New, ongoing, and future developments for WRF-Chem (V3.2)

Georg Grell

Steven E. Peckham, Stuart A. McKeen, Mariusz Pagowski + others from NOAA/ESRL

Jerome Fast, William Gustafson jr., + others from PNNL

+ Christine Wiedinmyer, Xue-Xi, Gabi Pfister, Mary Barth and others from NCAR

+ Saulo Freitas, Karla Longo (CPTEC, BRAZIL)

+ many more national and international collaborators

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

Structure of talk

- What is new in WRF/Chem – V3.2
  - Gas phase chemistry
  - GOCART and radiation
  - Lightning NO_X parameterization
  - Tracers and other options
  - Emissions preprocessors: new developments
- Ongoing and future work
  - Volcanoes, SOA, data assimilation, more

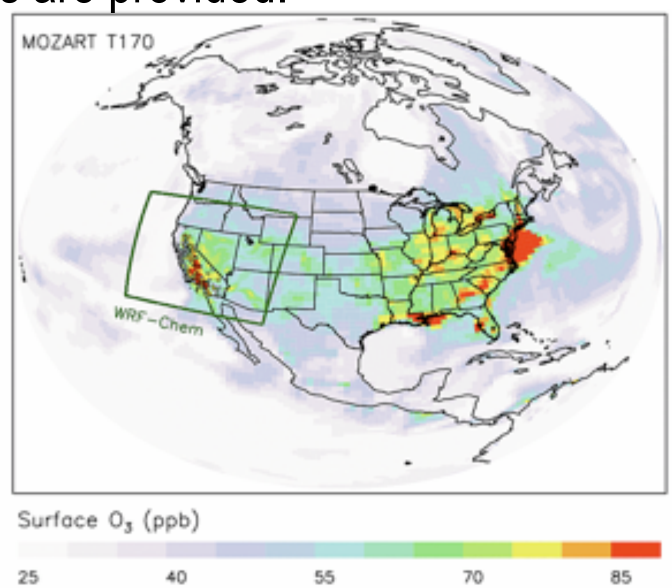
Gas Phase Chemistry Packages

- Chemical mechanism from RADM2 (Quasi Steady State Approximation method with 22 diagnosed, 3 constant, and 38 predicted species is used for the numerical solution)
- Carbon Bond (CBM-Z) based chemical mechanism, and the
- ***K***inetic ***P***re***P***rocessor (KPP)
  - RADm, **CBMZ**, various versions of RACM, **MOZART**
  - **MOZART also coupled to GOCART (MOZCART)**

WRF-Chem/MOZART & WRF-Chem/MOZCART

Provided and implemented by G. Pfister, S. Walters, C. Wiedinmyer, M. Barth, L. Emmons

- **MOZART-4 gas phase chemistry scheme included in WRF-Chem V3.2 through KPP (WRF-Chem/MOZART) and linked to GOCART aerosols (WRF-Chem/ MOZCART)**
- Updates to photolysis (FTUV) and dry deposition (Wesely), including:
  - Climatological overhead O3 and O2 columns for FTUV calculations
  - Seasonality in dry deposition
  - Preprocessors to produce the required additional inputs are provided.
- Works with MEGAN online biogenic emissions and plume rise fire emissions



MOZART-4 Gas Phase Chemical Mechanism:
included in the global MOZART-4 and CAM-Chem models
85 gas species, 39 photolysis reactions, 157 gas phase reaction
Details*: Emmons et al., Geosci. Model Dev., 3, 43–67, 2010.*

Preprocessors available to the WRF-Chem community

mozbc

- for setting space and time-varying chemical initial and boundary conditions from MOZART-4 or CAM-Chem output
- operates on the three most common map projections (Lambert, Mercator, Polar).
- mapping from MOZART species to any of the chemical/aerosol options in WRF-Chem is provided

see Poster P.77: "Defining Chemical Boundary Conditions in Regional Modeling" (G. Pfister et al.)

bio_emiss

- creates input files (wrfbiochemi) needed when running WRF-Chem with MEGAN online biogenic emissions (bio_emiss_opt=3).

see Poster P.73: "Using MEGAN Biogenic Emissions to Study the Fate of Isoprene on the Regional Scale (M. Barth et al.)

MOZCART preprocessor tools

- exo_coldens: creates an input file with O3 and O2 climatological overhead columns for FTUV
- season_wesely: creates an input file for seasonality in dry deposition

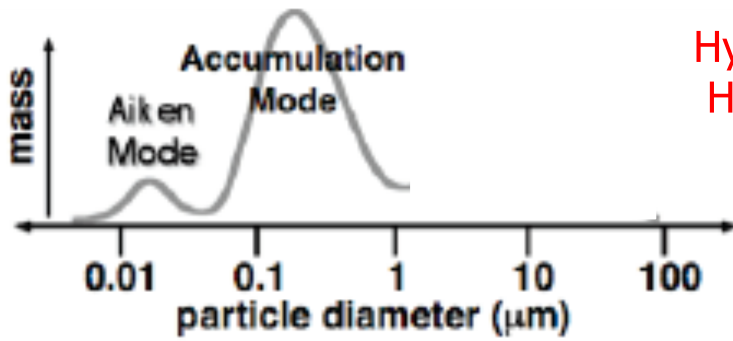
Codes, examples and instructions are available on:

www.acd.ucar.edu/wrf-chem/download.shtml

Hooking up GOCART with atmospheric radiation

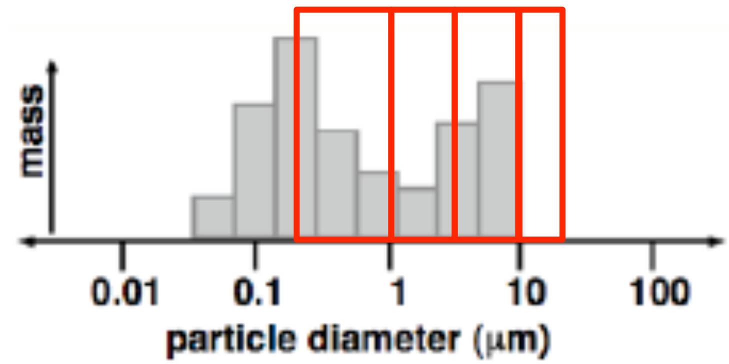
- Bulk scheme, much simpler than the sectional and model schemes
  - Only the total mass of the aerosol components
  - Provides no information on
    - Particle size
    - Particle concentration
  - Correction factors for OC and NH4 have been added for output of total pm2.5 as well as calculation of optical properties
- Numerically very efficient
- Now coupled with radiation

Apportioning GOCART species mass into 8-bins of MOSAIC



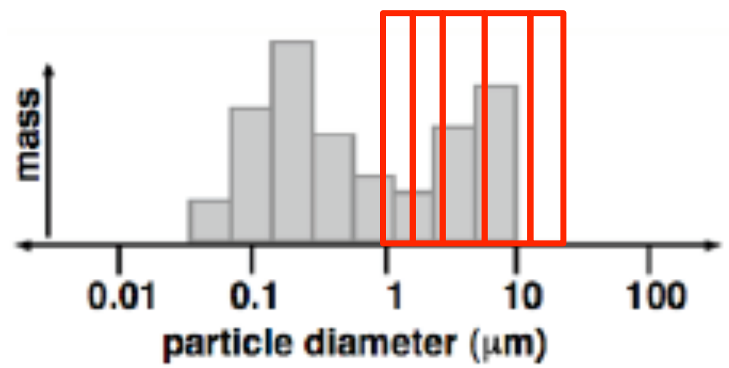
Primary Emitted $PM_{2.5}$, Sulfate, MSA,
Hydrophobic Organic Carbon & Elemental Carbon
Hydrophilic Organic Carbon & Elemental Carbon
75% to Accumulation, 25% to Aitken modes

Modal to 8-bin sectional apportioning



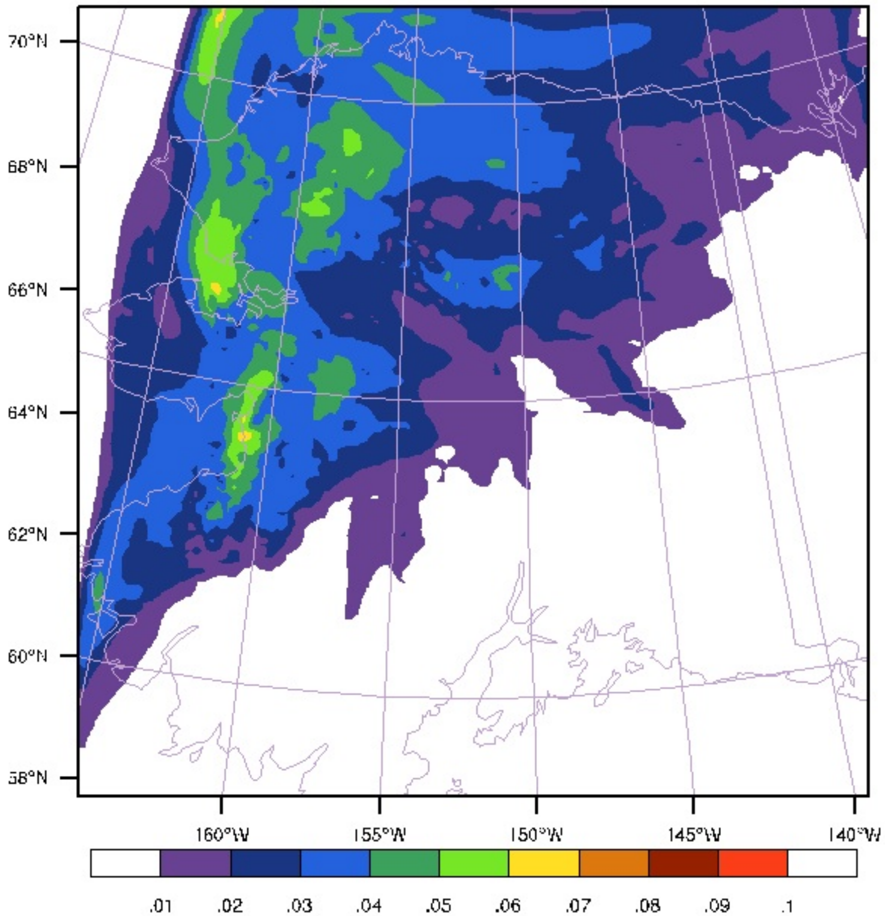
GOCART 4-bin_Seasalt

Fractional averaged over MOSAIC 8-bin

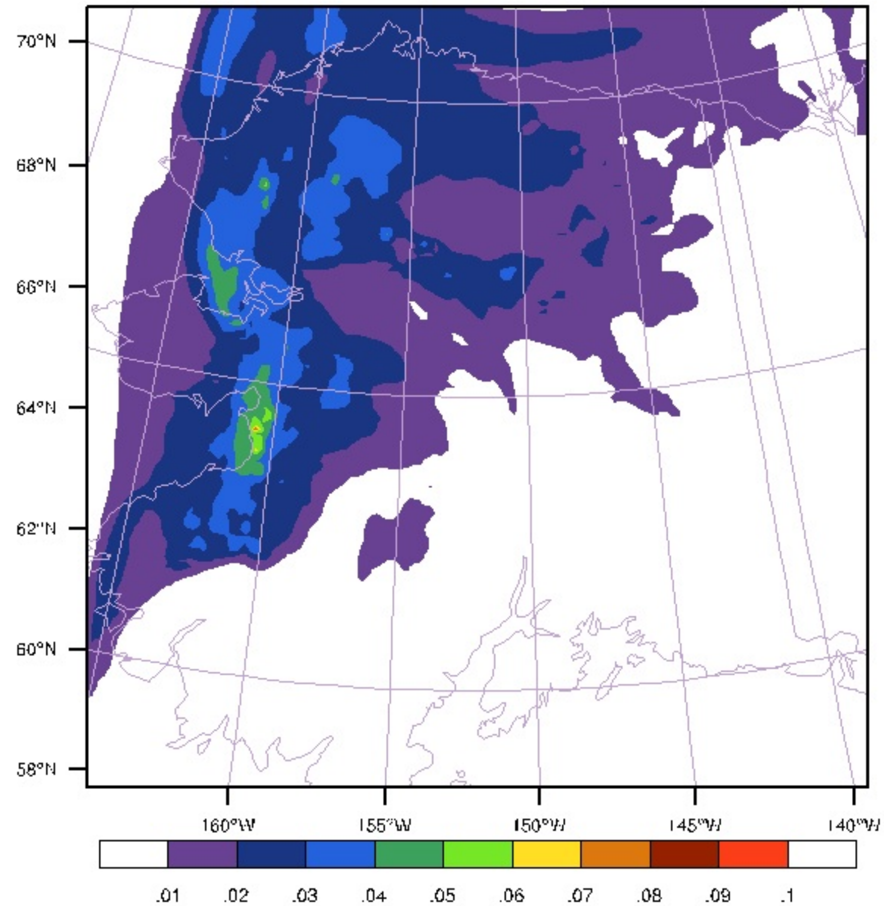


GOCART 5-bin Dust

Fractional averaged over MOSAIC 8-bin



Full Chemistry



GOCART

Comparison of integrated extinction coefficients (at .55um) when using bulk aerosol module (GOCART modules): a little smaller than in full chemistry run (a little less aerosol in the air)

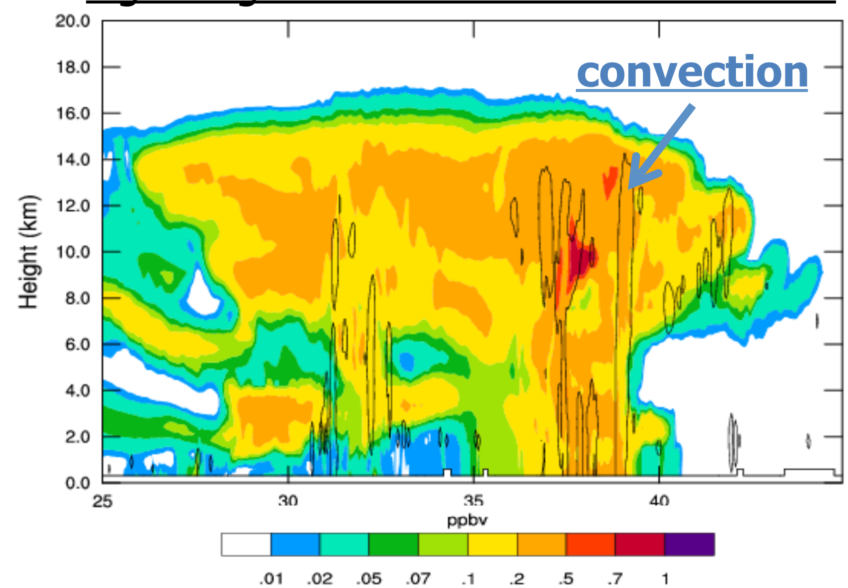
This run without correction factors!

Lightning NOx Production for Cloud Resolving Scales

Provided and implemented by M. Barth, C Barthe, K. Pickering, L. Ott, J. Lee

- Can choose method for predicting lightning flash rate
- Partitions between intracloud (IC) and cloud-to-ground (CG) flashes through climatology or prescribed fraction
- Distributes NO horizontally within reflectivity > 20 dBZ
- Distributes NO vertically using a Gaussian distribution
- The amount of NO produced per lightning can be specified through namelist parameter
- Includes Lightning NO_x tracers and IC and CG flash rate counters

Lightning-NOx tracer across a cold front



Other additions

- Reworked tracer option ("tracer_opt"), can run separately or in parallel to chemistry : Old tracer options (set with "chem_opt") will disappear in future version
- Inclusion of a driver that enables modular and interoperable dry deposition schemes for both MADE/SORGAM and MOSAIC. 4 deposition schemes are included: 2 from MADE/SORGAM, 1 from MOSAIC, and another based on Zhang et al., Atmos. Environ. (2001).
- Shallow convection (when using GD or G3 schemes)
- More general emissions input
- Aircraft emissions

*M*odel of *E*missions of *G*ases and *A*erosols from *N*ature (MEGAN) in WRFV3/Chem:

- MEGAN preprocessor now exists (poster P.73)

Provided and developed by S. Walters, C. Wiedinmyer, G. Pfister, T. Duhl

Volcanoes: new module for prep_chem_sources emissions preprocessor code

Collaboration with Saulo Freitas (CPTEC), Martin Stuefer (UAF), and Peter Webley (UAF)

1. New fortran module that contains the Mastin et al. dataset (more than 1500 volcanoes)
2. Provides collocation of the volcano at the nearest model grid box
3. Uses basic historic parameters
   - Was used by ESRL for Iceland volcano (“big E”) for global modeling

Future and **V3.2** line-up for WRF/Chem, with various groups working on these issues

- Much work with improving aerosol modules
- Chemical data assimilation
  - 4dvar, collaboration with U of Iowa, U of Colorado, ESRL/GSD, maybe more using WRF-var
  - 3dvar and EnsKF work at ESRL using GSI
- More choices for "interactive" parameterizations
- NMM-WRF/Chem could become available (mass conservation issue was fixed)
- Offline version exists, is still on the shelf
- Effects of volcanoes will be included - prediction of ash-fall (10 size bins) as well as ash concentrations(4 size bins)

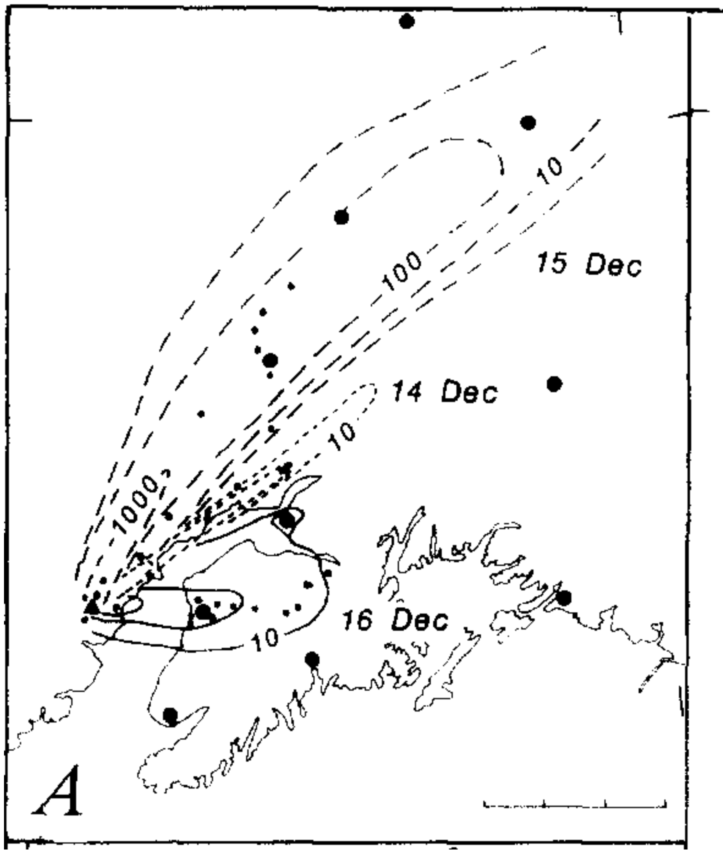
ASH and SO2 Volcanoes Prediction

- Historic cases
- Real-time predictions
  - Each volcano has a flag that turns color when an eruption is imminent, and then again when an explosive eruption occurs
  - Some emit constantly (ash as well as so2)
- Injection: vertical distribution below the umbrella section
  - Base of umbrella section is 27% of maximum height so 12 km plume, 3.24 km depth to umbrella.
  - The percentage below umbrella is around 20 – 30 % of total mass.
- New Particle size distribution based on MSH 1980

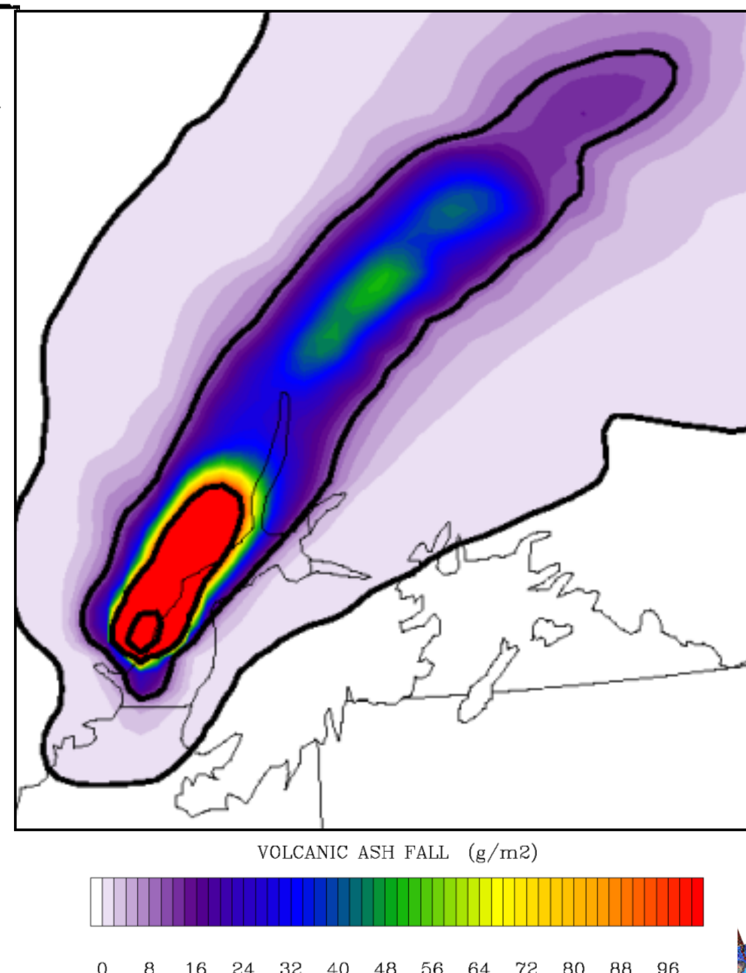
Particle Size Bin	Phi	Percentage of mass
1 – 2mm	-1 – 0	2
0.5 – 1 mm	0 – 1	4
0.25 – 0.5 mm	1 – 2	11
125 – 250 µm	2 – 3	9
62.5 – 125 µm	3 – 4	9
31.25 – 62.5 µm	4 – 5	13
15.625 – 31.25 µm	5 – 6	16
7.8125 – 15.625 µm	6 – 7	16
3.9065 – 7.8125 µm	7 – 8	10
< 3.9 µm	> 8	10

ESRL

Tephra-fall deposits (g/m²)
Redoubt Volcano, south-central Alaska
December 15, 1989



<u>Observed</u>



<u>Predicted by WRF-Chem,</u>
<u>using **RR setup**</u>

Plumerise will be modified:

including the environmental wind effect on cloud scale dilution- governing equations

dynamics for W

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

dynamics for U

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

thermo-dynamics

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

water_vapor conservation

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

cloud water conservation

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

rain/ice conservation

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

dynamic entrainment

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

equation for radius size

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

bulk microphysics

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

bulk microphysics:

Kessler, 1969; Berry,1967

Ogura & Takahashi,1971

See Freitas et al. (2010 ACPD) for 1d cloud model comparisons with fully 3D ATHAM simulations

Further modifications to prep_chem_sources

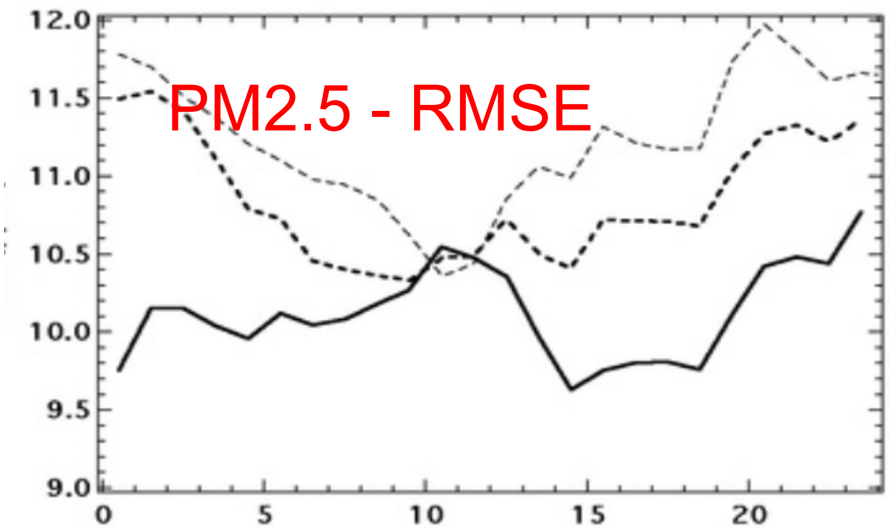
- biogenic emissions from MEGAN
- biomass burning from GFDV3.1
- anthropogenic emissions from EDGAR 4
- also works with icosahedral global grid

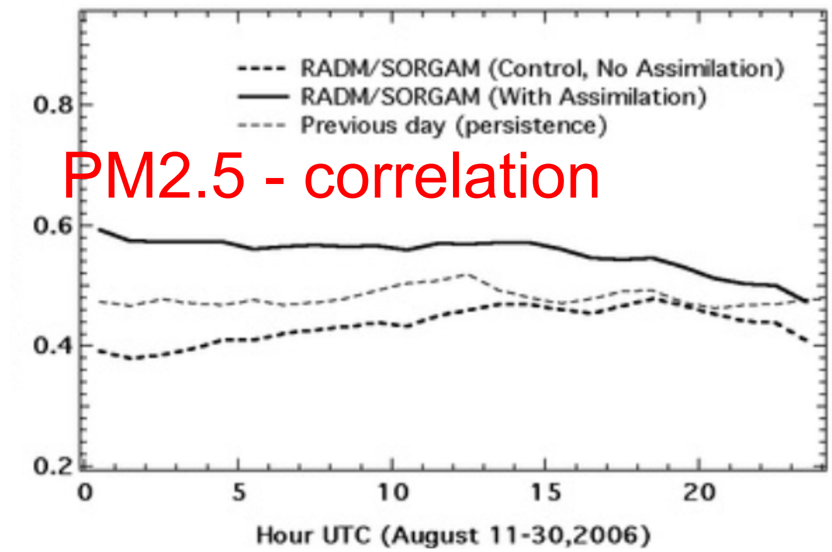
Release of new version expected in September of 2010, paper submitted to GMD

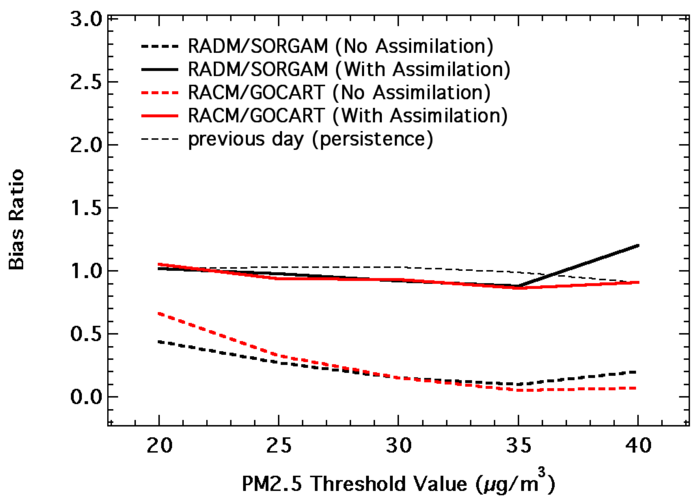
Chemical data assimilation: ARW-WRF/Chem and GSI

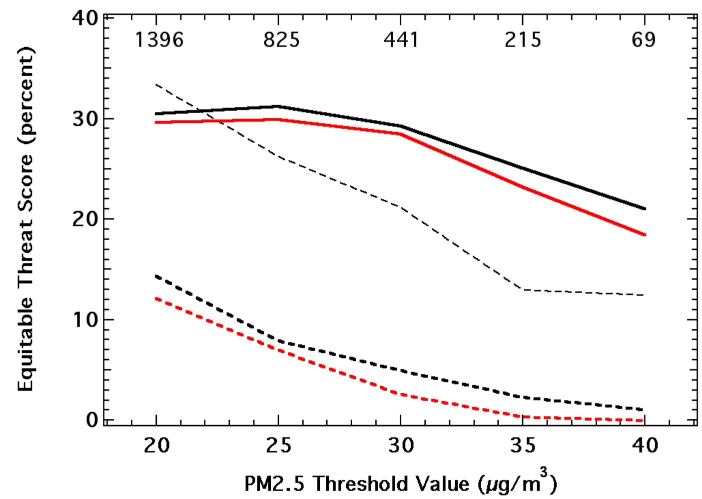
2 months worth of WRF/Chem runs:

1. New England 2004 to estimate background error covariances and lengthscales
2. Houston 2006 for evaluation









Chemical data assimilation: ARW-WRF/Chem and GSI

Current activity:

- Develop and deliver operational system for air quality and weather forecasting and assimilation of weather and aerosol data for Air Force Weather Agency
- Cooperative project AFWA/ESRL/NCAR
- Assimilation of AOD and surface PM data, using WRF-Chem and GSI
- Rapid Refresh framework (dx=13km for North American Grid)
- Also to be used for High Resolution Rapid Refresh (HRRR, dx=3km over continental US)

WRF/Chem ongoing and future work – PNNL

- Cloud-aerosol interactions to work with Morrison and Thompson microphysics schemes - currently being tested
- Package that couples MOSAIC with SAPRC99 photochemistry via KPP
- SOA using the volatility basis set approach has been coupled with MOSAIC; a computationally efficient version of this approach is being tested (talk 5B.1)
- Porting CAM5 physics suite to WRF, including its new aerosol model coupled with MOZART photochemistry (talk 6.2)
- coupling of GOCART dust emissions with MADE/SORGAM and MOSAIC (talk 5B.4)
- new aerosol model is planned (MOSAIC-ext), that simulates the evolution of the transition between internal and external aerosol mixing states
- ice-aerosol interactions to be included

WRF/Chem ongoing and future work – PNNL

- Aerosol modeling test bed is making progress

http://www.pnl.gov/atmospheric/research/aci/amt/index.stm

- Analysis Toolkit Software may be available via the web site later this summer, as well as test bed case data as they become available
- MILAGRO test bed data is finished,
- CHAPS, VOCALS, ISDAC/ARCTAS, CARES/CalNex integrated datasets (field campaign + routine monitoring) planned for the future

WRF/Chem current and future work – NCAR/ACD

- Add/improve wet scavenging of gases (hooked with MOZCART
- Create a pre-processor for wild fire emissions based on Wiedinmyer's fire emissions model
- Improve dust emission parameterizations
- Improve SOA gas chemistry and add SOA aqueous chemistry (likely to be hooked with MOZCART)

Aerosol/microphysics coupling from the microphysics guys

ESRL

WRF/Chem current and future work – ESRL/ GSD and/or CSD

- SOA: the volatility basis set approach has been coupled with modal aerosol scheme (talk 5B.2)
- Simplified wet deposition for resolved precipitation (if no aqueous phase option is used)
- Original GOCART optical property calculation has been implemented in optical driver and is being tested
- Aerosols will be coupled with convective parameterization (GD and G3)
- Graham Feingold, Hailong Wang, Jan Kazil (ESRL/CSD): Implementation of double moment bulk microphysics scheme (Feingold et al. 1998)
  - Coupling WRF/Chem/KPP gas phase chemistry with aqueous phase chemistry and aerosol microphysics
  - Coupling of the double-moment accumulation mode aerosol, and dissolved gas phase species with the Feingold 1998 double moment microphysics scheme (using it for LES simulations to see how these changes will affect the CCN population, drizzle, and POC's).
  - New nucleation scheme (neutral and charged nucleation of H_2SO_4/ H_2O based on CSD laboratory measurements)

Thank you!

Chem session is Thursday morning if you would like to find out more, posters are Wednesday afternoon