Introduction to WRF-Chem

Georg Grell

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

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

+ Saulo Freitas, Karla Longo (CPTEC, BRAZIL)

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

+ many more national and international collaborators

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

ESRL

WRF-Chem

Community effort

Largest contributing groups: ESRL, PNNL, NCAR

Other significant contributions from: University of Chile, CPTEC Brazil, University of Fairbanks, NASA

WRF-Chem

The help desk:

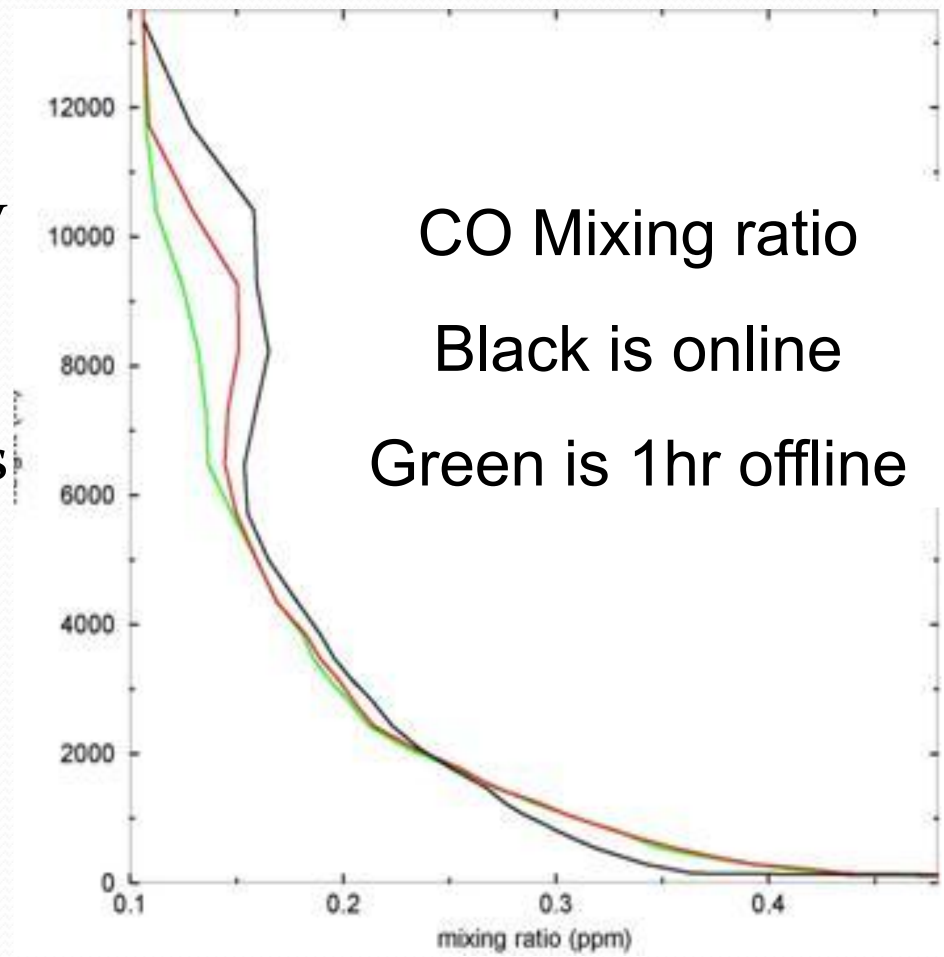
wrfchemhelp.gsd@noaa.gov

WRF-Chem

- 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)
- Very modular approach
  - Chemistry subdirectory has been implemented in version of HIRLAM
  - Is being implemented now into FIM global model (icosahedral in horizontal, vertical adaptive coordinates

Why Online?

- In models, with increasing horizontal resolution, the variability of the vertical velocity becomes much more important
- Offline might introduce a large error in estimate of vertical mass transport
- If dependent on offline, power spectrum analysis should be performed to determine necessary offline frequency



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)
  - RADM2, versions of RACM, MOZART, CBMZ, SAPRC99,...

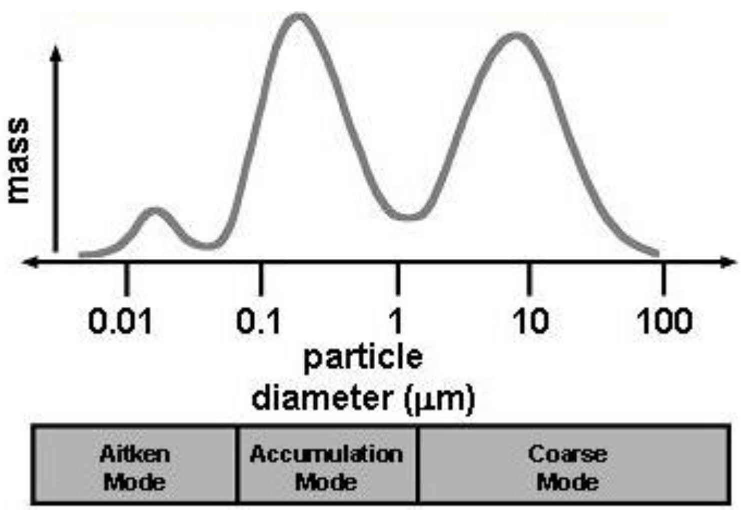
Available Aerosols modules

1. PM advection, transport, emissions and deposition only
2. GOCART
3. Modal approach (MADE/SORGAM)
4. Sectional approach (MOSAIC)

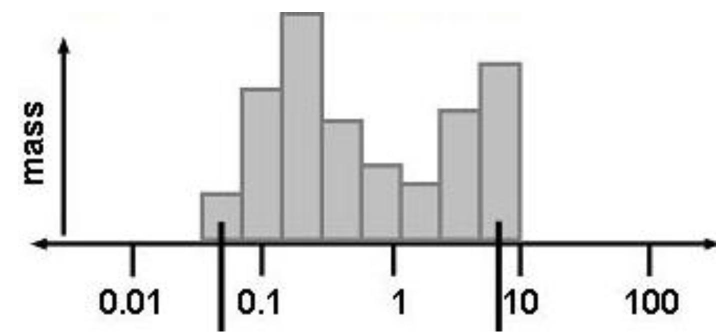
Aerosol modules comparison

(1) Modal

(2) Sectional



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



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

For NWP a bulk scheme is very attractive GOCART (Currently used in real-time FIM-Chem, RR-Chem, and HRRR-Chem

- Much simpler than the sectional and model 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)

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

Selection of radiation parameterizations for aerosol direct effect

For V3.3 all aerosol modules were hooked up to Goddard short wave radiation, and RRTMG short and long wave scheme.

More to come for V3.4

Selection of microphysics parameterizations for aerosol indirect effect

For V3.3

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

Photolysis Packages – all coupled to aerosols and hydrometeors

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

Biogenic emissions

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

Model of ***E***missions of ***G***ases and ***A***erosols from ***N***ature (MEGAN) in WRF-Chem

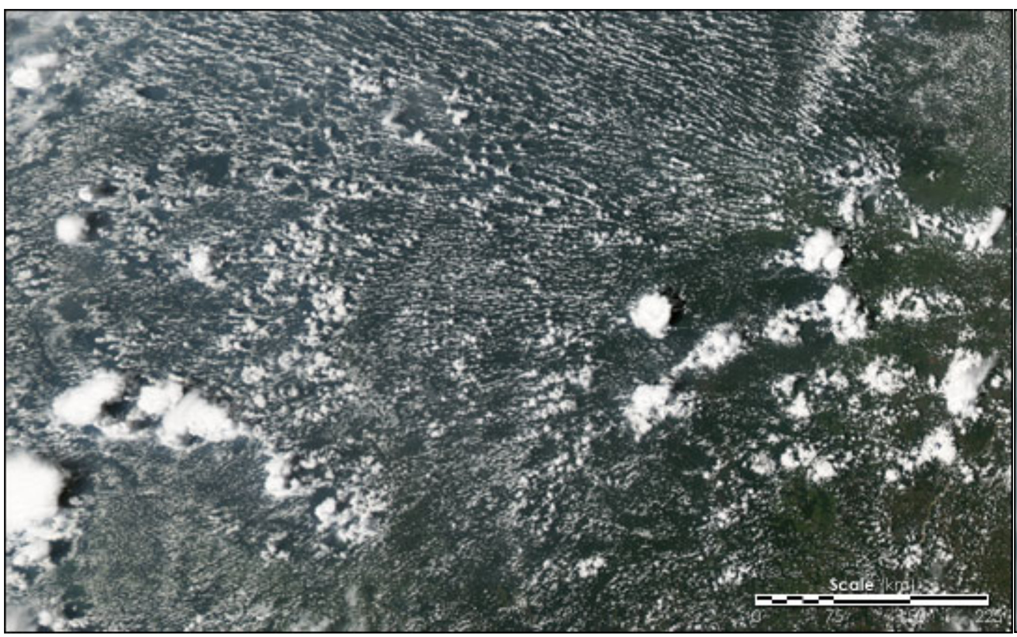
Global, high resolution biogenic emissions

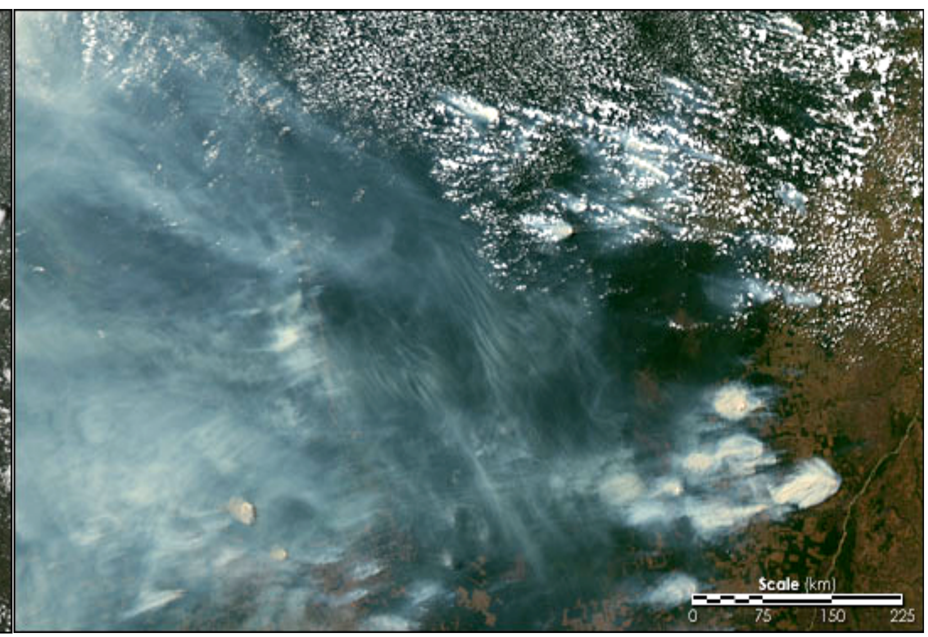
Out of available biogenic emissions modules only BEIS and MEGAN are actively being worked on (developed)

Preprocessor for MEGAN exists and can be downloaded from NCAR

Fire Plumerise - Collaboration with Saulo Freitas from CPTEC in Brazil

1-D Cloud model

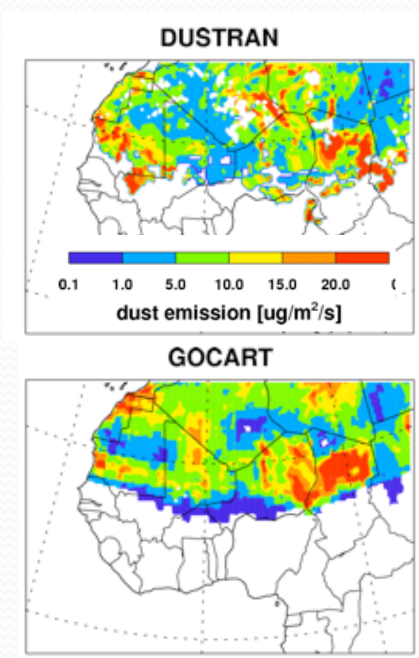




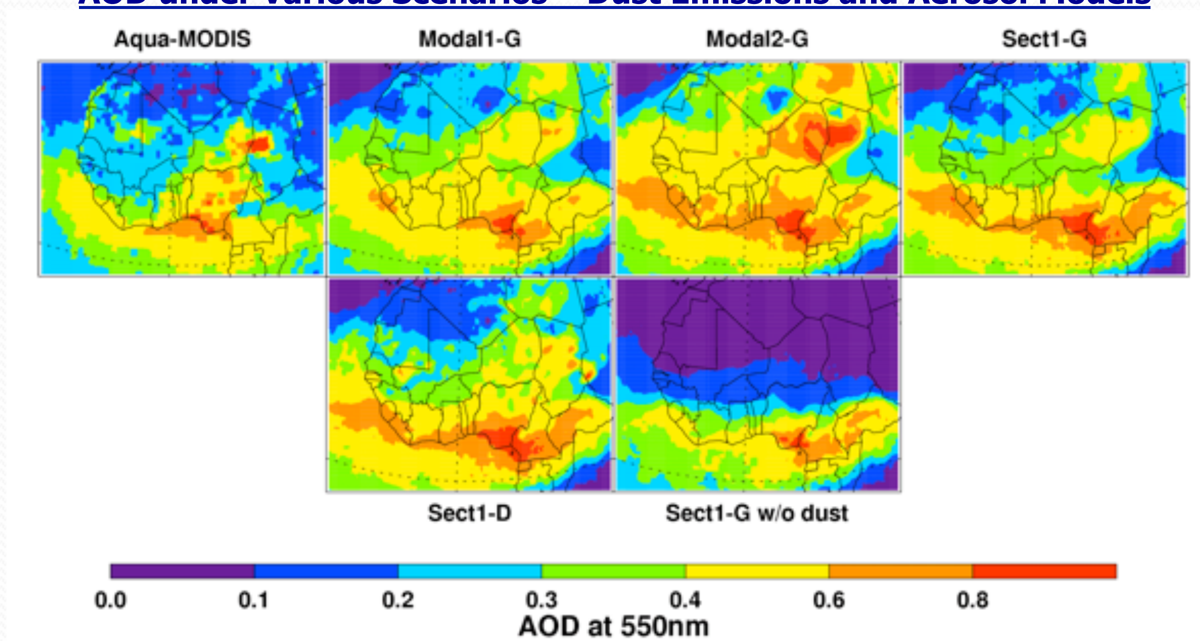
New in V3.3: Coupling of Aerosols to RRTMG Radiation (implemented by PNNL)

- Extended modular optical property module to compute information needed for both shortwave and longwave RRTMG radiation scheme
- Works for all aerosol modules
- 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



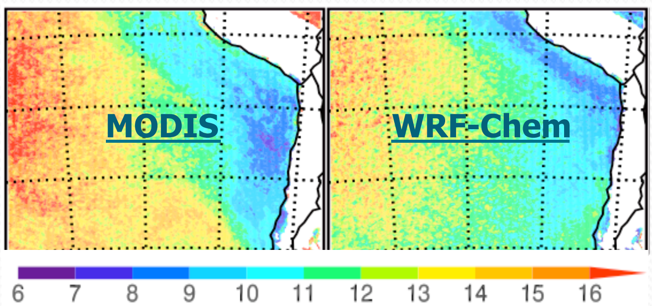
AOD under Various Scenarios – Dust Emissions and Aerosol Models



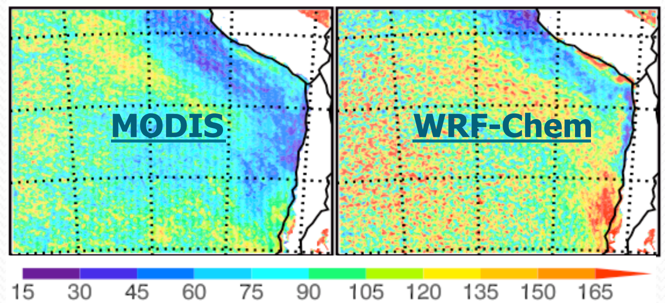
Aerosol-Cloud Aerosol Interactions: What's new in V3.3

- Morrison microphysics scheme now coupled with either prescribed aerosols or predicted aerosols from both MADE/SORGAM or MOSAIC (PNNL + Hugh Morrison(NCAR))
- Using same treatment for aerosol activation as implemented previously with Lin microphysics scheme, as described in *Chapman et al., ACP, 2009*
- Current applications (publications in progress):
  - Effect of aerosols on marine stratocumulus during VOCALS-Rex

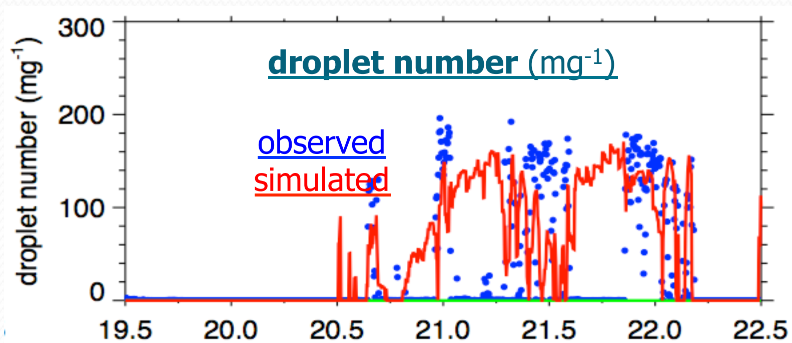
Effective radius

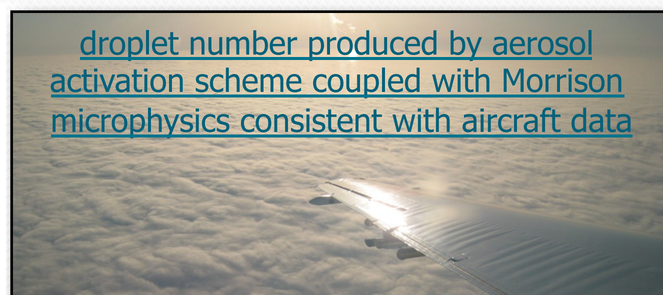


Liquid Water Path



- **Effect of aerosols on mixed phase clouds during ISDAC / ARCTAS**





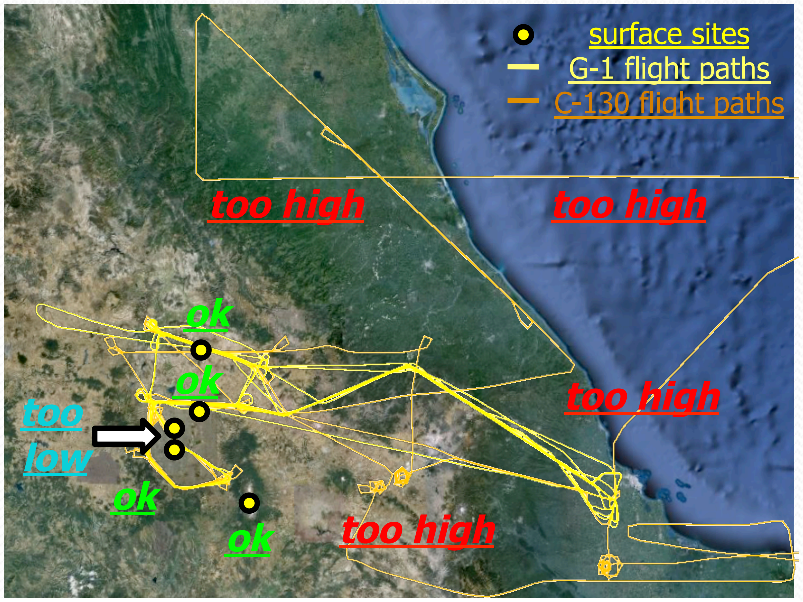
Secondary Organic Aerosols: New in V3.3

Added 'volatility basis set' approach to MOSAIC (PNNL)

- Based on *Robinson et al. (2007)* and *Shrivastava et al. (2008)*
- Coupled with SAPRC99 photochemistry – which has also been added as a separate stand alone package, in collaboration with Pablo Saide (Univ. Iowa)
- Release version uses 2 volatility bins for simplicity and 4 size bins, 8 volatility bins approach available on request (computationally expensive)
- Oxygen and carbon species treated separately to compute O:C ratios
- Anthropogenic, biomass burning, and biogenic sources of organics tracked

Like all SOA parameterizations, it should be treated with caution

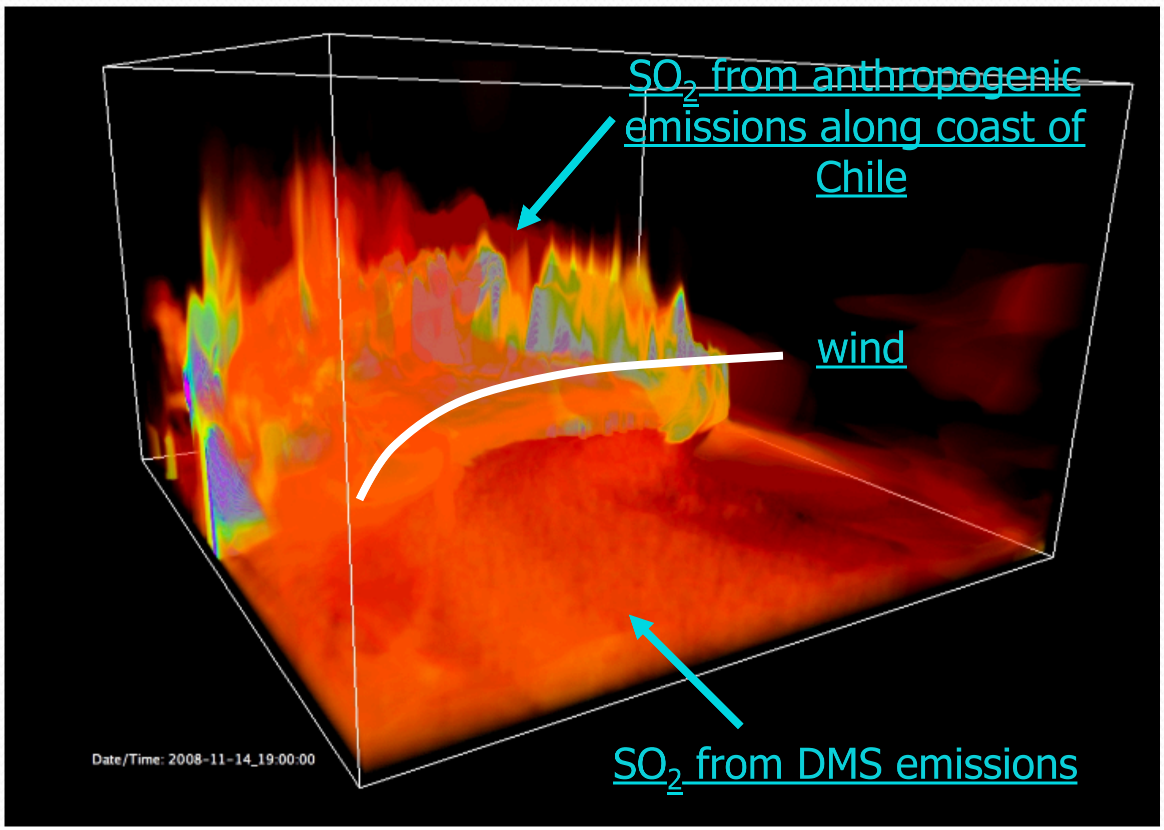
- Predictions not perfect, but better than simulating non-volatile POA only
- Evaluated against surface and aircraft data collected during MILAGRO field campaign – see *Shrivastava et al., ACPD, 2010* and *Fast et al. ACP 2009* for more details
- Optical properties for SOA treated the same as POA – for now
- Aerosol-cloud interactions not treated for SOA presently



DMS and Sea-Salt Emissions

- DMS chemistry now included in MOSAIC
- Fixed bugs with DMS rate constants for MOSAIC and bugs for GOCART DMS emissions
- Fixed minor bug in sea-salt emissions in smallest size bins of MOSAIC

SO_2 over the Southeastern Pacific Ocean during VOCALS-Rex, looking Southeast



Volcanic ash in WRF-Chem V3.3

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

Publications in progress

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)

ASH Volcanoes Prediction

Based on Mastin et al. (2009) dataset

1. 1535 volcanoes with lat, lon, elevation, eruption classification (ESP)
2. Table describing injection height, duration, eruption rate, volume and mass fraction (<63um)

ESP	Type	Example	H km above vent	Duration hr	Eruption rate (kg/s)	Volume (km3)	mass fraction less than 63 micron
M0	Standard mafic	Cerro Negro, Nicaragua, 4/13/1992	7	60	1,E+05	0,01	0,05
M1	small mafic	Etna, Italy, 7/19-24/2001	2	100	5,E+03	0,001	0,02
M2	medium mafic	Cerro Negro, Nicaragua, 4/9-13/1992	7	60	1,E+05	0,01	0,05
M3	large mafic	Fuego, Guatemala, 10/14/1974	10	5	1,E+06	0,17	0,1
S0	standard silicic	Spurr, USA, 8/18/1992	11	3	4,E+06	0,015	0,4
S1	small silicic	Ruapehu, New Zealand, 6/17/1996	5	12	2,E+05	0,003	0,1
S2	medium silicic	Spurr, USA, 8/18/1992	11	3	4,E+06	0,015	0,4
S3	large silicic	St. Helens, USA, 5/18/1980	15	8	1,E+07	0,15	0,5
S8	co-ignimbrite silicic	St. Helens, USA, 5/18/1980 (pre-9 AM)	25	0,5	1,E+08	0,05	0,5
S9	Brief silicic	Soufrière Hills, Montserrat (composite)	10	0,01	3,E+06	0,0003	0,6
U0	default submarine	none	0	--	--	--	

Vertical source distribution and particle size bin

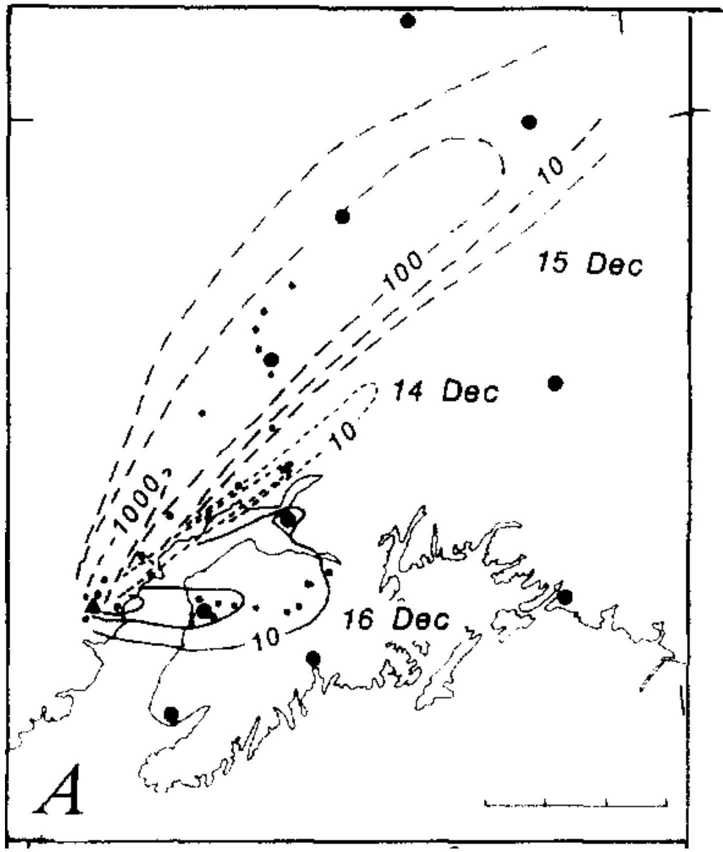
Particle Size Bin	Phi	Percentage of mass
1 – 2mm	-1 – 0	2
0.5 – 1 mm	0 – 1	4
0.25 – 0.5 mm	1 – 2	11
125 – 250 μm	2 – 3	9
62.5 – 125 μm	3 – 4	9
31.25 – 62.5 μm	4 – 5	13
15.625 – 31.25 μm	5 – 6	16
7.8125 – 15.625 μm	6 – 7	16
3.9065 – 7.8125 μm	7 – 8	10
< 3.9 μm	> 8	10

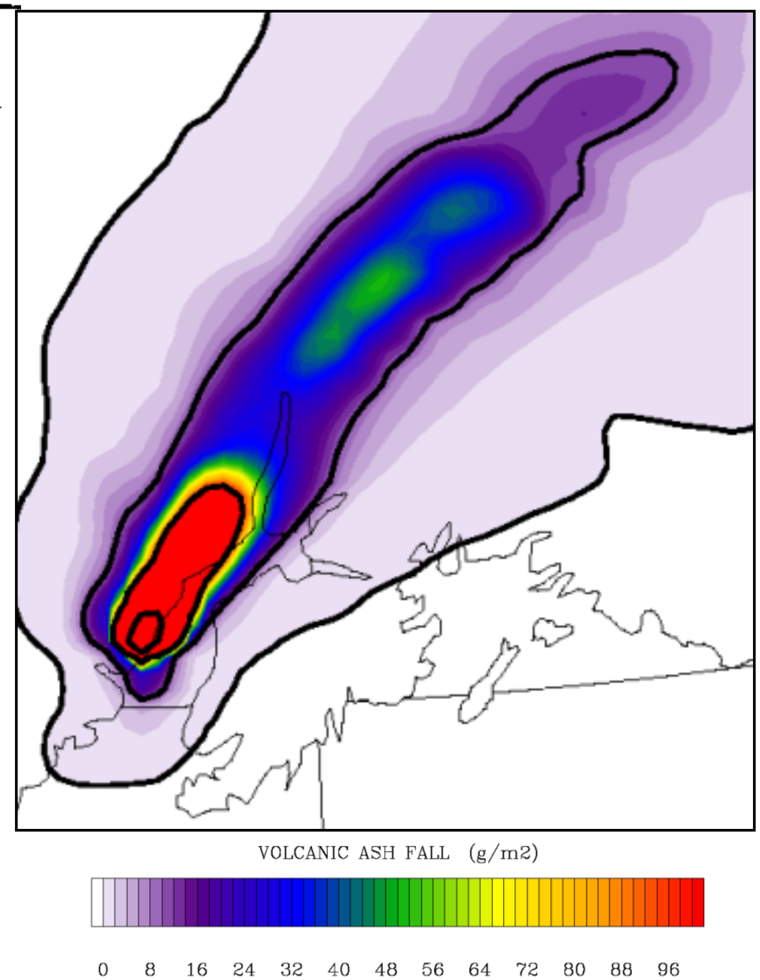
10 size bins for prediction of ash-fall and transport of volcanic ash

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

Percentage of mass will change in V3.4, emissions of SO2 will also be added depending on type of Volcano

Tephra-fall deposits (g/m^2)
Redoubt Volcano, south-central Alaska
December 15, 1989





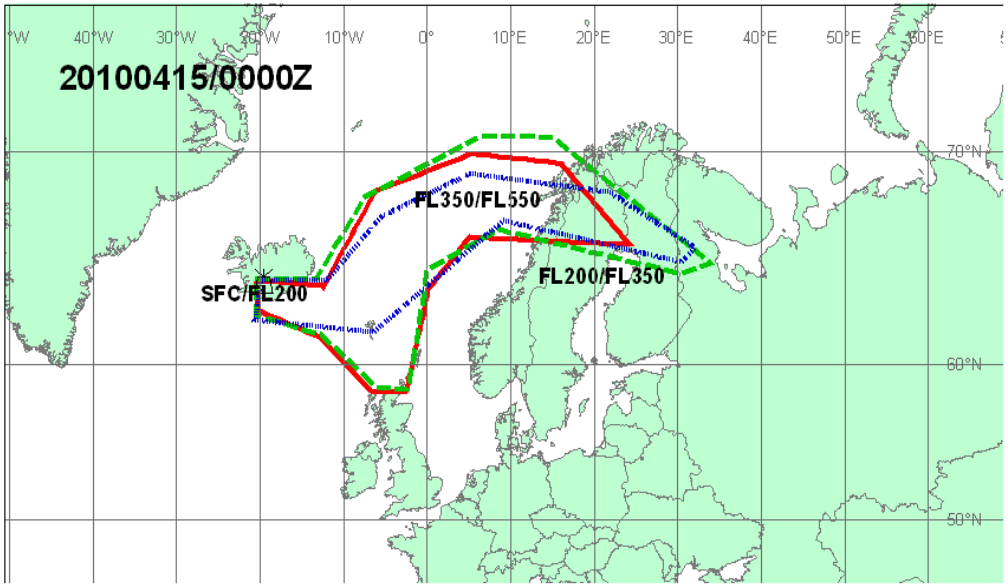
<u>Observed</u>

<u>Predicted by WRF-Chem</u>

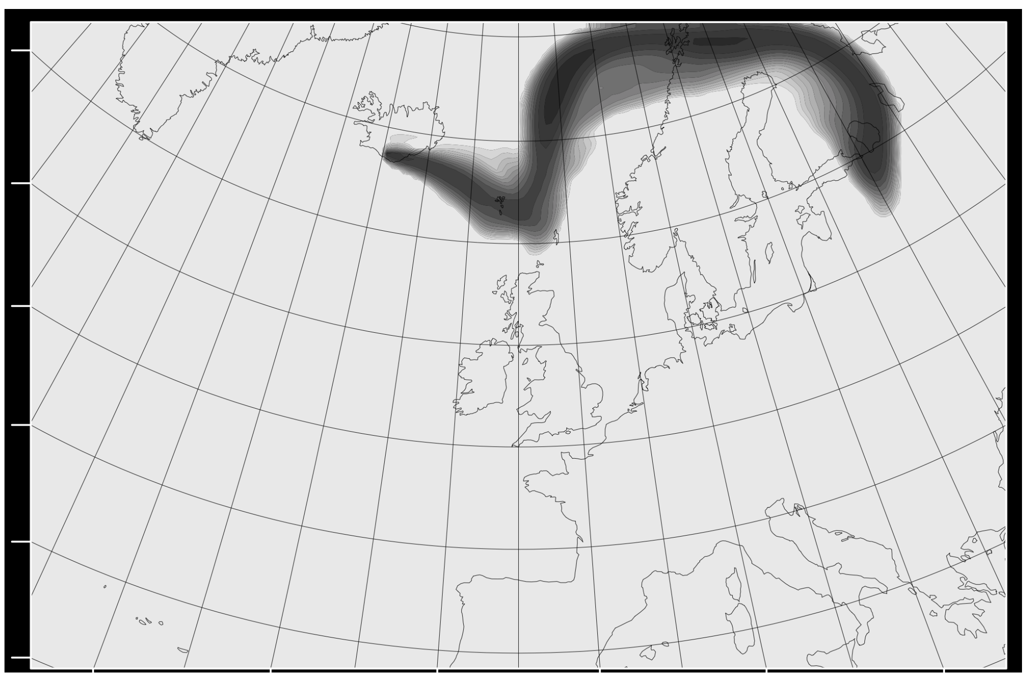
First WRF-Chem runs for “Big E”

- 30km horizontal resolution
- 10 ash bins
- Ash settling, dry deposition, and wet deposition included
- Aerosol optical properties easily implemented for ash

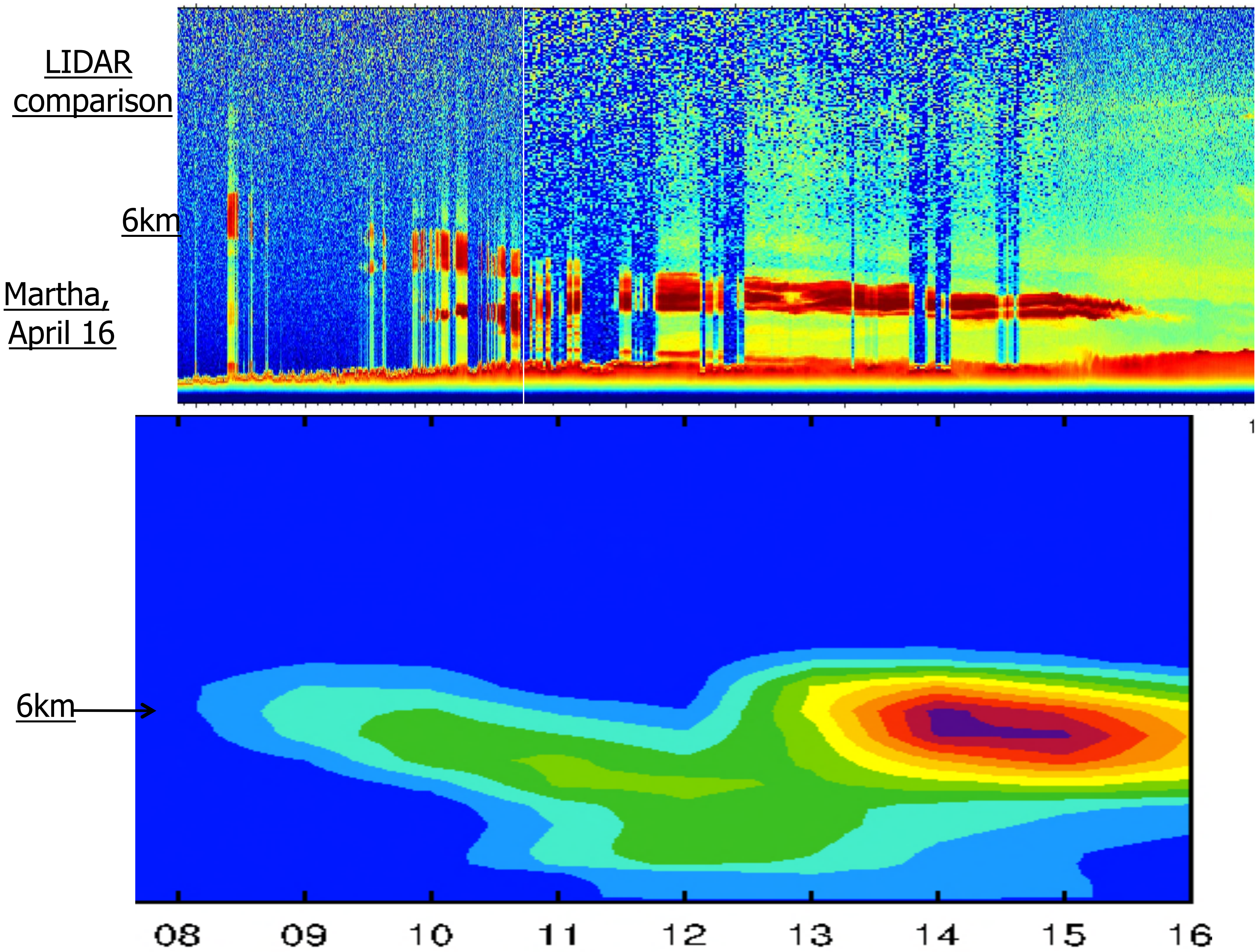
Comparison of ash forecasts (London VAAC and WRF-Chem) at 0000Z, April 15



VA advisory from London



WRF-Chem


LIDAR
comparison
6km
Martha,
April 16
6km
08
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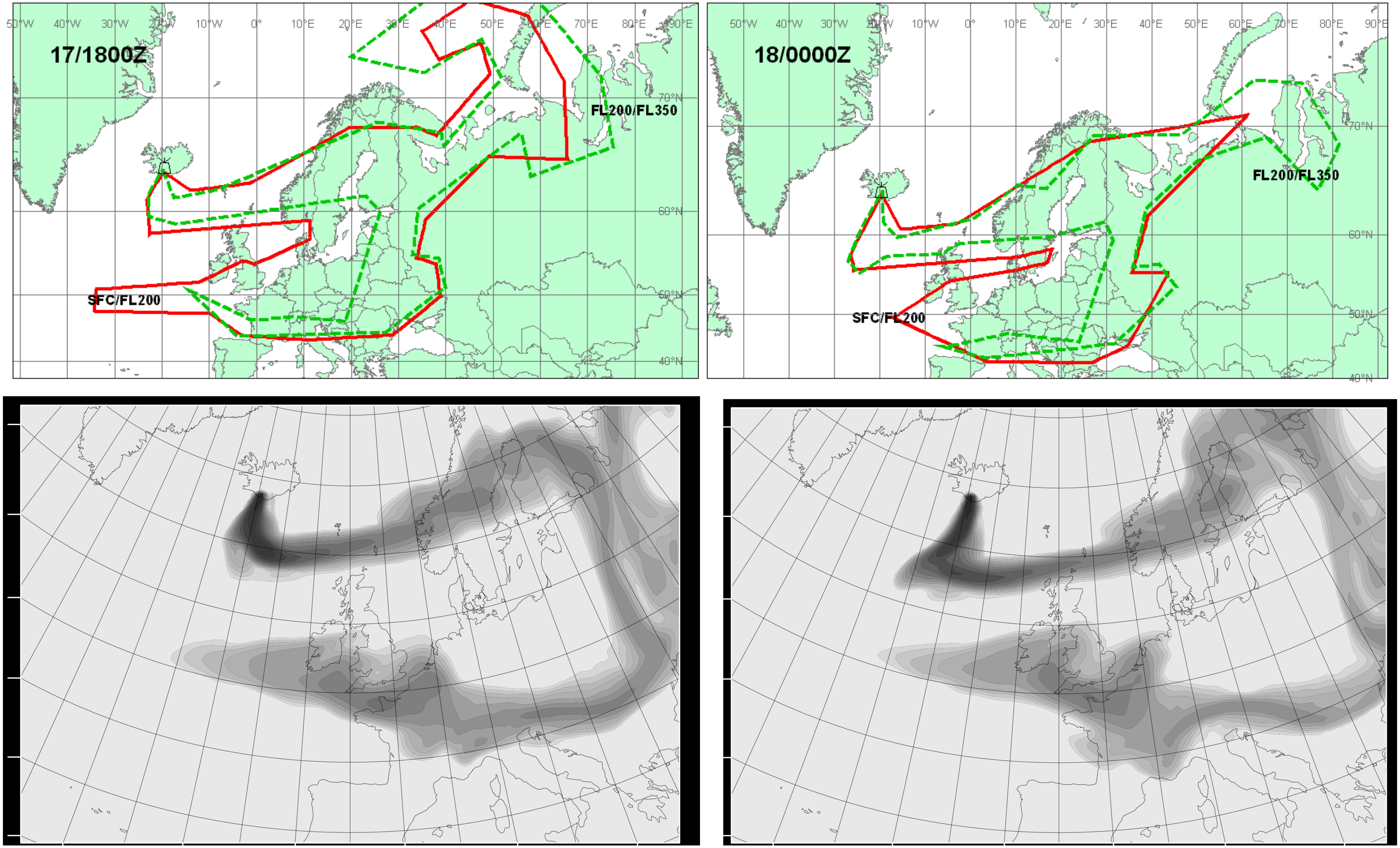
Comparison of ash forecasts (London VAAC and WRF-Chem) at1800Z, April 17 and 0000Z, April 18



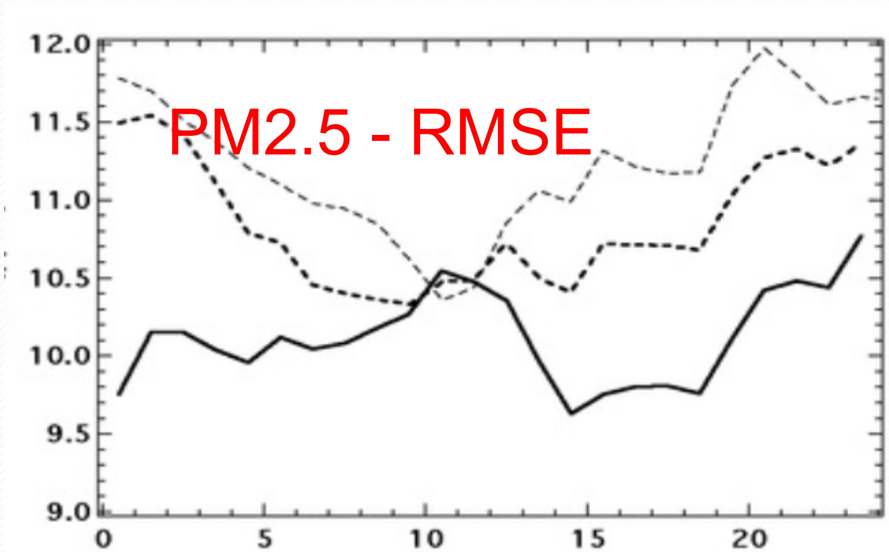
How is the meteorological forecast affected by aerosol?

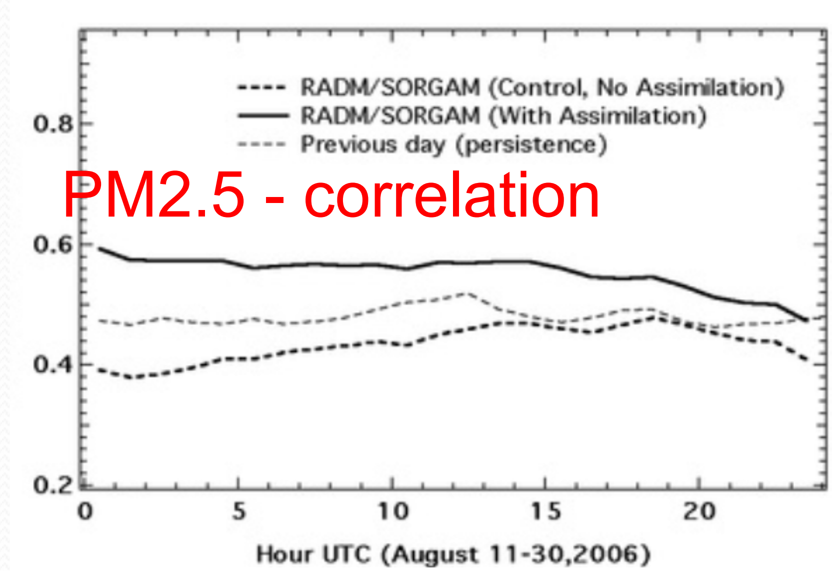
- In general large importance for climate simulations is recognized (when integrating models over 100's of years, small differences in the earth's energy budget are extremely important)
- Weather forecasting for only a few days?
  - Much research needed, but direct effect may positively influence forecasts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

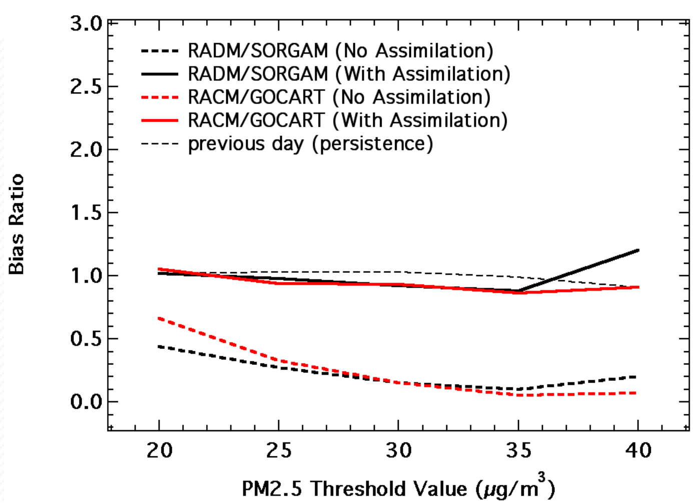
Chemical data assimilation: WRF-Chem and PM2.5

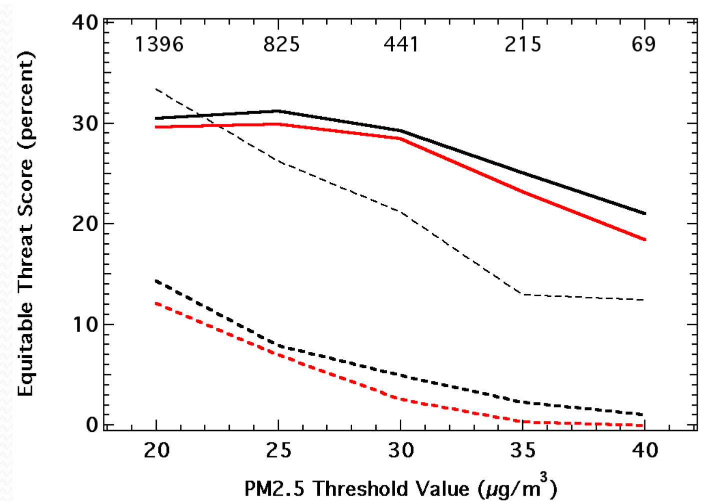
2 months worth of WRF-Chem runs:

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









Chemical data assimilation: ARW-WRF/Chem and PM2.5

Much work in progress at ESRL (EnKF) as well as at NCAR (AOD assimilation with GSI), not released to community yet

If you need chemical data assimilation, contacts: wrfchemhelp desk will tell you who and when

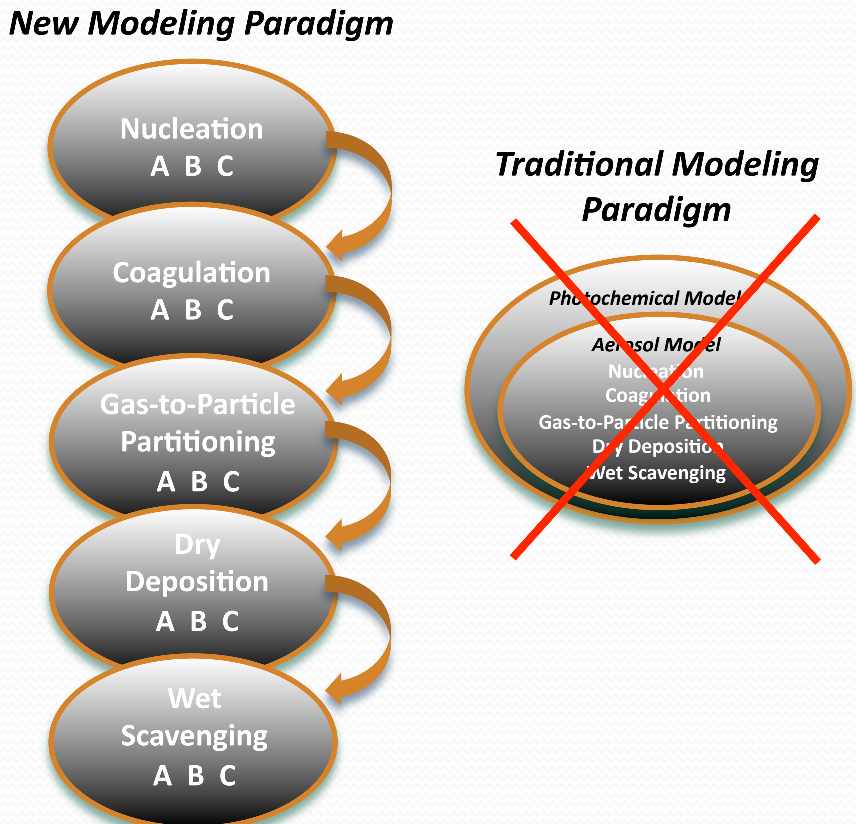
Resources

- WRF project home page
  - http://www.wrf-model.org
- WRF users page (linked from above)
  - http://www.mmm.ucar.edu/wrf/users
- On line documentation (also from above)
  - http://www.mmm.ucar.edu/wrf/WG2/software_v2
- WRF users help desk
  - wrfhelp@ucar.edu
- WRF-Chem users help desk
  - wrfchemhelp.gsd@noaa.gov

PNNL Aerosol Modeling Testbed (Fast et al. 2011 in BAMS)

Create a computational framework, the **Aerosol Modeling Testbed**, that streamlines the process of testing and evaluating aerosol process modules over a range of spatial / temporal scales

- **Systematically and objectively** evaluate aerosol process modules
- Provide **tools** that facilitate science by minimizing redundant tasks
- **Document** performance and computational expense
- Better **quantify uncertainties** by targeting specific processes
- Build an **internationally-recognized capability** that fosters collaboration



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