Introduction to WRF-Chem

Georg Grell

Steven E. Peckham, Stuart A. McKeen, Jan Kazil, R. Ahmadov + others from
NOAA/ESRL

Jerome Fast, William Gustafson jr., P.L. Ma, B. Singh+ many others from **PNNL**

+ Alma Hodzic, Christine Wiedinmyer, Gabi Pfister, Mary Barth and many others
from **NCAR**
other **University contributions**
+ Saulo Freitas (**CPTEC, BRAZIL**)

+ many more national and international collaborators

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

WRF-Chem

Community effort

Largest contributing groups: ESRL, PNNL, NCAR

Other significant contributions from: National and international Universities, CPTEC Brazil, NASA, AFWA

Structure of Talk

1. Brief description of only the *general features* of WRF-Chem
2. Some applications of what the model may be used for are mixed in

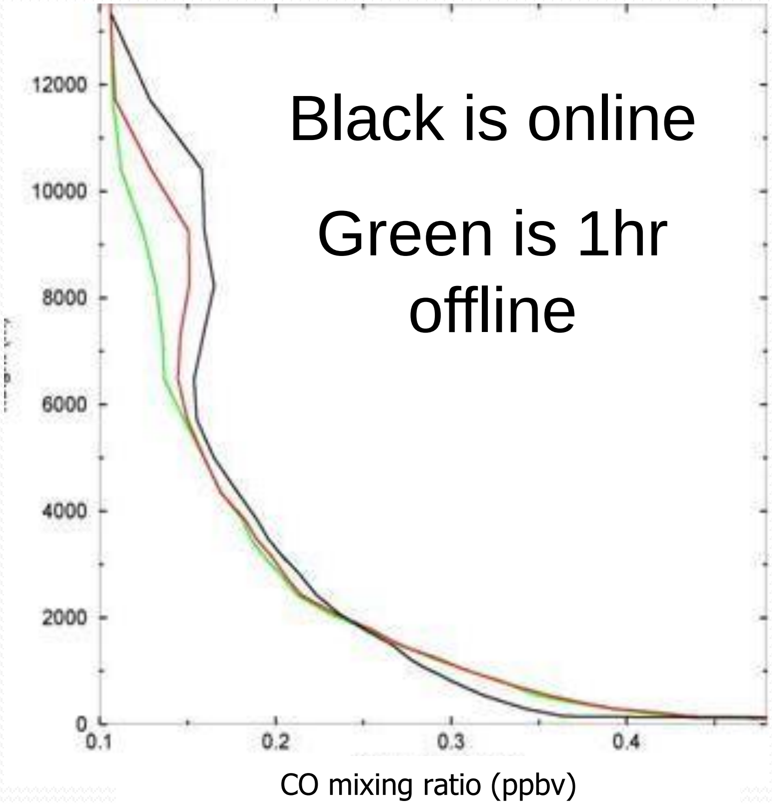
There are more than 50 chemistry options for the main gas phase chemistry and aerosol modules!

WRF-Chem

- Chemistry is online, completely embedded within WRF CI
- Consistent: all transport done by meteorological model
  - Same vertical and horizontal coordinates (no horizontal and vertical interpolation)
  - Same physics parameterization for subgrid scale transport
  - No interpolation in time
- Easy handling (Data management)
- Ideally suited to study feedbacks between chemistry and meteorology
- Ideally suited for air quality forecasting on regional to cloud resolving scales

Why Online?

- Offline modeling introduces errors for air quality applications
  - Error for offline modeling is increasing with increasing horizontal resolution
  - Power spectrum analysis can show the amount of information that is lost in offline runs
- 2-way feedback in-between chemistry and meteorology
  - Process studies relevant for global climate change
  - Ultimately it should lead to improved data assimilation (meteorology) and improved weather forecasts



What is needed for this type of modeling system?

1. Advection and diffusion (all done by WRF)
2. Sub-grid scale transport (WRF parameterizations, PBL, convection)
3. Some processes that are specific for chemical constituents, but need meteorology: emissions (biogenic, fire, sea salt, dust, volcanic, anthropogenic), dry deposition, wet scavenging
4. Treatment of chemical reactions, aqueous phase chemistry, gas phase species and aerosols
5. "Chemical" radiation routines (photolysis routines) that provide photolysis rates necessary for (4)
6. Capability of feedback from chemistry to meteorology (meteorological radiation and microphysics parameterizations, possibly also convective parameterizations)

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Gas Phase Chemistry Packages

Complex part of the modeling system: Many additional species that are fully prognostic variables and require transport - costly

- Hard coded: chemical mechanism from RADM2
- Hard coded: Carbon Bond (CBM-Z) based chemical mechanism
- ***K***inetic ***P***re***P***rocessor (KPP) – Many different equations files exist (also for RADM2 and CBM-Z). KPP will generate the modules from equation files. These generated modules will then be used by WRF-Chem
- IN V3.5.1/ V3.6: CRIMech gas phas scheme (U. of Manchester, 240 species, 652 reactions)

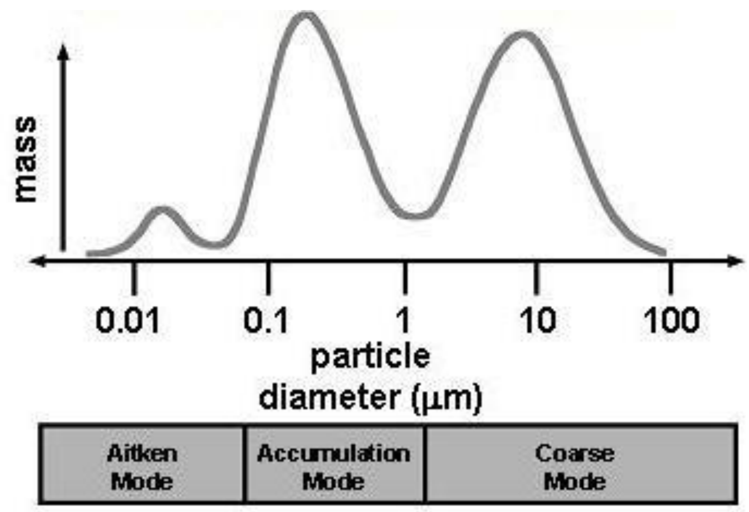
Ravan Ahmadov will fill in some details later in the tutorial

Photolysis Packages – all coupled to aerosols and hydrometeors

- Madronich Photolysis
- Madronich F-TUV
- Fast-j photolysis scheme

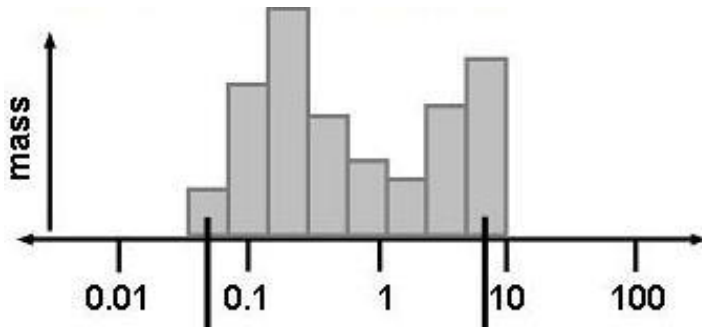
Available aerosol modules

(1) Modal



composition
sulfate
nitrate
ammonium
chloride
carbonate
sodium
calcium
other inorganics
organic carbon
elemental carbon

(2) Sectional



(3) Bulk: Sections for dust and sea salt, otherwise total mass only

Aerosols may have a significant impact on weather forecasts through interaction with radiation (sometimes also called "direct effect") and microphysics (sometimes also called "indirect effect")

Aerosols may also impact meteorological data assimilation

For NWP a bulk scheme is very attractive: GOCART (Currently used in real-time high resolution global (dx=30km) and regional modeling (up to dx=3km) at ESRL

- Much simpler than the sectional and modal schemes
  - Calculates only with the total mass of the aerosol components
  - Provides no information on
    - Particle size
    - Particle concentration
  - E.g., when particles grow, the aerosol mass increases but we don't know how their size/number changes
- Numerically very efficient
- Coupled with radiation (Mie scattering and extinction calculations)
- Will be coupled to microphysics in future versions

For research on aerosol direct and indirect effects modal and sectional approaches are more attractive

Less assumptions are made when coupled to atmospheric radiation and/or microphysics

Interaction processes are very complex, they will not work for every radiation and microphysics scheme in WRF ! (takes time to implement)

ESRL

Selection of radiation parameterizations for aerosol “direct effect”

For V3.6 all aerosol modules were hooked up to Goddard short wave radiation, and RRTMG short and long wave scheme, CAM radiation.

Selection of microphysics parameterizations for aerosol "indirect effect"

For V3.6

Modal and sectional schemes only can be used in combination with a version of the Lin et al. Microphysics scheme as well as the Morrison scheme

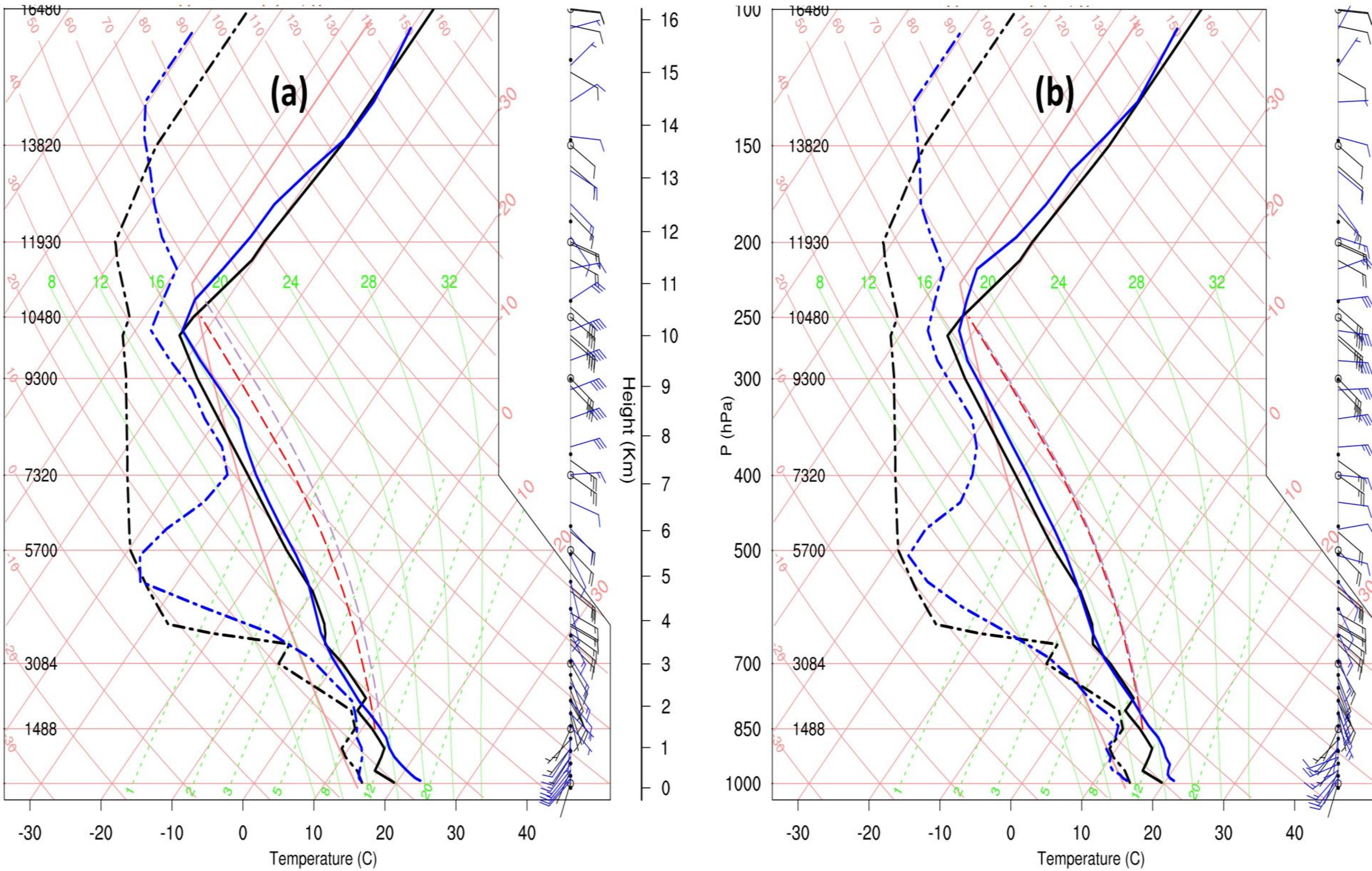
More to come in future

The microphysics schemes must be double moment for QC. The above schemes are only double moment when using WRF-Chem: care must be taken when studying impacts of aerosol indirect effect!

How is the meteorological forecast affected by aerosol?

- Large importance for climate simulations is recognized (when integrating models over 100's of years, small differences in the earth's energy budget are extremely important)
- Weather forecasting for only a few days?
  - Much research needed, but chemistry may positively influence forecasts when strong signals exist
  - Influence on meteorological data assimilation

No fires **24-hr forecast** **Very Strong Signal: With fires**



Observed (black) and predicted (blue) sounding for Fairbanks, Alaska, on July 4, 0000UTC.

Biogenic emissions

- May be calculated "online" based on USGS landuse
  - Easy to use
- May be input
- BEISv3.13 (offline reference fields, online modified)
  - Good choice, but difficult to use
- Use of MEGAN
  - Best choice!!

***M*odel of *E*missions of *G*ases and *A*erosols from *N*ature (MEGAN)**

Global, high resolution biogenic emissions

Out of available biogenic emissions modules only BEIS and MEGAN are actively being worked on (developed)

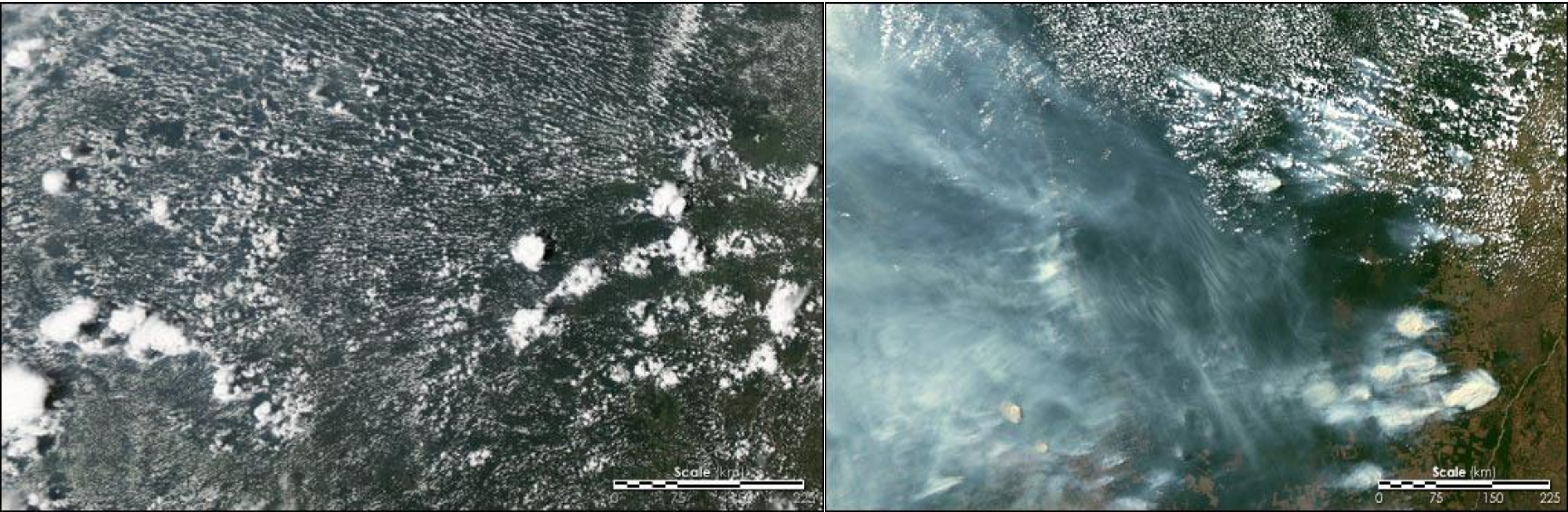
Preprocessor for MEGAN exists and can be downloaded from NCAR

Fire Plumerise

1-D Cloud model used in WRF-Chem to determine injection height, wind shear effects are included

Satellite information (other aerial and ground observations may also be used) to determine fire location and fire properties

Emissions preprocessing may be done by (1) CPTEC preprocessor, or (2) NCAR's FINN preprocessor



New in V3.5.1:

The 1D cloud model to calculate injection height: **including the environmental wind effect**

$$\frac{\partial w}{\partial t}+w\frac{\partial w}{\partial z}=\gamma gB-\frac{2\alpha}{R}w^2-\delta_{entr}w$$

$$\frac{\partial u}{\partial t}+w\frac{\partial u}{\partial z}=-\frac{2\alpha}{R}|w|(u-u_e)-\delta_{entr}(u-u_e)$$

$$\frac{\partial T}{\partial t}+w\frac{\partial T}{\partial z}=-w\frac{g}{c_p}-\frac{2\alpha}{R}|w|(T-T_e)+\left(\frac{\partial T}{\partial t}\right)_{micro-physics}-\delta_{entr}(T-T_e)$$

$$\frac{\partial r_v}{\partial t}+w\frac{\partial r_v}{\partial z}=-\frac{2\alpha}{R}|w|(r_v-r_{ve})+\left(\frac{\partial r_v}{\partial t}\right)_{micro-physics}-\delta_{entr}(r_v-r_{ve})$$

$$\frac{\partial r_c}{\partial t}+w\frac{\partial r_c}{\partial z}=-\frac{2\alpha}{R}|w|r_c+\left(\frac{\partial r_c}{\partial t}\right)_{micro-physics}-\delta_{entr}r_c$$

$$\frac{\partial r_{ice,rain}}{\partial t}+w\frac{\partial r_{ice,rain}}{\partial z}=-\frac{2\alpha}{R}|w|r_{ice,rain}+\left(\frac{\partial r_{ice,rain}}{\partial t}\right)_{micro-physics}+\mathrm{sedim}-\delta_{entr}r_{ice,rain}$$

dynamic entrainment

$$\delta_{entr}=\frac{2}{\pi R}|u_e-u|$$

$$\frac{\partial R}{\partial t}+w\frac{\partial R}{\partial z}=+\frac{6\alpha}{5R}|w|R+\frac{1}{2}\delta_{entr}R$$

$$\left(\frac{\partial \xi}{\partial t}\right)_{micro-physics}(\xi=T,r_v,r_c,r_{rain},r_{ice}),\quad \mathrm{sedim}$$

bulk microphysics:
Kessler, 1969; Berry,1967
Ogura & Takahashi,1971

Impact of Volcanoes

- Ash-fall near eruption
- Transport of fine ash in high concentrations for long distances
- Impact on weather, climate, and air quality

The plume of the 30 Sept/1 Oct 1994 eruption of Kliuchevskoi Volcano, Kamchatka taken from the space shuttle STS-68 mission (Russia)

10 size bins for prediction of ash-fall and transport of volcanic ash

Particle Size Bin	Phi	Percentage of mass
1 – 2mm	-1 – 0	2
0.5 – 1 mm	0 – 1	4
0.25 – 0.5 mm	1 – 2	11
125 – 250 μm	2 – 3	9
62.5 – 125 μm	3 – 4	9
31.25 – 62.5 μm	4 – 5	13
15.625 – 31.25 μm	5 – 6	16
7.8125 – 15.625 μm	6 – 7	16
3.9065 – 7.8125 μm	7 – 8	10
< 3.9 μm	> 8	10

- Options for transport only (4 bins or 10 bins +so2) – aerosol direct effect may be included
- Coupled with chemistry/aerosol modules (only using up to three bins – depending on size)

4 size bins for prediction if transport only is of interest

Particle Size Bin	Phi	Percentage of mass
15.625 – 31.25 μm	5 – 6	16
7.8125 – 15.625 μm	6 – 7	16
3.9065 – 7.8125 μm	7 – 8	10
< 3.9 μm	> 8	10

3 size bins for coupling with other aerosol modules

WRF-Chem Greenhouse Gas Packages *(chem_opt =17)-new in WRF-ChemV3.4*

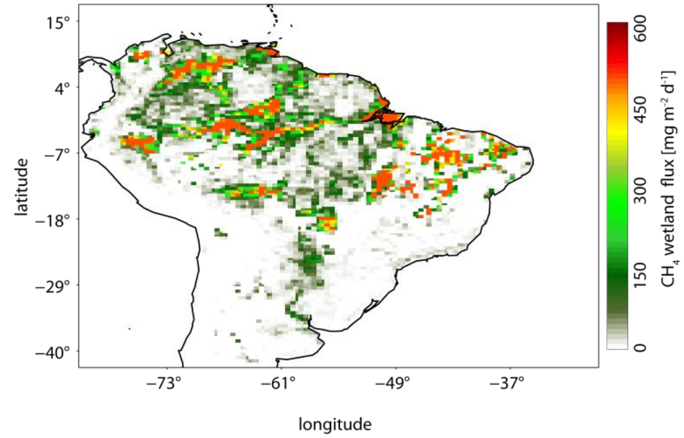
- **Online calculation of biospheric CH_4 fluxes**
  wetland – Kaplan (2002)
  termite – Sanderson (1996)
  soil uptake – Ridgwell et al. (1999)

- **Passive tracer simulations for CO_2, CH_4, and CO**
  (including all options of CO_2 tracer package, chem_opt=16)

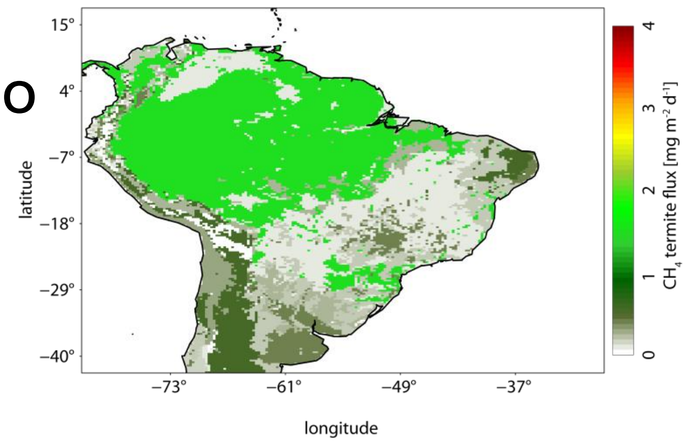
- **Tuning of wetland fluxes** through namelist options wpeat and wflood possible

- **Separate biomass burning option** for CO_2, CH_4, and CO including plumerise calculation (biomass_burn_opt = 5)

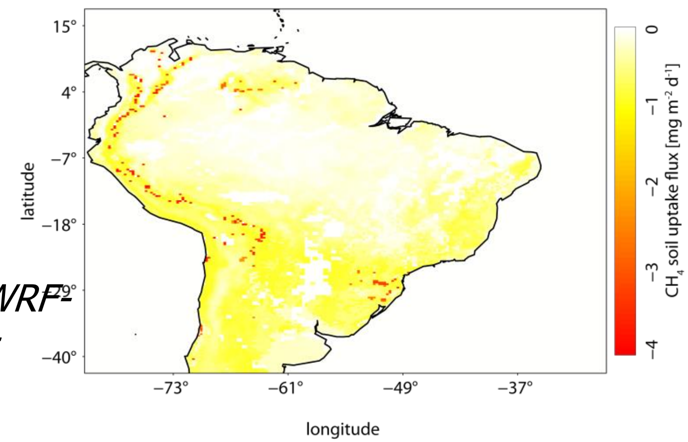
- **Detailed description**
  Beck et al., (2011): The WRF Greenhouse Gas Model (WRF-GHG) Technical Report No. 25, Max Planck Institute for Biogeochemistry, Jena, Germany, available online at http://www.bgc-jena.mpg.de/bgc-systems/index.shtml



wetland CH_4 flux



termite CH_4 flux



soil uptake CH_4 flux

Direct connection to NCAR's climate modeling system: Implementation of the Community Atmosphere Model version 5 (CAM5) Physics/Chemistry

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle *Since 1965*

- **Includes different physics options for deep and shallow convection, microphysics, boundary layer**
- **Aerosols:** *Liu et al*. (GMD, 2012), Modal Aerosol Model (MAM)
- **Gas-Phase Chemistry:** MOZART used by "CAM-Chem" already implemented in WRF-Chem by NCAR
- **PNNL** has coupled MAM with CBM-Z photochemistry in WRF-Chem

overview paper of CAM5 and coupling of these parameterizations (Rasch et al., 2013)

This Climate Model package also includes aerosol direct and indirect effect, but is limited on combinations with other packages

Several dust and sea-salt models, used for bulk, modal, and sectional approaches

Lightning parameterization for NOx emissions

Aerosol interaction with convective parameterization (GF scheme)

University of Manchester: CRIMech

- Common Represetative Intermediate Mechanism (CRIMech) (CRIv2-R5; 240 species, 652 rxns) (Watson et al., 2008)
- N_2O_5 heterogeneous chemistry in WRF-Chem sectional aerosol (Bertram & Thornton, 2009)
- Sea-spray emission scheme with organics (Fuentes et al., 2011)
- Organic Partial Derivative Fitted Taylor Expansion (PD-FiTE) added to MOSAIC sectional aerosol (Topping et al., 2009; 2012)

Douglas Lowe, Steven Utembe*, Scott Archer-Nicholls, David Topping, Mark Barley, Gordon McFiggans

Publications are being prepared for inter-journal special issue on WRF-Chem (GMD and ACP)

Chemical data assimilation

- NCEP's Grid Point Statistical Interpolation (GSI, 3DVAR) assimilation system can be used with surface chemical data as well as with AOD: Significant improvements in forecasts.
- EnKF assimilation system has been used for WRF-Chem
- Work is on-going with hybrid EnKF/GSI system (ESRL and NCAR)
- Work is also ongoing with WRF-Chem adjoint development (project lead by Greg Carmichael)

These approaches are not released to community yet

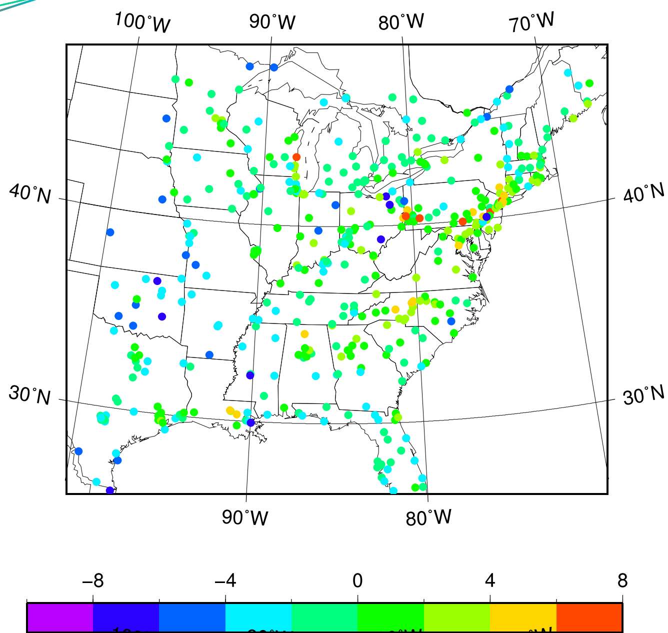
If you need chemical data assimilation to help develop or use, email wrfchemhelp for contact information

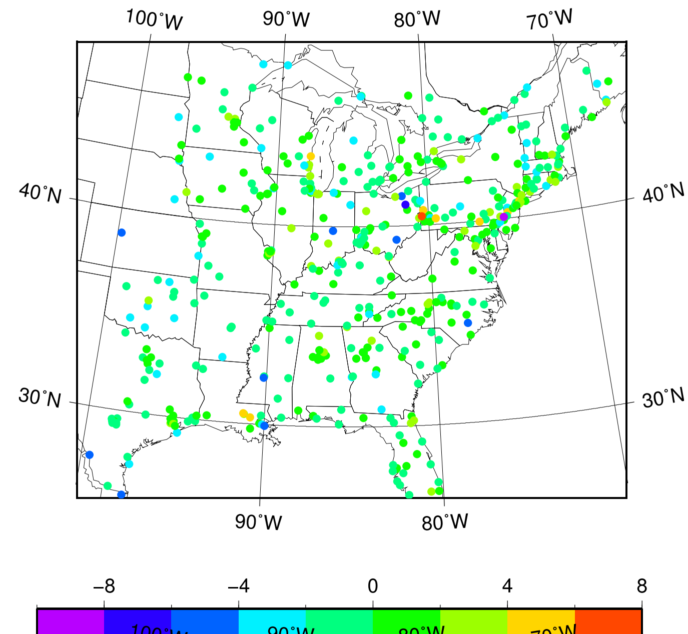
Aerosol assimilation: verification statistics against surface PM2.5
June 1 – Aug 31, 2012

without aerosol assimilation

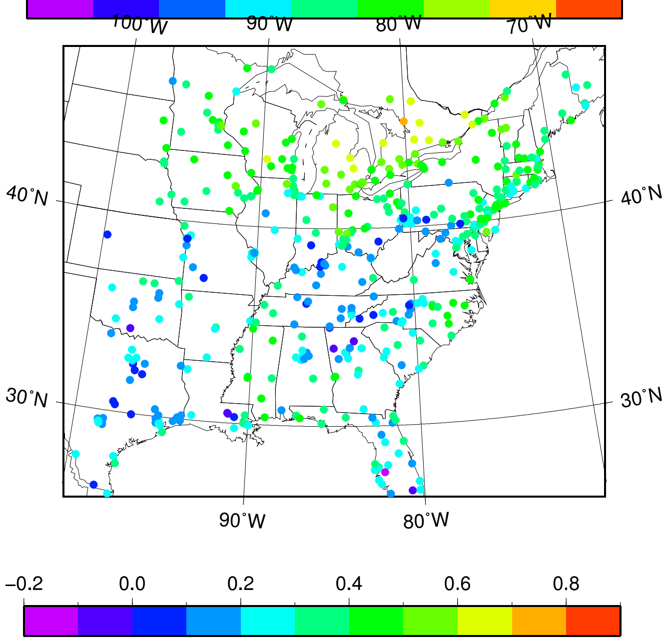
with aerosol assimilation

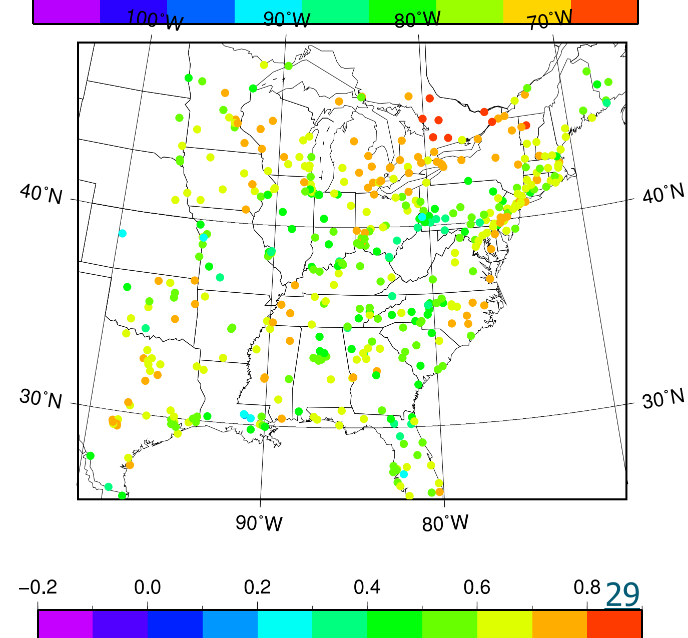
bias





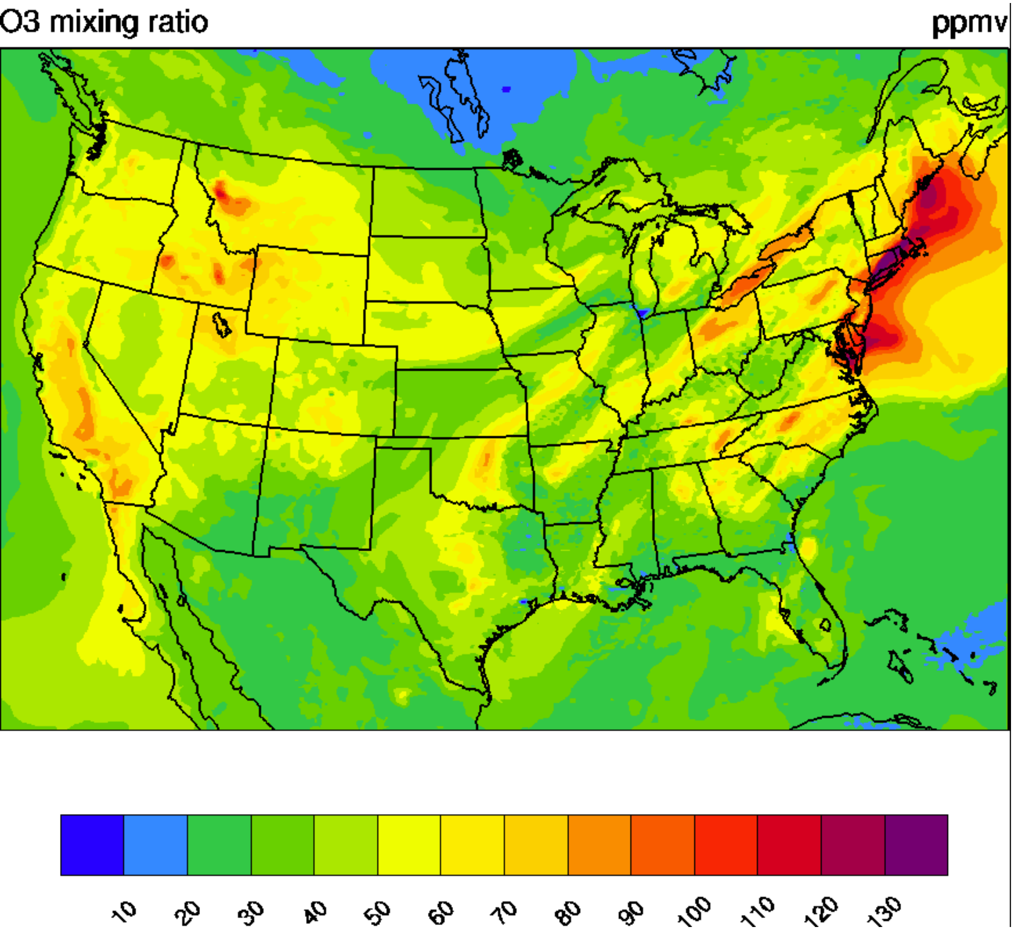
correlation



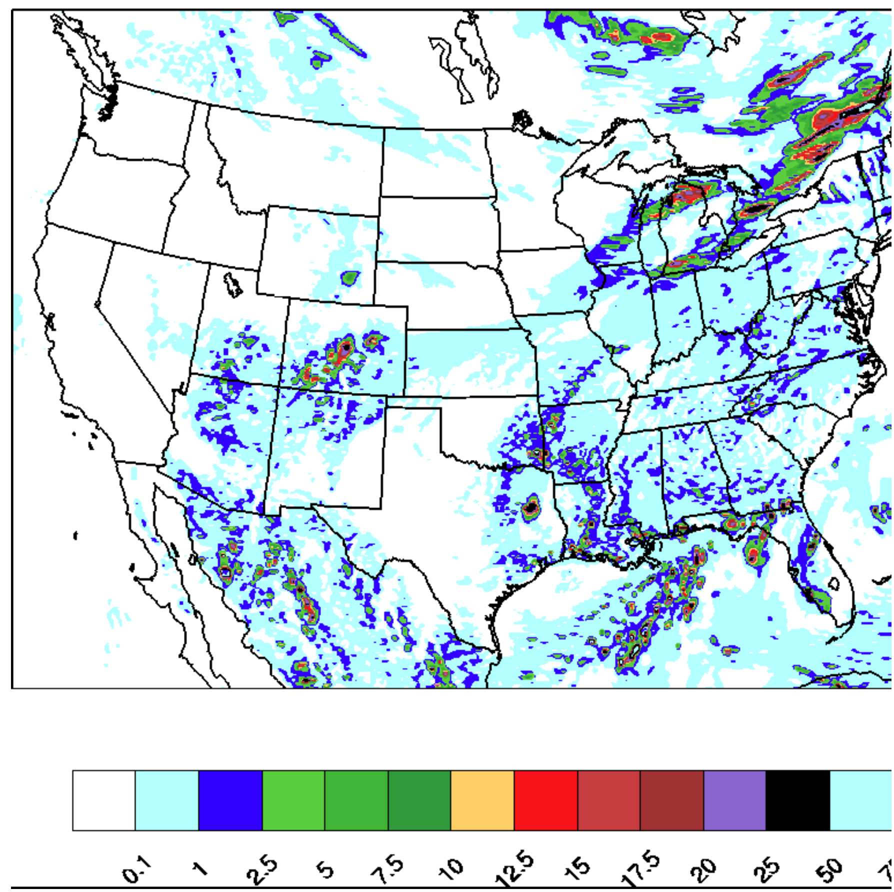


Real-time AQ forecasting with WRF-Chem

http://ruc.noaa.gov/wrf/WG11_RT/



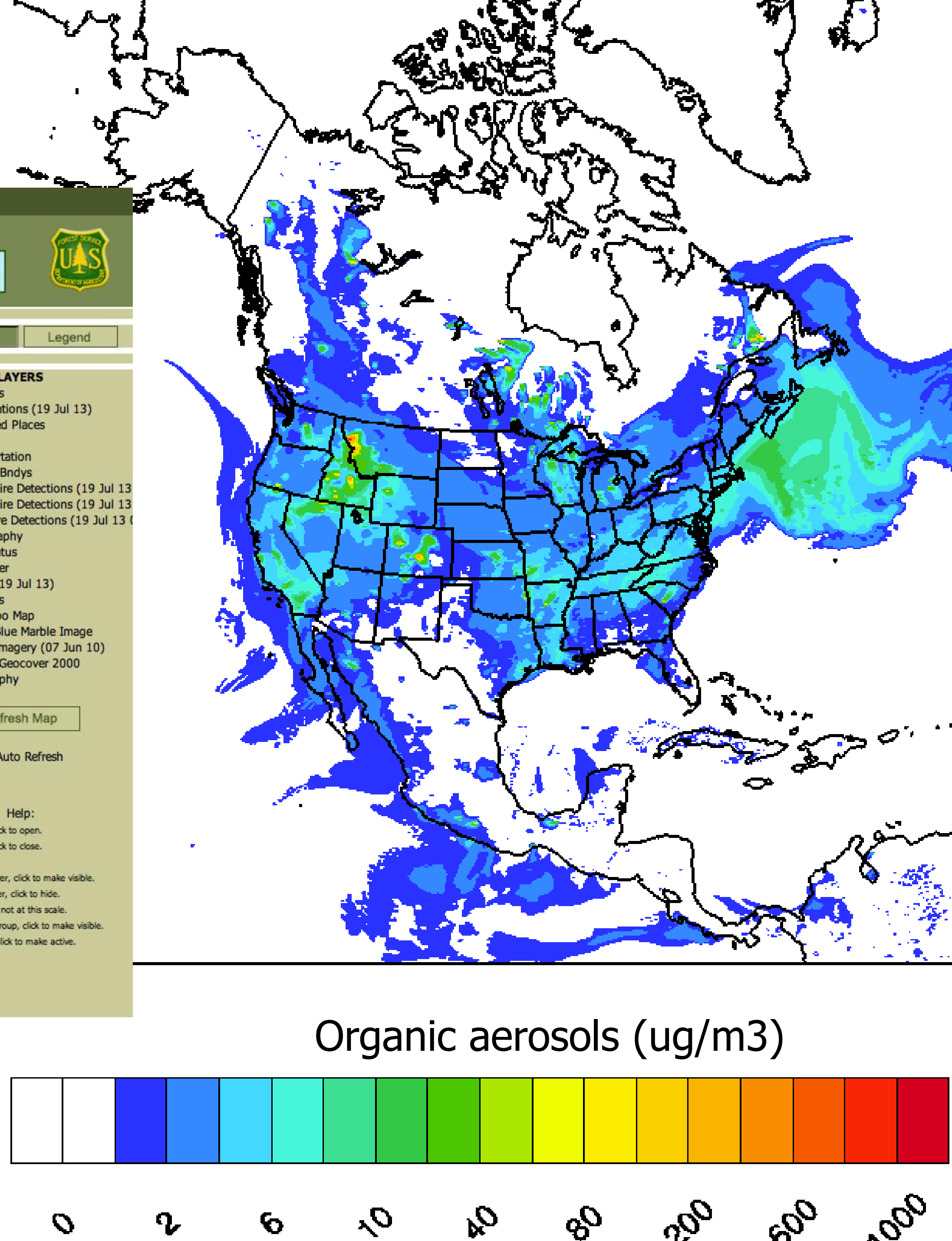
Ozone at 21Z



3-hr precip at 00Z

WRF-Chem using MADE/VBS/RACM on Rapid Refresh Domain, DX=13km

wildfires



Organic aerosols, 36hr forecast, 12Z, July 20

Real-time forecasting examples

RAP-Chem WEB site, **full ozone chemistry**, aerosols, **VBS for Secondary Organics**, wildfires

- http://ruc.noaa.gov/wrf/WG11_RT/

Using WRF-Chem for operational and semi-operational forecasting in other areas of the world

- http://ruc.noaa.gov/wrf/WG11/Real_time_forecasts.htm

Ongoing research examples

Aerosol direct and indirect effect, impact of wildfires, chemical composition, lightning NOx, emissions, transport of ash and ash-fall predictions……….

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. Also, please send us info on your peer reviewed WRF-Chem publications

http://ruc.noaa.gov/wrf/WG11/References/WRF-Chem.references.htm

Resources and final remarks

- WRF-Chem users help desk
  - wrfchemhelp.gsd@noaa.gov
- Publications (please send us yours)
  - http://ruc.noaa.gov/wrf/WG11/References/WRF-Chem.references.htm

Inter-journal special issue on WRF-Chem now also opened: ACP and GMD

Please consider: no support currently exists for preparation of tutorials and documentation. The wrfchem help desk is also only minimally supported. **If you plan to provide development work back to the community, please make it easy for us (provide documentation, follow coding standards)**

Thank you for inviting us!! Questions?