Georg Grell

S.A. McKeen, S. E. Peckham, R. Ahmadov (**NOAA/ESRL**), J. D. Fast, W. I. Gustafson Jr., R. C. Easter, M. Shrivastava, Q. Yang, C. Zhao (all **PNNL**), M. Barth, G. Pfister, S. Wolters (all **NCAR**), J. Wong (University of Colorado), S. Freitas (**CPTEC, Brazil**), P. Webley, M. Stuefer (**University of Alaska**), G. A. Creighton (**AFWA**), S. L. Jones (**AER** and **AFWA**)

\+ *many more national and international collaborators*

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

Structure of talk

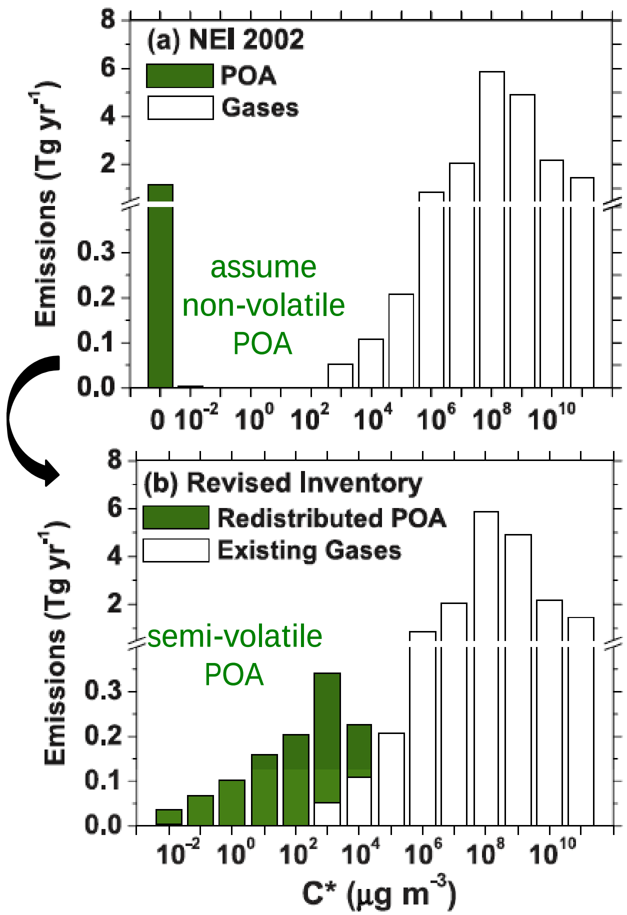
- What is new in WRF/Chem – V3.3
- Emissions preprocessors: new developments
- Ongoing and future work

Adding Gas Phase Chemistry and Aerosol Packages (all implemented by **PNNL**)

- New gasphase chemistry KPP packages include
  - SAPRC99 (by itself and coupled to MOSAIC + VBS2
  - 7 CBMZ packages (coupled to MADE/SORGAM, MOSAIC_DMS, with and without aqueous phase chemistry)

Secondary Organic Aerosols in MOSAIC

Volatility Basis Set Approach

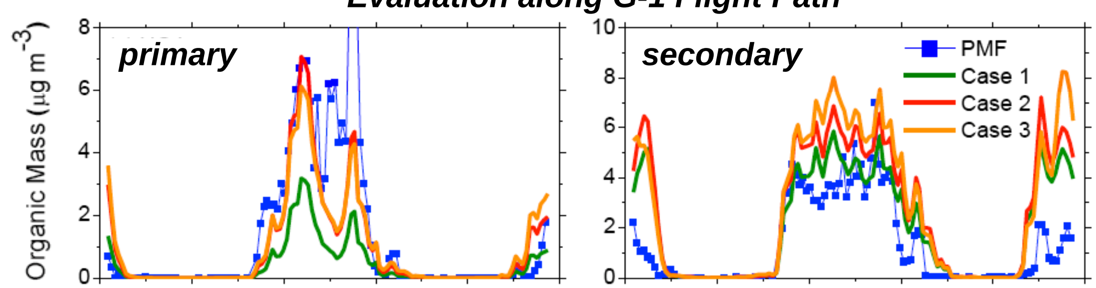


Description

Shrivastava, M., et al., 2010: Simplifying a secondary organic aerosol formation mechanism for global models using the WRF-Chem regional model. *Atmos. Chem. Phys. Discuss.*, 10, 30205-30277.

- 9 and 2 volatility bins versions developed, but only 2-bin version released in WRF v3.3
- Works with only 4-size bin version of MOSAIC
- Computationally expensive, since O and C treated separately so that O:C ratios can be determined and compared with observations
- 2-bin version could be made simpler by reducing the # of transported arrays
- Tested using organic aerosol components in Mexico City during MILAGRO campaign

Evaluation along G-1 Flight Path



NOTE: Users should be aware of assumptions and limitations of this approach. SOA treatments are changing monthly.

Improving Aerosol Modules: Secondary Organic Aerosols in MOSAIC: Volatility Basis Set Approach (VBS) as implemented by PNNL

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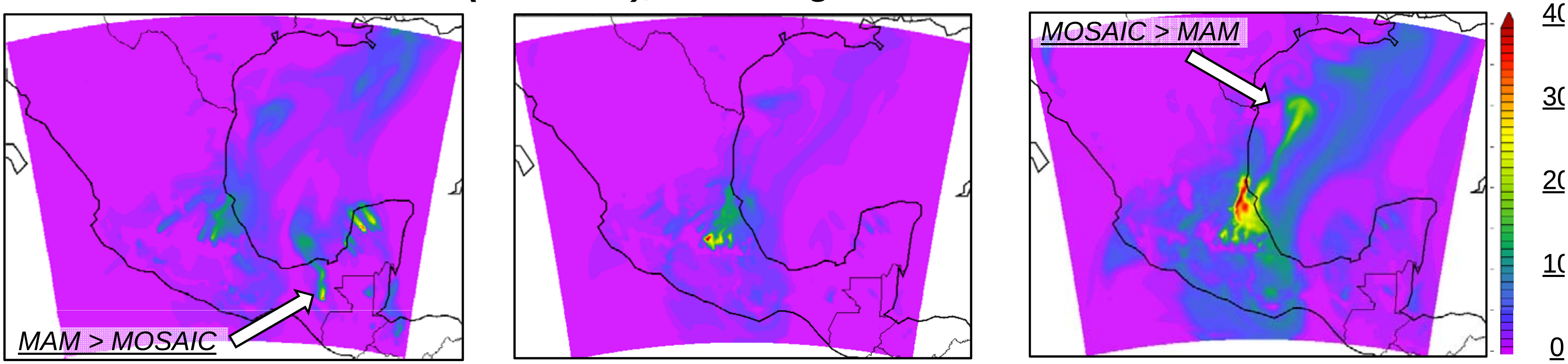
Aerosol Model from CAM5 Ported to WRF-Chem

MAM (from CAM5)	**MADE/SORGAM**	**MOSAIC**
modal – 3 modes, **18** species	modal – 3 modes, **38** species	sectional – 4 bins, **164** species
'simple'	*9 times more species*	**'complex'**
1 simulation day ~ 21 min	*~ 24 min*	*~ 60 min*

fine PM (< 2.5 mm), excluding dust ~1800 m AGL



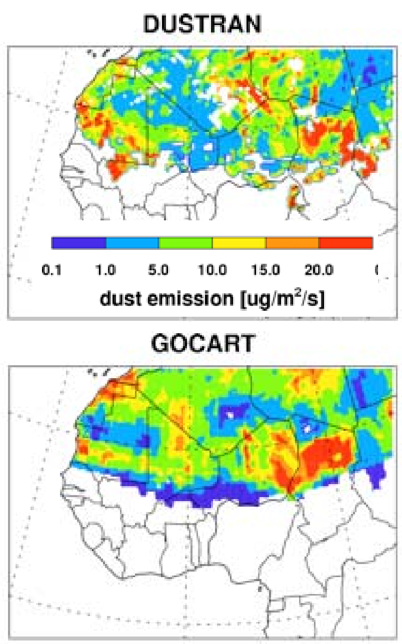
- Identical emissions, meteorology, chemistry, dry deposition, boundary conditions
- Differences due to secondary aerosols (SO_4, NO_3, NH_4, organics)
- Treatment of organics:
- **MAM**: POA - non-volatile, SOA – simple yields
- **MADE/SORGAM**: POA - non-volatile, SOA - 2-product approach
- **MOSAIC**: 'volatility basis set' approach, volatile POA & SOA

See Poster P80, Fast et al. for more details

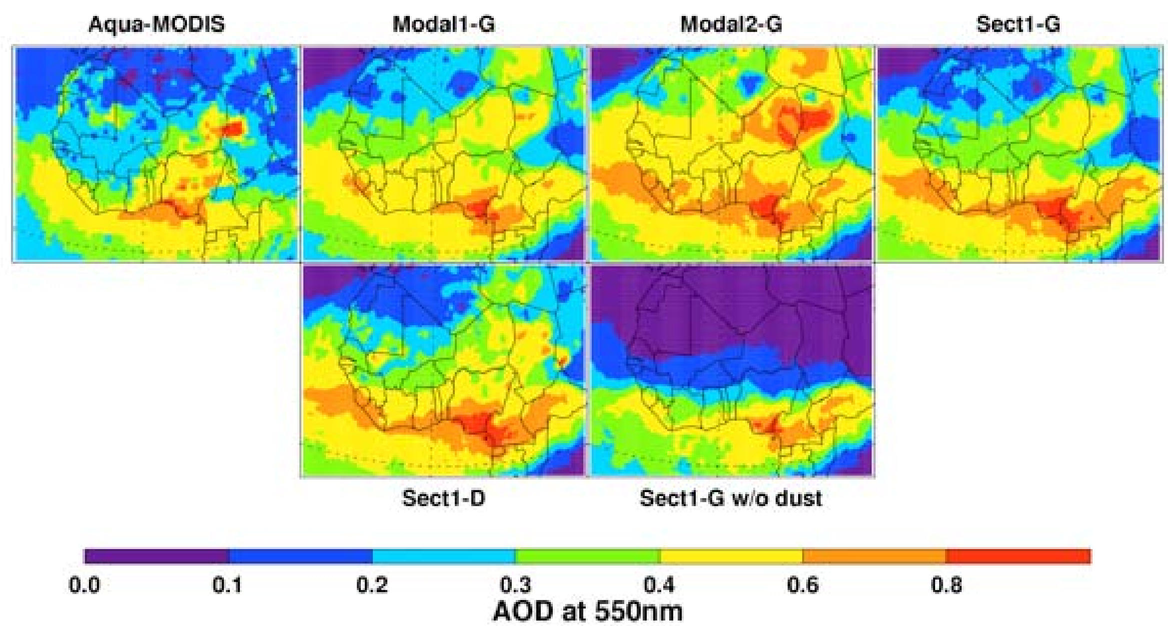
Aerosol direct effect capabilities were expanded: New in V3.3: Coupling of Aerosols to RRTMG Radiation (implemented by PNNL)

- Extended modular optical property module to compute information needed for both shortwave and longwave RRTMG radiation scheme
- Works for both MADE/SORGAM and MOSAIC
- Evaluated using AOD and extinction profile data over northern Africa associated with Saharan dust
  - GOCART dust emission module also extended to work with MADE/SORGAM and MOSAIC
  - See *Zhao et al., ACP, 2010* for more details

Dust Emissions from 2 Treatments



AOD under Various Scenarios – Dust Emissions and Aerosol Models



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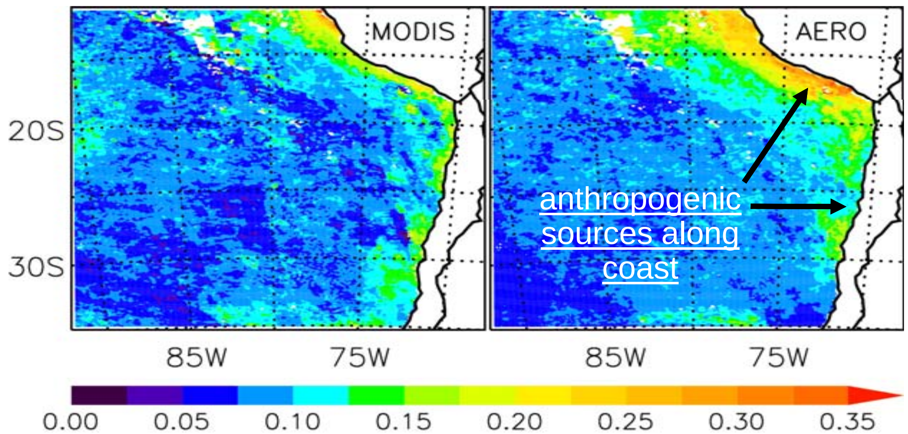
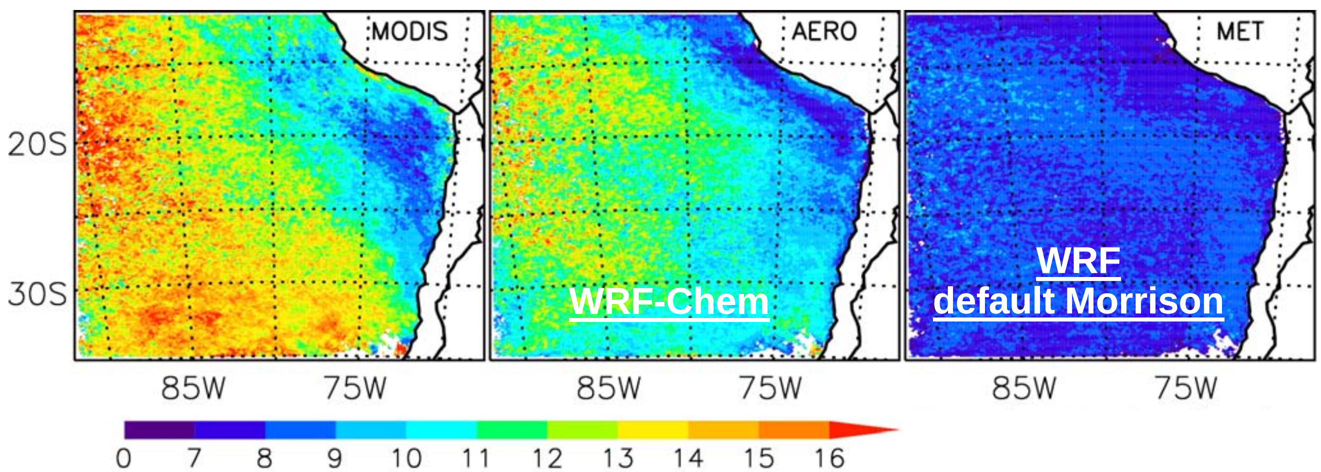
Aerosol Indirect Effect: Cloud-Aerosol Interactions with Morrison Microphysics (PNNL)

Average AOD Oct 15 – Nov 15, 2008 during VOCALS-REx



- Cloud-aerosol interactions, aqueous chemistry, wet removal, and indirect effects implemented with Morrison scheme, similar to Lin et al. scheme
- Works with MADE/SORGAM and MOSAIC
  - Coupling aerosols with clouds improves many cloud properties
- Affects cloud albedo, radiation, and drizzle rate as expected

Average Droplet Effective Radius Oct 15 – Nov 15, 2008



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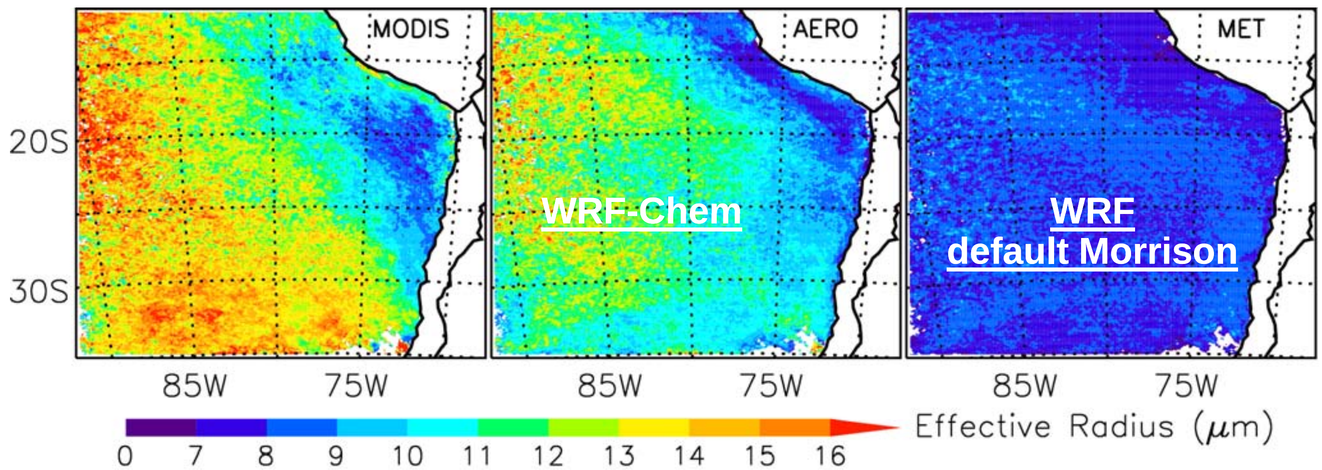

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Other minor additions

- GOCART now also coupled with RRTMG for SW and LW (Stu Mc Keen)
- Additional option for dust only simulation – no chemistry
- Shallow convection (when using GD or G3 schemes) is being improved and evaluated
- Experimental very simple wet deposition scheme is in V3.3 and is being evaluated
- More general emissions input

Volcanic ash in WRF-Chem V3.3

Collaboration with University of Alaska in Fairbanks as well as INPE/CPTEC in Brazil,

Publications in progress

New module avilable in prep_chem_sources that contains the Mastin et al. dataset (more than 1500 volcanoes) and provides collocation of the volcano at the nearest model grid box

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

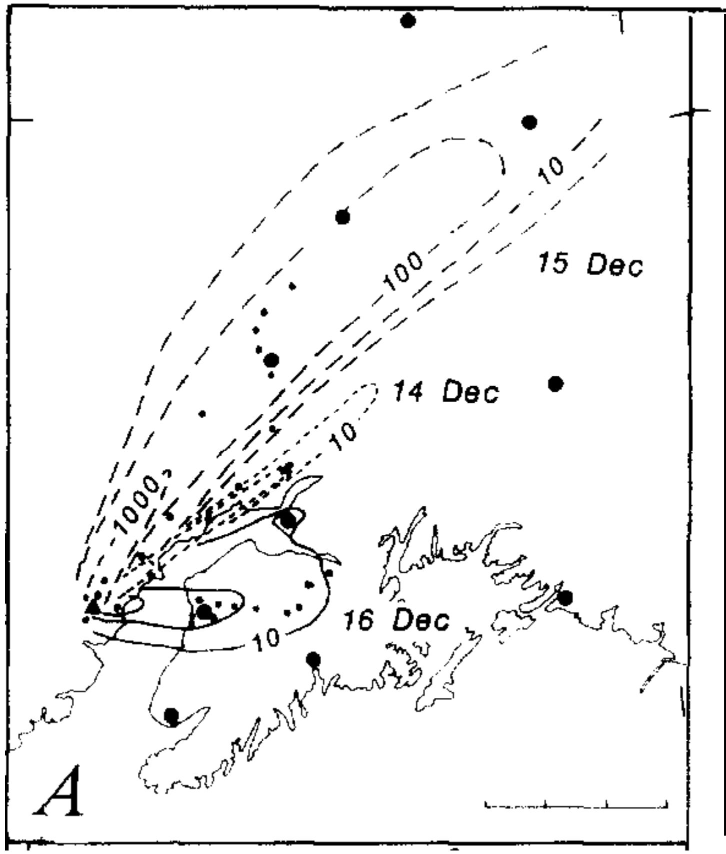
4 size bins for prediction if transport only is of interest

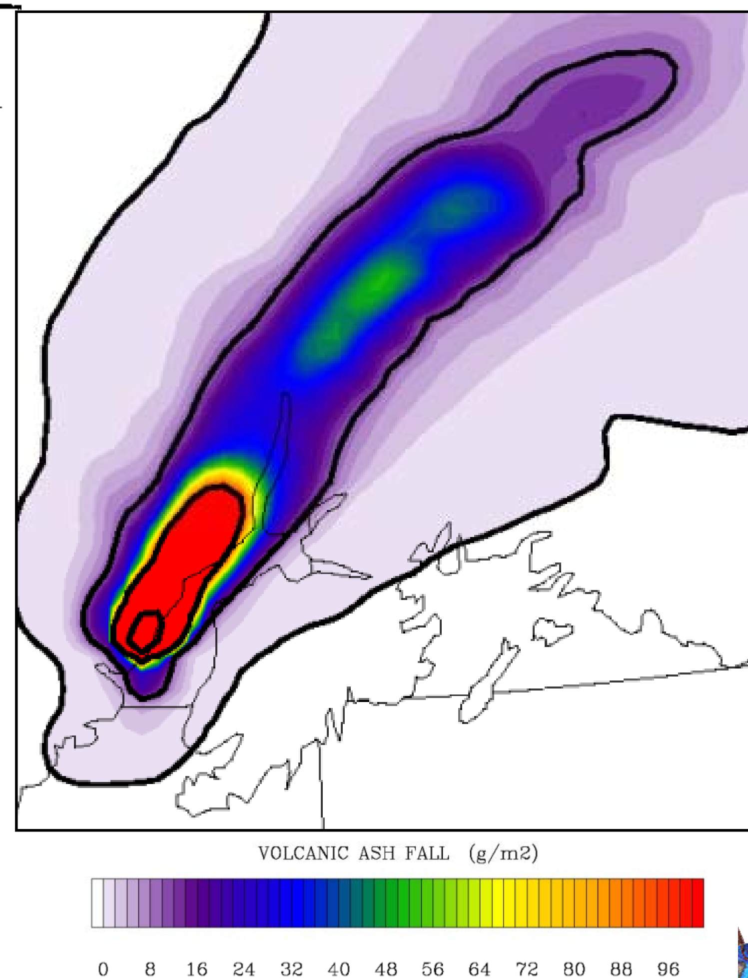
Particle Size Bin	Phi	Percentage of mass
15.625 – 31.25 µm	5 – 6	16
7.8125 – 15.625 µm	6 – 7	16
3.9065 – 7.8125 µm	7 – 8	10
< 3.9 µm	> 8	10

Volcanic ash

- **What we get in real-time application**: info that a volcano has erupted, with name and time, some Satellite info possible
- **Initial emissions** based on Mastin et al data set (includes 1523 Volcanoes, injection height and total mass of injected ash)
- May be adjusted with radar or Satellite observations
- Transport includes sub-grid scales (PBL, Convection), also settling, wet and dry deposition

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

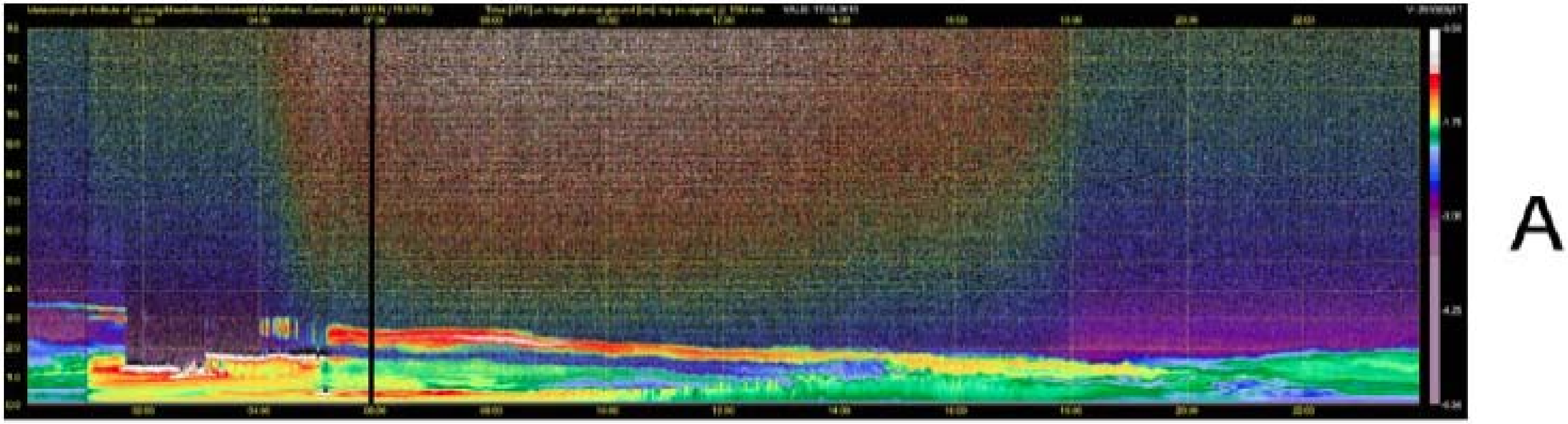


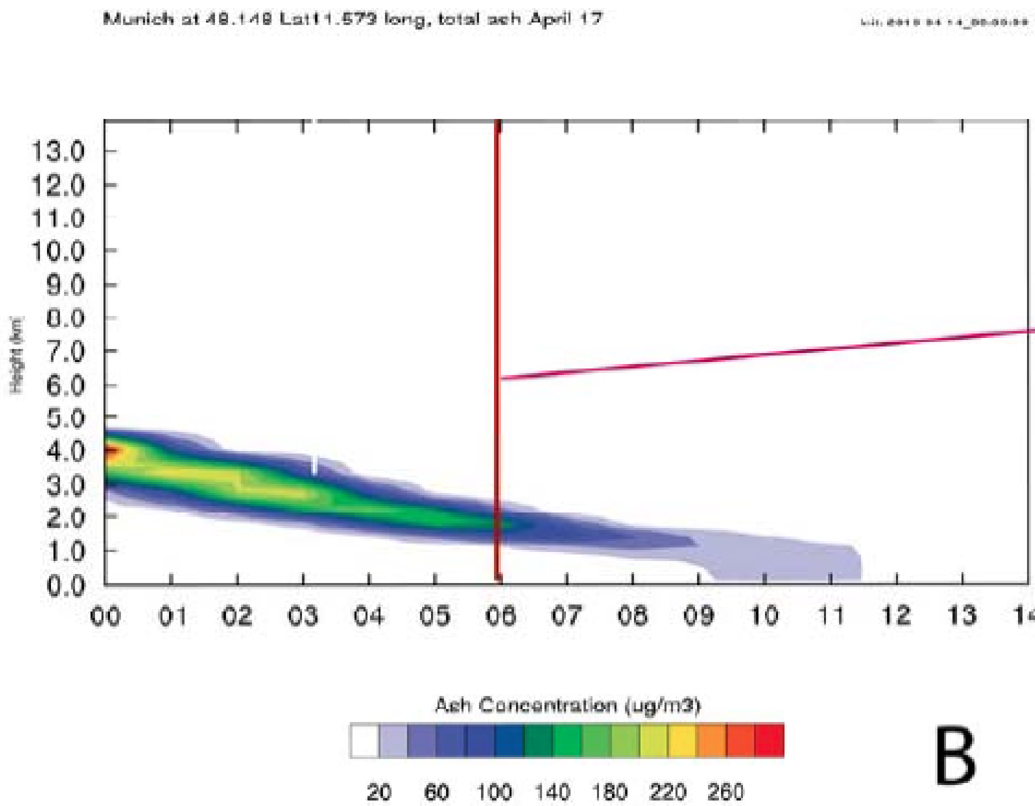


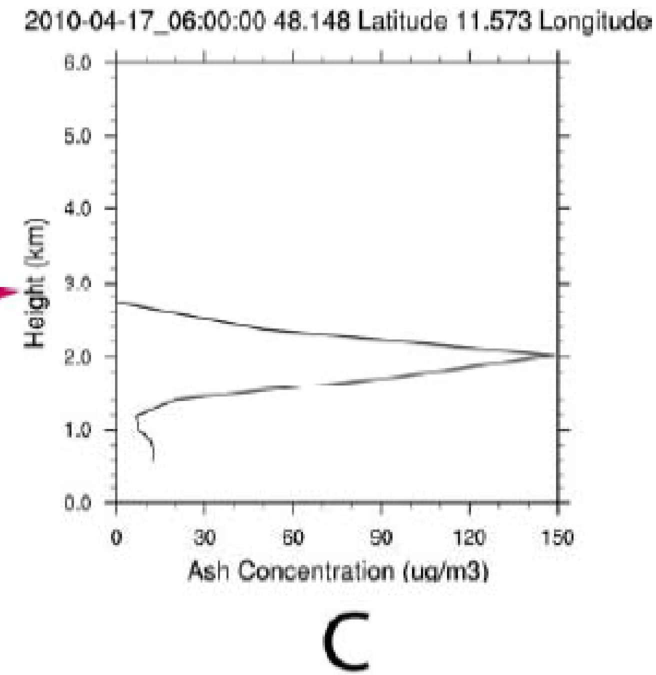
Observed

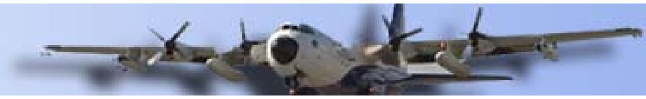
Predicted by WRF-Chem, using **RR setup**

Forecast compared to Munich Lidar, April 17, 06Z









Additional Fire Emissions Preprocessor “Fire_Emis”

- For creating wrffirechemi_<domain> files when running WRF-Chem with online plume rise. Emissions are based on the NCAR Fire Model (FINN; C. Wiedinmyer). Download from http://www.acd.ucar.edu/wrf-chem/
- For MOZART, SAPRC, or GEOS-Chem specification
- Currently only used by MOZART – other chem options will be added

Further modifications to prep_chem_sources

- biomass burning from GFDV3.1
- anthropogenic emissions from EDGAR 4.1
- Volcanic ash
- also works with icosahedral global grid

Chemical data assimilation: ARW-WRF/Chem and GSI

- Assimilation of AOD (Zhiquan Liu, NCAR talk on Thursday in WRF-Chem session) and surface PM data (Mariusz Pagowski), using WRF-Chem was included in GSI
- Used at ESRL in Rapid Refresh framework (dx=13km for North American Grid)
- Also used for High Resolution Rapid Refresh (HRRR-chem-fire, dx=3km over western US)

WRF/Chem ongoing and future work – PNNL

- Continued work on cloud-aerosol interactions
- 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

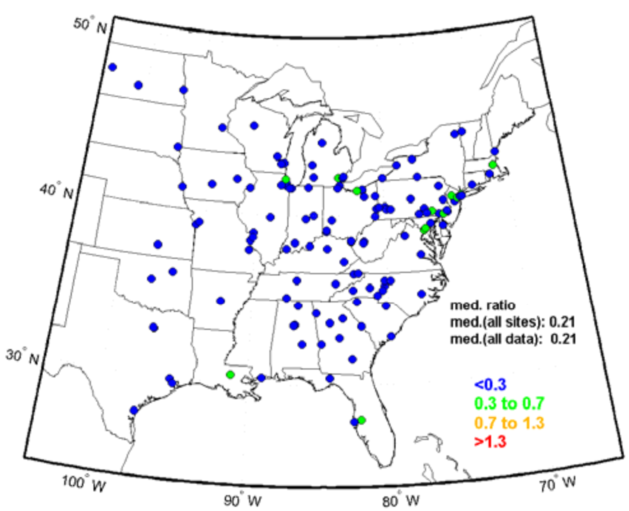
- Some of the Analysis Toolkit Software available via the web site
- MILAGRO test bed data is finished,
- CHAPS, VOCALS, ISDAC/ARCTAS, CARES/CalNex integrated datasets (field campaign + routine monitoring) planned for the future

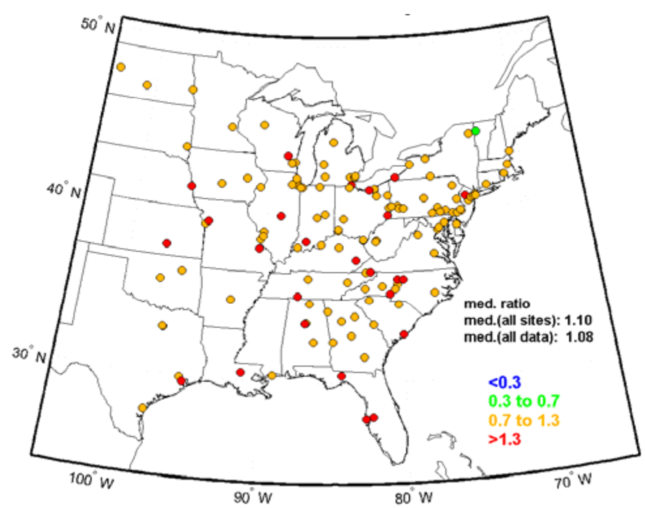
WRF/Chem current and future work – NCAR/ACD

- Add wet scavenging of gases (see talk by Gabi Pfister, Thursday, June 23)
- Improve SOA gas chemistry and add SOA aqueous chemistry (likely to be hooked with MOZCART)
- **Upper Chemical Boundary Conditions**
  Chemical UBC are taken from WACCM climatology for past, present and future (talk by M. Barth et al., Thursday, June 23)
- **Reduced Chemistry**
  Implemented reduced chemical mechanism (Howeling et al., 1998); useful for long climate runs and compatible with CAM-Chem (-> talk by Jerome Fast in Physics Section, Thursday, June 23)
- **Aircraft Tracking Tool**
  Enables output for specified location in model time steps

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

- Simple aqueous chemistry and wet deposition for resolved precipitation as well as convective parameterization (CMAQ module), see also talk by Ravan Ahamadov, WRF-Chem session)
- CO2 emissions module- Includes a high spatiotemporal resolution biospheric flux model –Vegetation and Photosynthesis (uses MODIS reflectances as input)
- SOA: the volatility basis set approach has been coupled with modal aerosol scheme





WRF/Chem current and future work – ESRL + other groups

- CH_4 emissions module
  - Different CH_4 tracers (anthropogenic, biospheric, …)
  - Several CH_4 flux models are implemented: Wetland fluxes (Kaplan, 2002), Soil uptake (Ridgwell et al.,1999), Termite fluxes (Sanderson, 1996)
- Dust parameterization from AFWA (S. Jones and G Creighton) is working and is being evaluated
- Aerosols will be coupled with convective parameterization (G3, collaboratively with S. Freitas)
- Volcanic SO_2 emissions will be added this summer
- Using WPS to run WRF-Chem off global FIM-Chem

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

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

equation for radius size

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

dynamic entrainment

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

bulk microphysics

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

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

Thank you!

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

ESRL