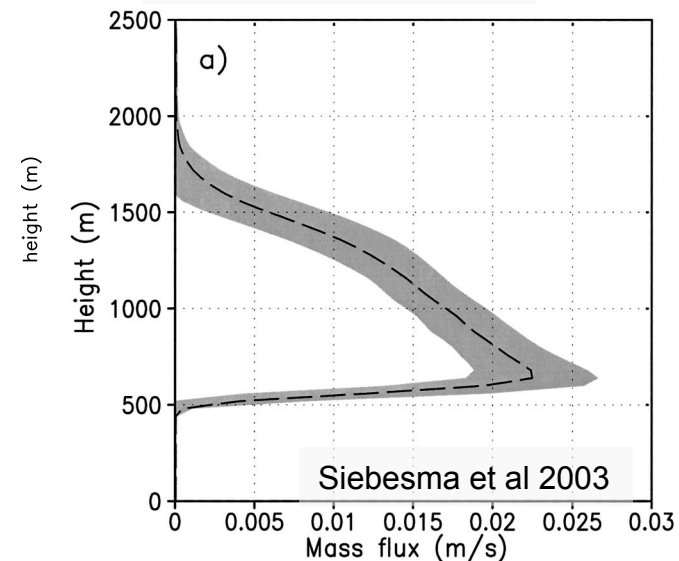
- Non-precipitating
- Transport of moisture, heat and tracers
- Mass flux profile given by a PDF (easy to adjust profile, and/or to apply stochasticism)
- Three closures – BLQE (Raymond, 1995), W^* (Grant, 2001) and convection as natural heat engine (Rennó and Ingersoll, 1996).
- Completely mass conserving
- Scale awareness implemented so far with Honnert approach

Diurnal cycle of shallow convection and diffusion in PBL



updraft mass flux: shaded TKE: contour

Mass flux Profile



- Similar with LES
- Sharp increase, peaking just above boundary layer
- Smooth decrease above

Coupling Aerosols and Parameterized Convection



- ▶ Modified Kain-Fritsch (deep convection) coupled with Cumulus Potential (CuP) (shallow convection) (Berg et al., 2013)
- ▶ Aerosol activation
- ▶ Transport
- ▶ Aqueous chemistry
- ▶ Wet removal
- ▶ See Berg et al., GMD, 2015

Talk by Jerome Fast,
Thursday morning

Missing - will be added in the future

- ▶ Feedback to radiation (indirect effects)
- ▶ Feedback on precipitation and cloud lifecycle

New implementations from NCSU (Yang Zhang and Kai Wang)

- (1) CBo5
- (2) CBo5 coupled with MADE/VBS
- (3) CBo5 coupled with MADE/VBS and Jan Kazil's AQCHEM use

Tested and evaluated on 10 year regional climate simulations

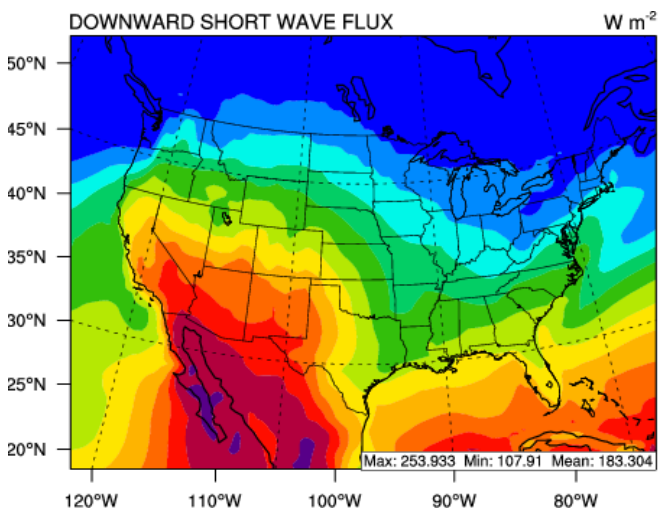
WRF/Chem pre-released v. 3.7 model configurations and set-up

Model Attribute	Configuration Option	Reference (s)
Domain and Resolutions	36km × 36km, 148 × 112 horizontal resolution over CONUS, with 34 layers vertically from surface to 100 hPa	-
Simulation Period	January 2001 to December 2010	-
Chemical and Meteorological IC/BCs	Downscaled from the NCSU's CESM/CAM5 v1.2.2. Meteorological IC/BCs bias-corrected NCEP FNL	He et al. (2014) Glotfelty et al. (2015)
Anthropogenic Emissions	RCP 4.5 emission scenarios	van Vuuren et al., 2011
Biogenic Emissions	MEGAN2	Guenther et al. (2006)
Dust Emissions	AER/AFWA	Jones and Creighton (2011)
Sea-Salt Emissions	Gong et al. parameterization	Gong et al. (1997)
Radiation	RRTMG SW and LW	Clough et al. (2005), Iacono et al. (2008)
Boundary Layer	Yonsei University (YSU)	Hong et al. (2006); Hong (2010)
Land Surface	NOAH	Chen and Dudhia (2001), Ek et al. (2003), Tewari et al. (2004)
Microphysics	Morrison two moment module	Morrison et al. (2009)
Cumulus Parameterization	Grell 3D Ensemble	Grell and Freitas. (2014)
Gas-phase chemistry	Modified CB05 with updated chlorine chemistry	Yarwood et al. (2005), Sarwar et al. (2006, 2007)
Photolysis	Fast Troposphere Ultraviolet Visible (FTUV)	Tie et al. (2003)
Aqueous-phase chemistry	CMAQ v5.0 's AQChem for both resolved and convective clouds	Sarwar et al. (2011)
Aerosol module	MADE/VBS	Ahmadov et al. (2012)
Aerosol Activation	Abdul-Razzak and Ghan	Abdul-Razzak and Ghan (2000)

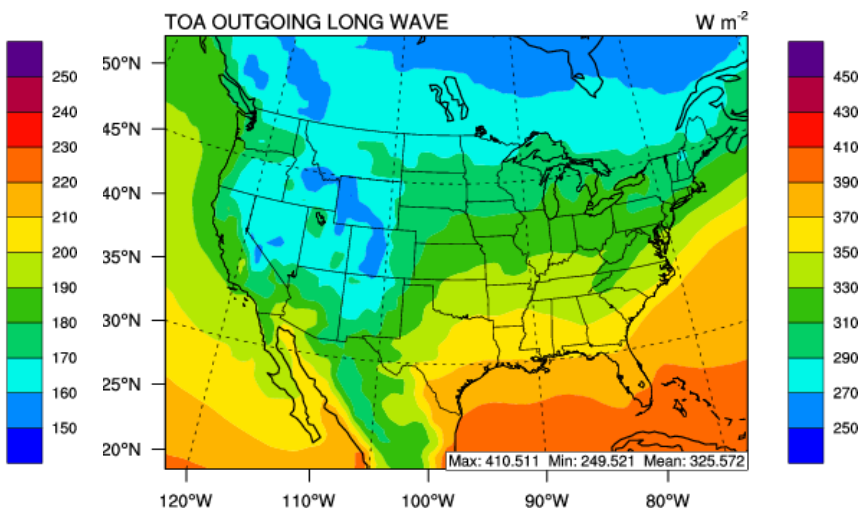
10-yr Avg. RCP 4.5 Meteorological Evaluation: Short- and Long-wave Radiation

CERES

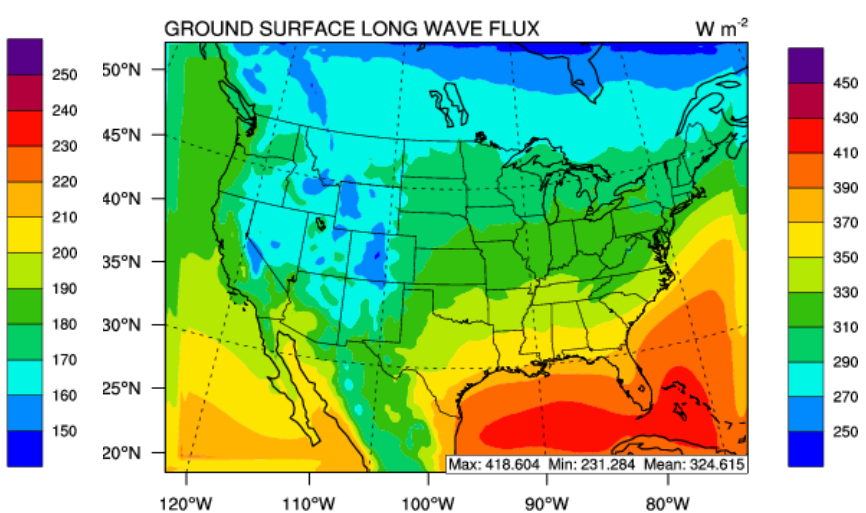
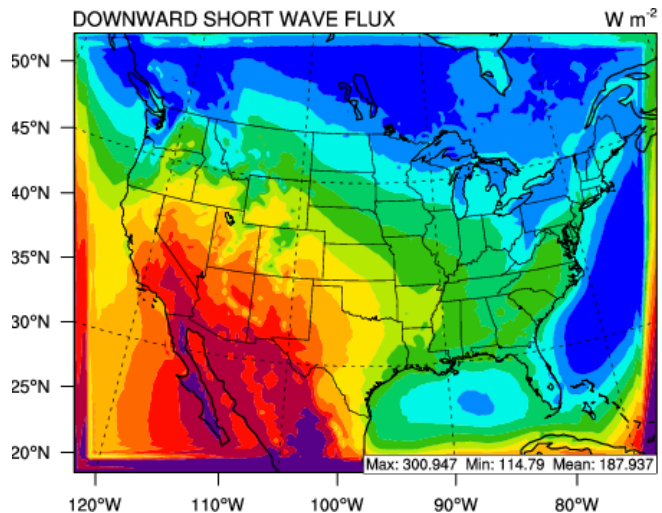
SWDOWN



GLW



WRF/Chem



MB = -0.1 $W m^{-2}$, NMB = 0.0%

MB = 1.2 $W m^{-2}$, NMB = 0.4%

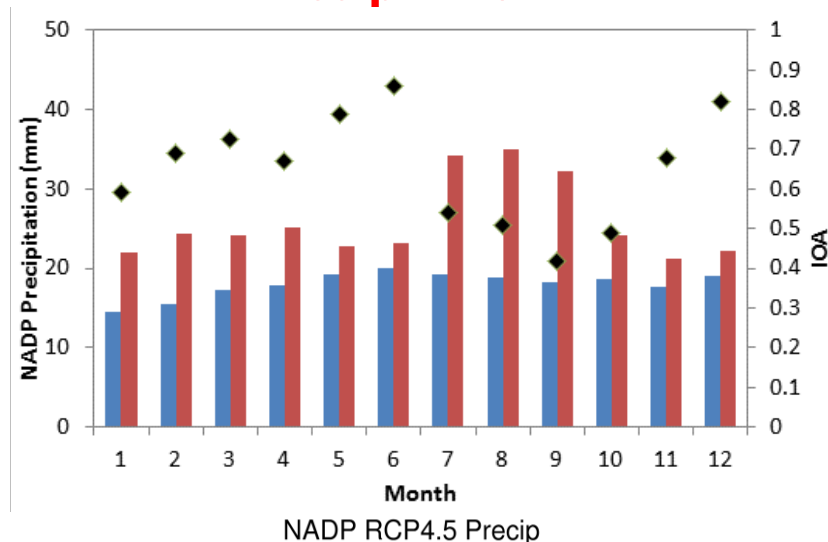
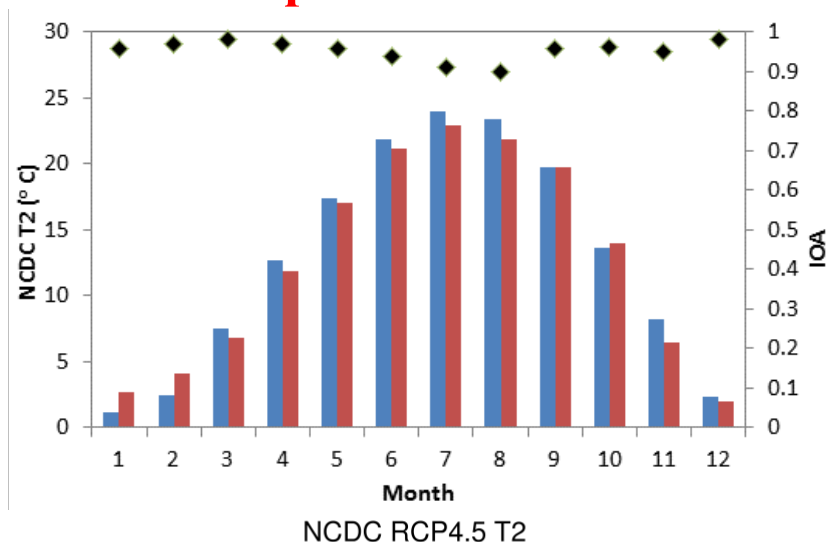
Good performance in terms of both performance statistics and spatial correlation

10-yr Avg. RCP 4.5 Meteorology Evaluation: Monthly Variation and Probability

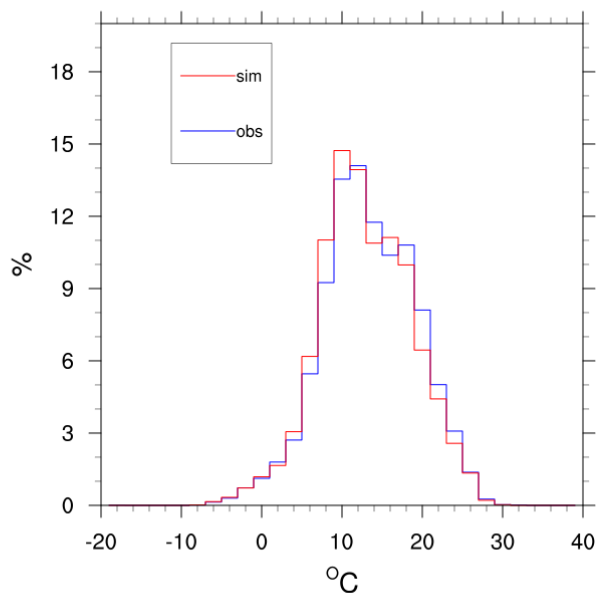
Temperature at 2-m

Precipitation

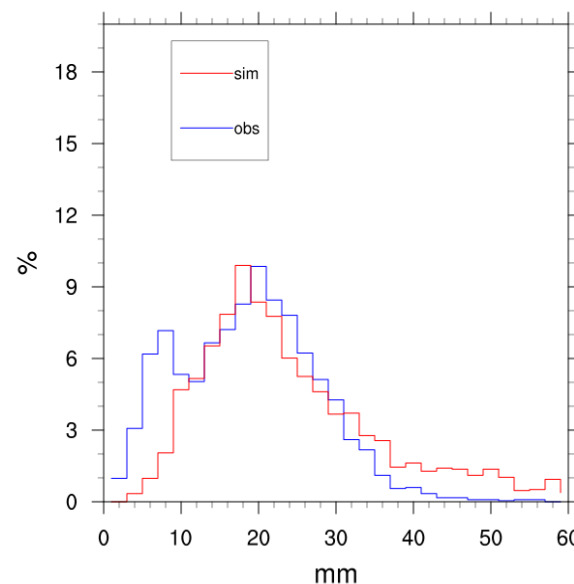
Monthly



Probability



MB = -0.5 °C, NMB = -3.7%



MB = 7.9 mm day⁻¹, NMB = 44.2%

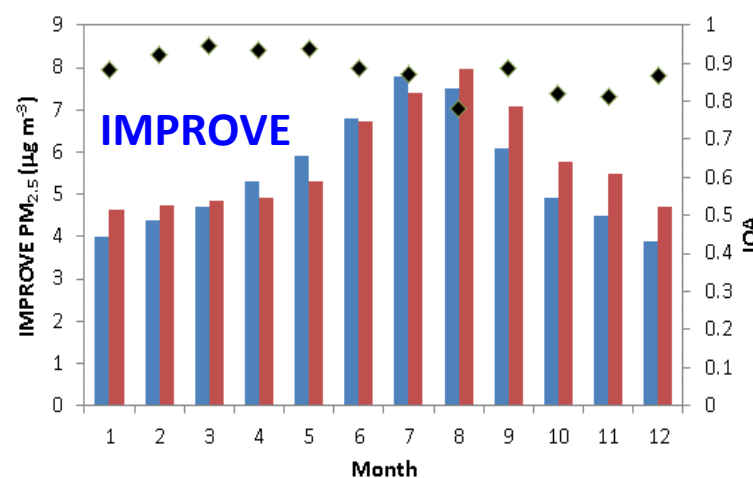
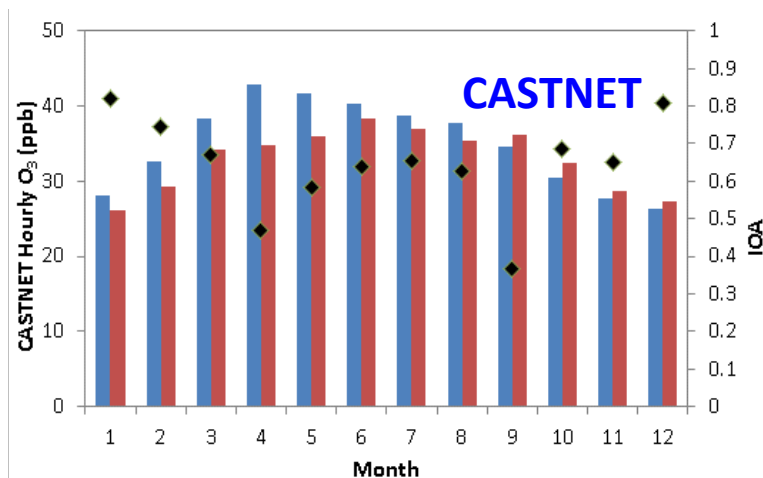
Good performance for T2 with slight cold bias and large wet biases in Precipitation

10-yr Avg. RCP 4.5 Chemical Evaluation: Monthly Variation of O₃ and PM_{2.5}

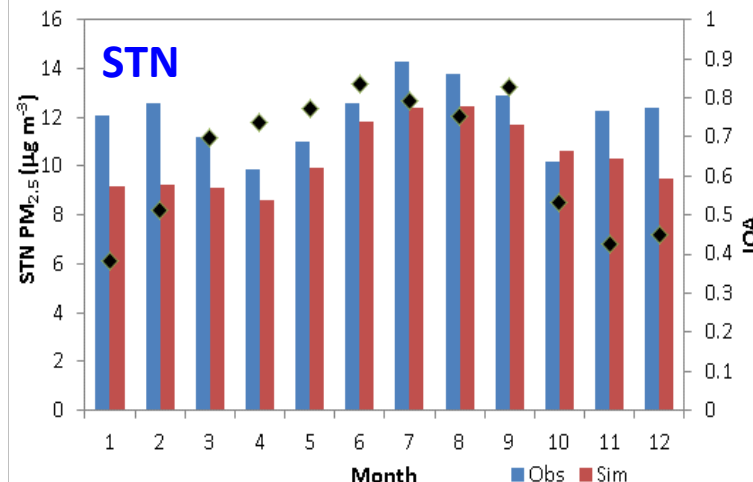
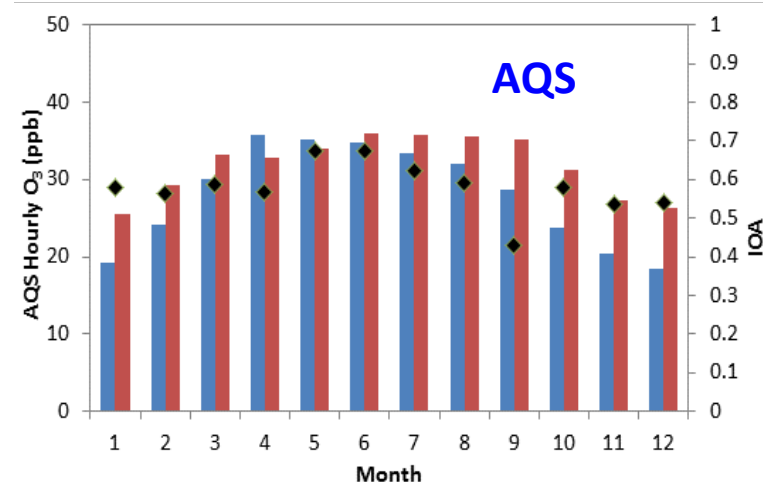
Hourly O₃

24-hr average PM_{2.5}

Rural
Remote
Sites



Urban
Suburban
Sites



CASTNET: MB=-2.4 ppb, NMB=-6.7%

IMPROVE: MB=0.3 µg m⁻³, NMB=6.0%

AQS: MB=2.8 ppb, NMB=9.2%

STN: MB=-1.6 µg m⁻³, NMB=-13.2%

Good performance for both hourly O₃ and daily PM_{2.5} at all types of sites

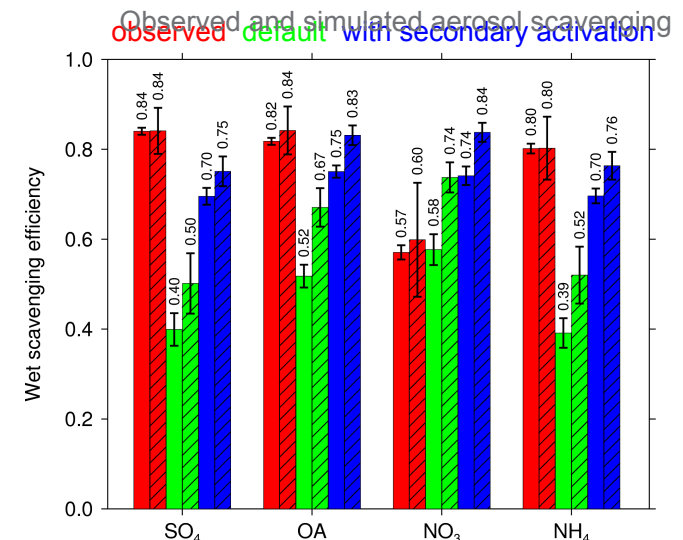
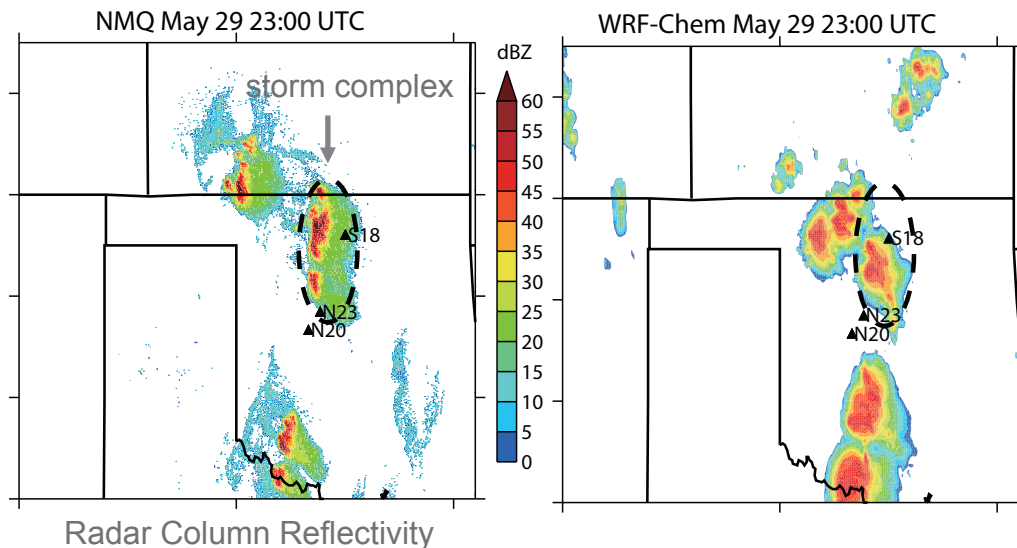
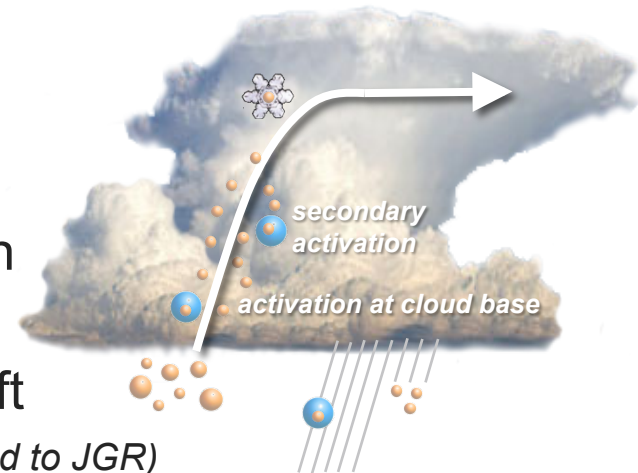
Other Important Developments at PNNL

- ▶ **Secondary Activation**
- ▶ **Ice-Borne Aerosols**
- ▶ **Explicit Nucleation and Ultrafine Particles**
- ▶ **Biogenic VOC Emissions**

With the exception of ice-borne aerosols, these may be implemented in v3.7.1

Added Secondary Activation to Resolved Cloud-Aerosol Interactions

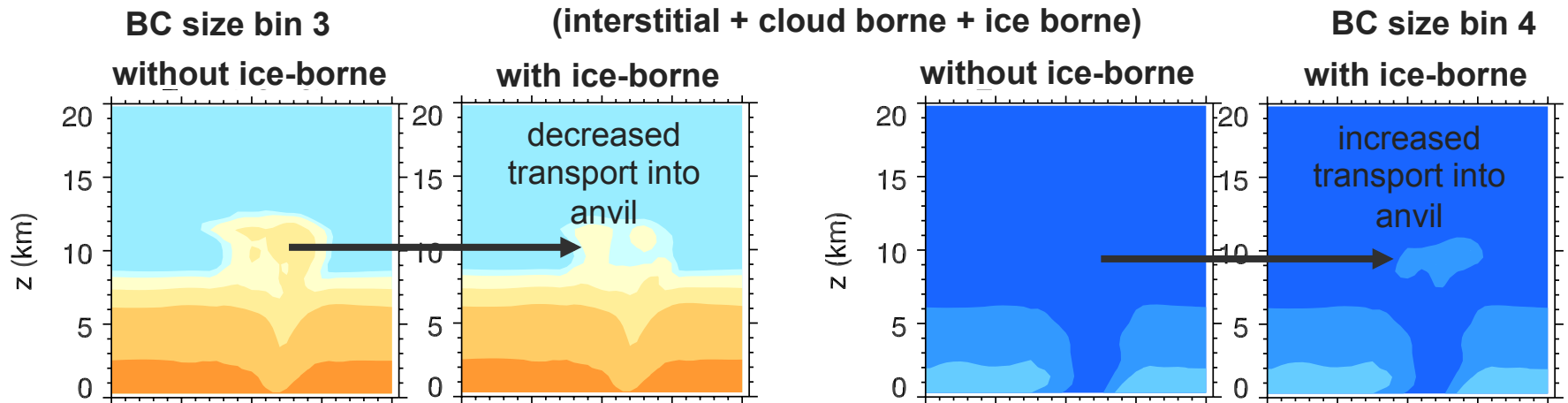
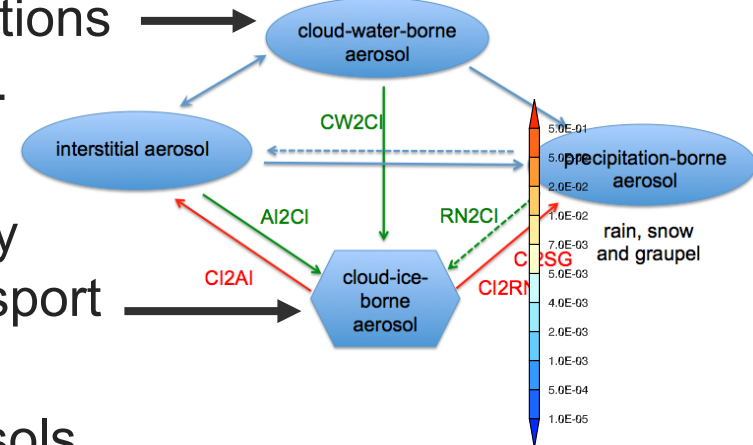
- ▶ Current treatment activates aerosols at cloud base, which is appropriate for shallow and stratiform clouds, but ...
- ▶ Activation could occur aloft for deep convection
- ▶ Therefore a treatment for secondary activation has been implemented and tested using aircraft data during the DC3 campaign (*Yang et al., submitted to JGR*)



Simulated wet scavenging efficiency improved with inclusion of secondary activation

Ice-Borne Aerosols

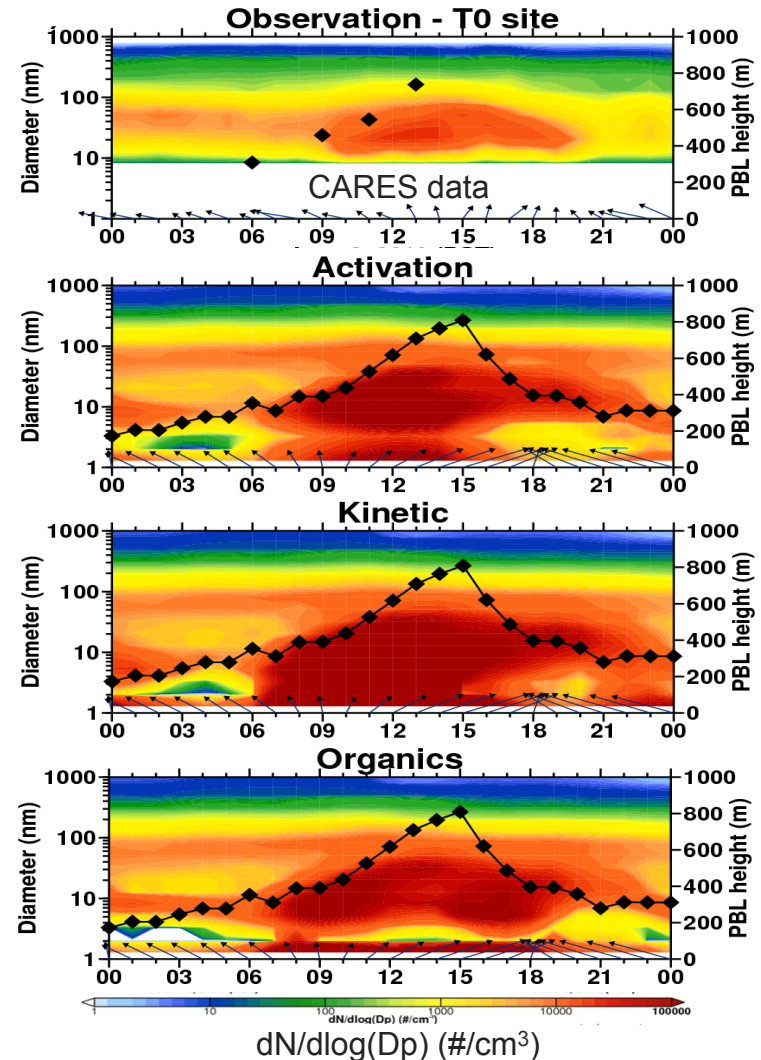
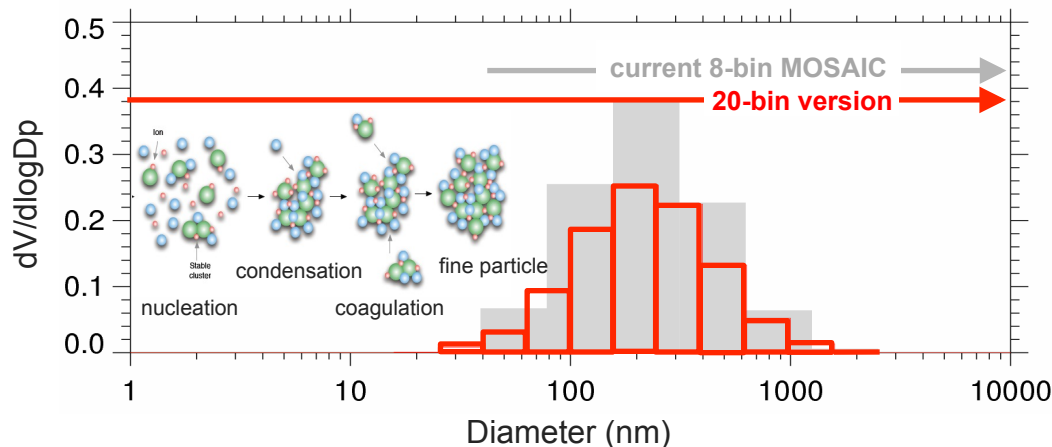
- ▶ Current treatment of cloud-aerosol interactions only considers liquid cloud droplets, but ...
- ▶ In reality, aerosol residuals in droplets may freeze into ice crystals, which affects transport and lifetime of aerosol particles
- ▶ PNNL testing treatment of ice-borne aerosols using idealized 2-D thunderstorm case



Inclusion of ice-borne does affect details of spatial distribution and size distribution of aerosols

Explicit Treatment of Ultrafine Particles

- ▶ Particle number is challenging to predict accurately and depends on formation growth, and coagulation from nanometer sizes and upwards
- ▶ The lowest size bin in the MOSAIC model is currently 0.39 μm and does not explicitly treat nucleation and ultrafine particle growth
- ▶ MOSAIC extended to have 20 size bins from 1 nm to 10 μm to resolve this issue
- ▶ 3 nucleation schemes tested: two depending on H_2SO_4 and one depending on H_2SO_4 and organic vapors from volatility basis set SOA approach (*Lupascu et al., submitted to ACPD*)

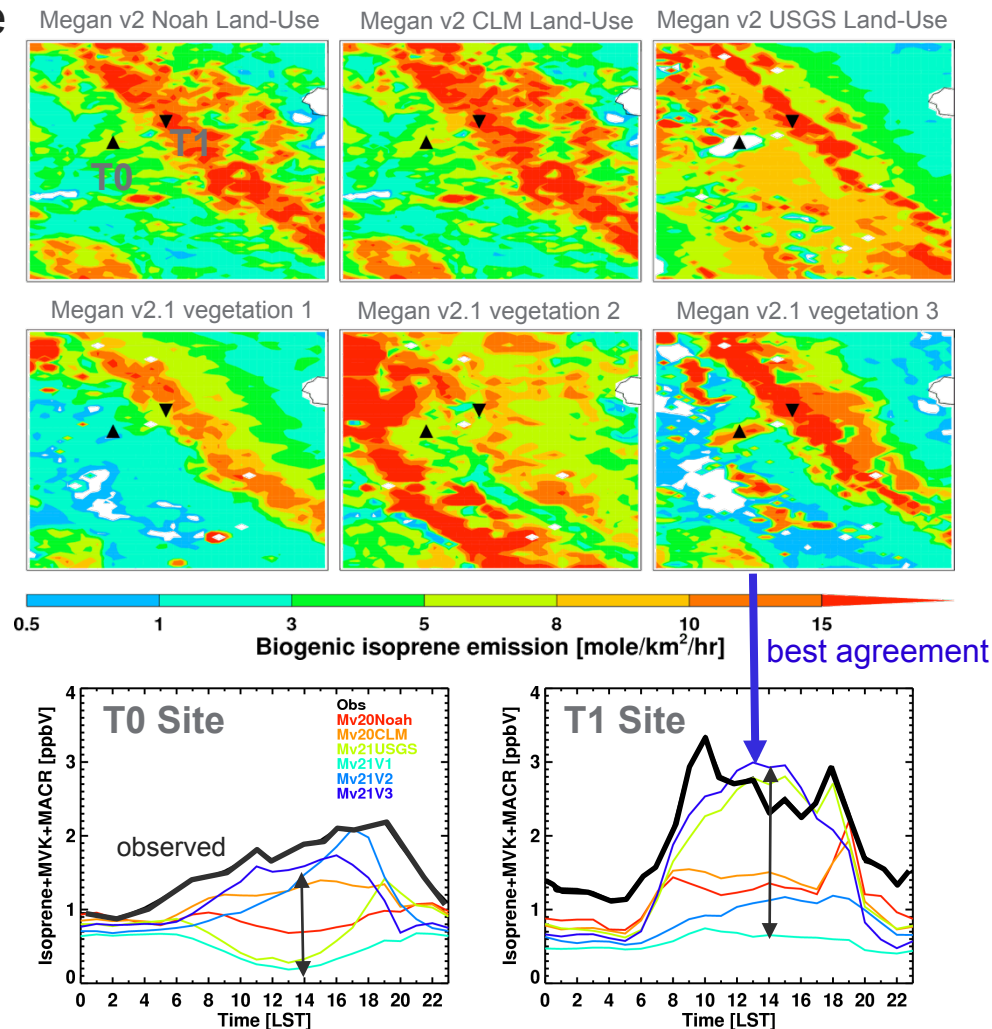


Linking CLM to Biogenic Emissions

(in collaboration with NCAR)

- ▶ Biogenic volatile organic compounds (BVOCs) in the atmosphere play an important role in atmospheric chemistry, and therefore can significantly affect SOA formation and ultimately climate
- ▶ The Community Land Model (CLM) was ported to WRF previously, but the linkages to biogenic emissions were not; therefore, ...
- ▶ CLM now implemented in a manner more consistent with CAM5 that includes biogenic emissions from MEGAN v2.1
- ▶ Tested with BVOC data from CARES campaign, and found that CLM+MEGAN v2.1 with an improved vegetation map performed better than current implementation of MEGAN and Noah land surface scheme

(Zhao et al., to be submitted)

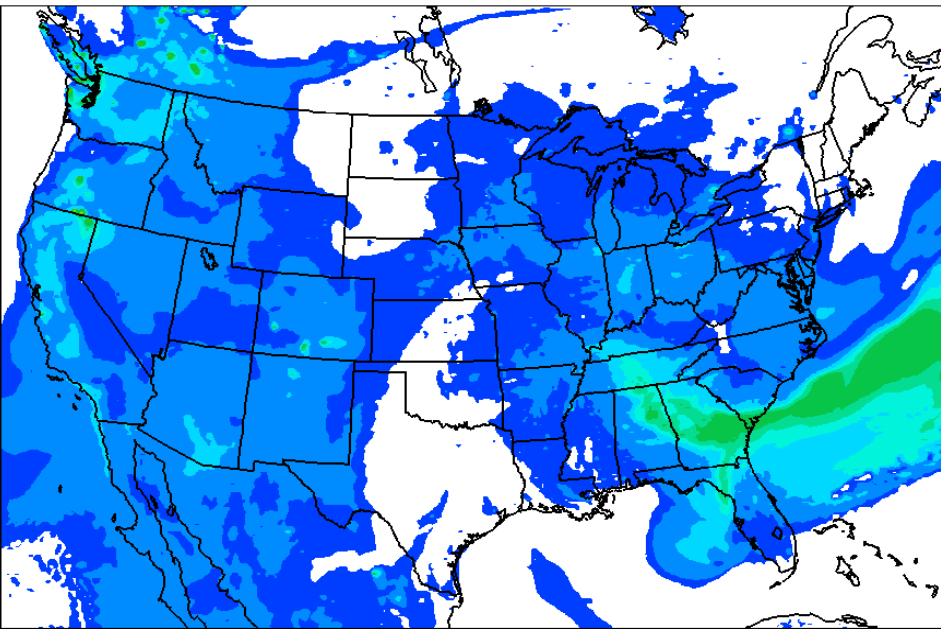


Another new chemistry option was implemented by Paolo Tuccella

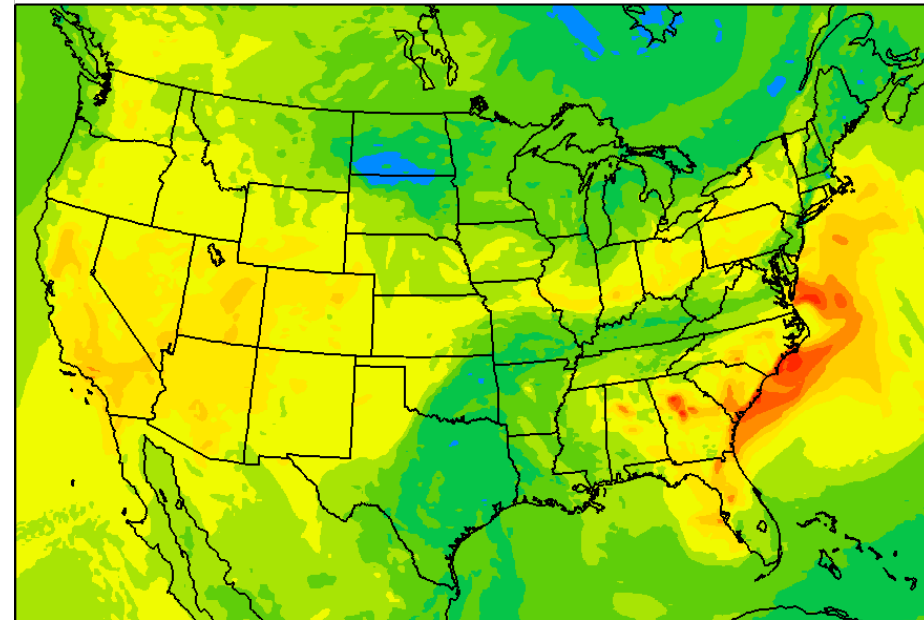
- RACM/MADE/VBS with aerosol indirect effect (using CMAQ AQCHEM module)
- Evaluated in Europe with data from field campaign

Paper currently in GMDD: Tuccella et al.: A new chemistry option in WRF/Chem V3.4 for the simulation of direct and indirect aerosol effects using VBS: evaluation against IMPACT-EUCAARI data

Your real-time AQ forecast for today



Organic aerosols



WRF-Chem using MADE/VBS/RACM on Rapid Refresh Domain,
DX=13km, soon with **aerosol aware microphysics**

Will probably change to HRRR (dx=3km) in near future, HRRR already has a "smoke" version, soon to be expanded to smoke/dust, also for application with aerosol aware microphysics scheme (Greg Thompson)

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

<http://ruc.noaa.gov/wrf/WG11/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 - <http://wrf-model.org/WG11>

Thank you!

