Introduction to WRF-Chem

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

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+ 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

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

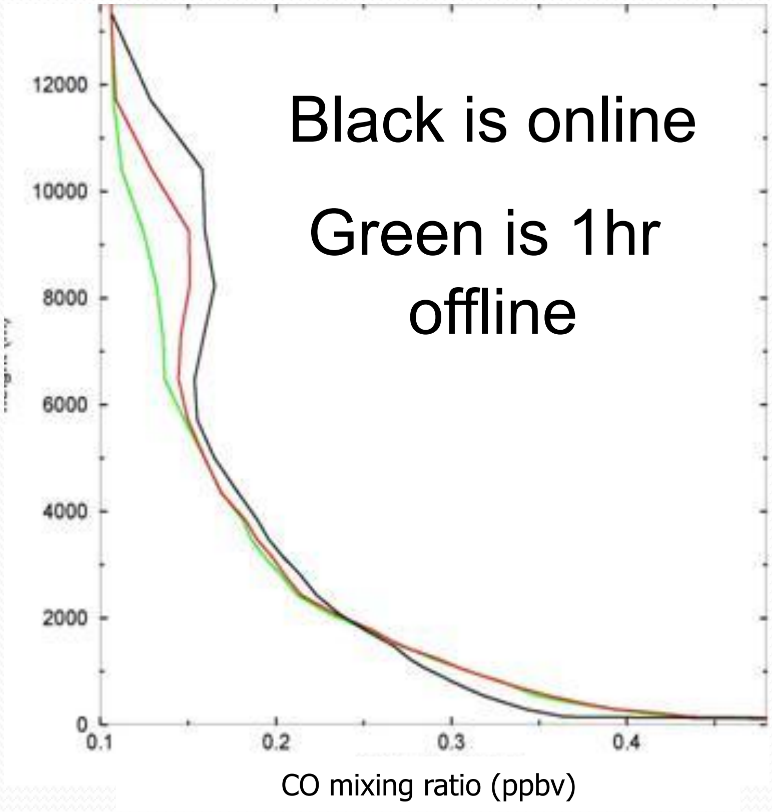
There are almost 50 chem_options for the main gas phase chemistry and aerosol modules!

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)
- 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
- Power spectrum analysis can show the amount of information that is lost in offline runs
- In models, with increasing horizontal resolution, the variability of the vertical velocity becomes much more important, especially with less and less (or no) activity from convective parameterization
- 2-way feedback in-between chemistry and meteorology



Grell and Baklanov, 2011, AE

Gas Phase Chemistry Packages

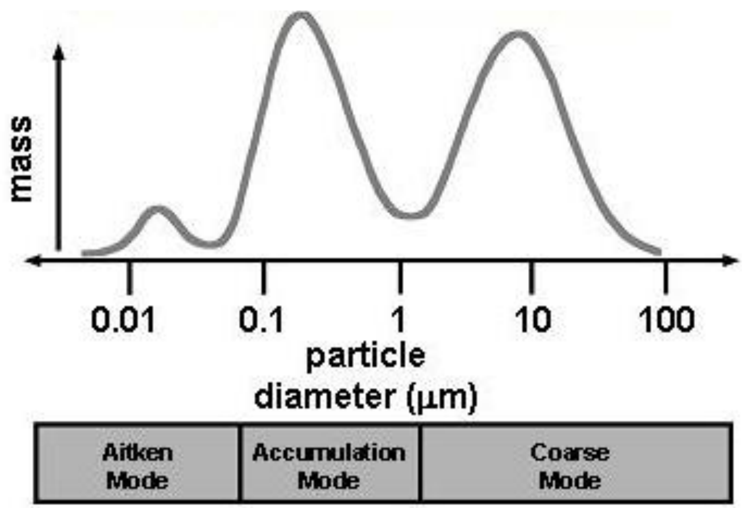
- Hard coded: chemical mechanism from RADM2
- Hard coded: Carbon Bond (CBM-Z) based chemical mechanism
- ***K***inetic ***P***re***P***rocessor (KPP) – Many different equations files exist. KPP will generate the modules from equation files. These generated modules will then be used by WRF-Chem

Photolysis Packages – all coupled to aerosols and hydrometeors

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

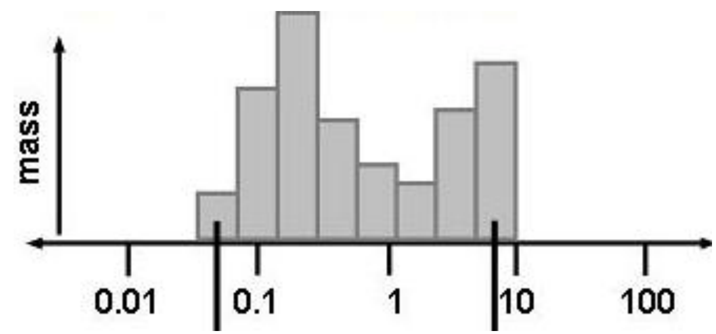
Available aerosol modules

(1) Modal



<u>composition</u>
sulfate
nitrate
ammonium
chloride
carbonate
sodium
calcium
other inorganics
organic carbon
elemental carbon

(2)



(3) Bulk: 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, 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)
- 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

Selection of radiation parameterizations for aerosol "direct effect"

For V3.4 all aerosol modules were hooked up to Goddard short wave radiation, and RRTMG short and long wave scheme.

More to come for V3.5

Selection of microphysics parameterizations for aerosol "indirect effect"

For V3.4

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

More to come for V3.5

"indirect effect" is a result of the interaction aerosols/microphysics

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) in WRF-Chem

Global, high resolution biogenic emissions

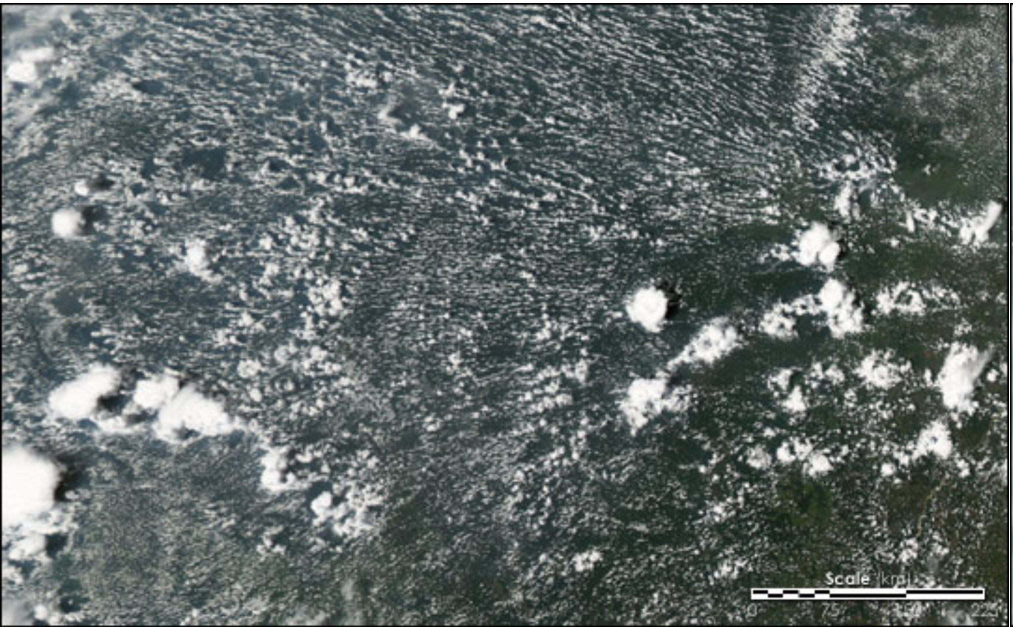
Out of available biogenic emissions modules only BEIS and MEGAN are actively being worked on (developed)

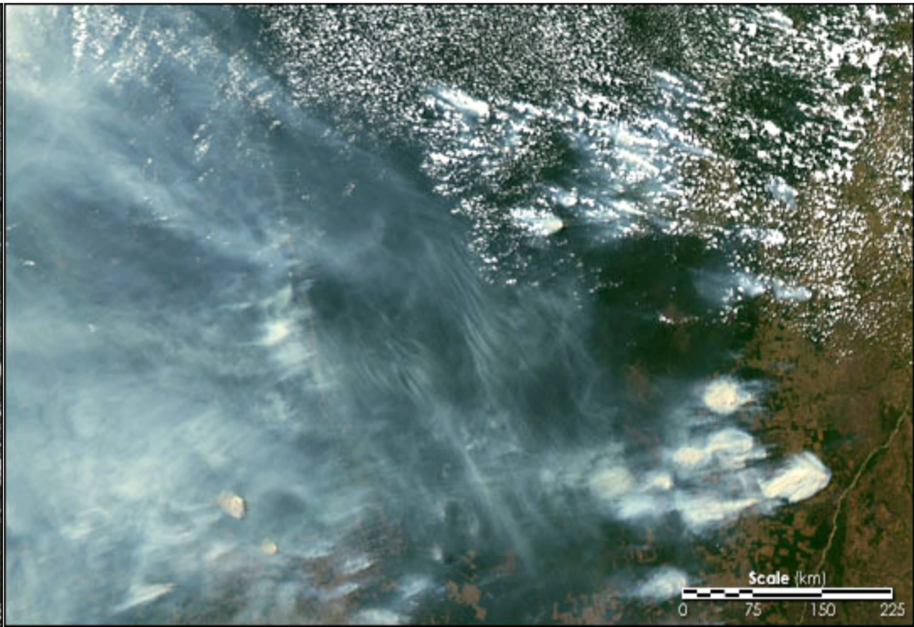
Preprocessor for MEGAN exists and can be downloaded from NCAR

Fire Plumerise

1-D Cloud model used in WRF-Chem to determine injection height

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





Volcanic ash in WRF-Chem V3.4

- Options for transport only (4 bins), transport + ash-fall (10bins +so2) – aerosol direct effect may be included
- Coupled with chemistry/aerosol modules (only using up to three bins – depending on size), interaction with meteorology included for these options

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	--	--	--	

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

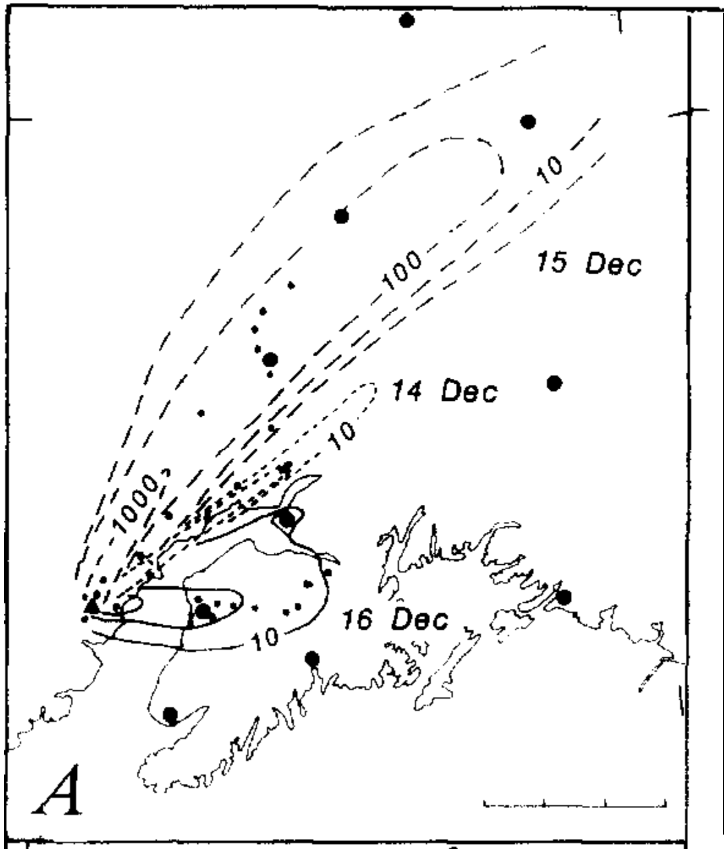
Particle Size Bin	Phi	Percentage of mass
1 – 2mm	-1 – 0	2
0.5 – 1 mm	0 – 1	4
0.25 – 0.5 mm	1 – 2	11
125 – 250 µm	2 – 3	9
62.5 – 125 µm	3 – 4	9
31.25 – 62.5 µm	4 – 5	13
15.625 – 31.25 µm	5 – 6	16
7.8125 – 15.625 µm	6 – 7	16
3.9065 – 7.8125 µm	7 – 8	10
< 3.9 µm	> 8	10

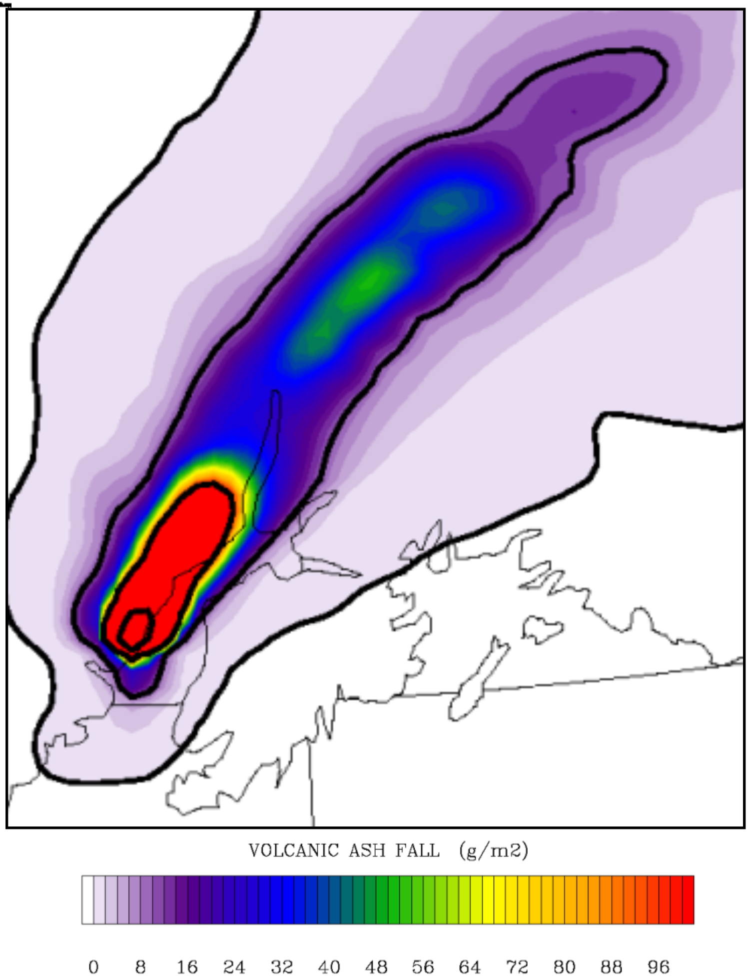
4 size bins for prediction if transport only is of interest

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

3 size bins for coupling with other aerosol modules

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





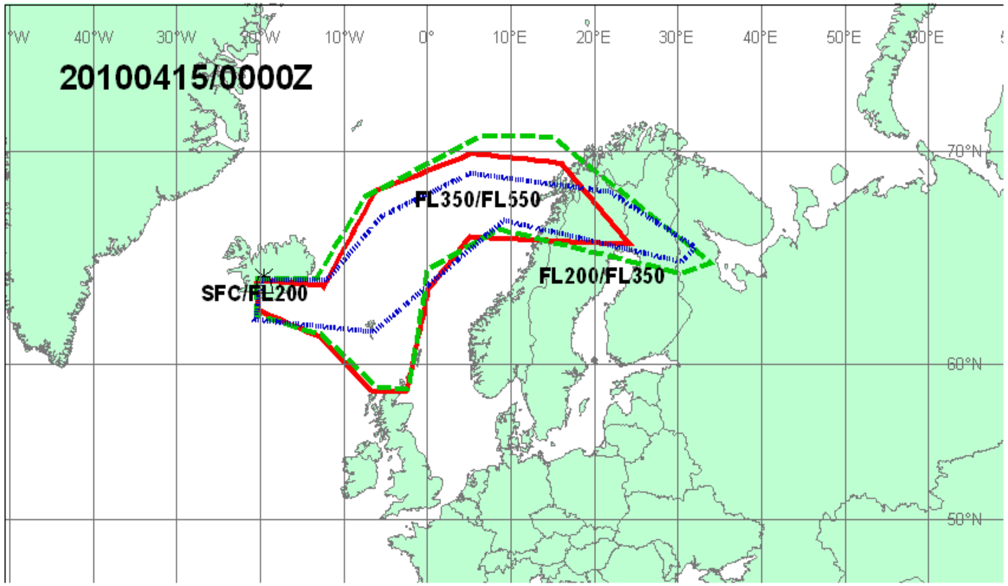
Observed

Predicted by WRF-Chem

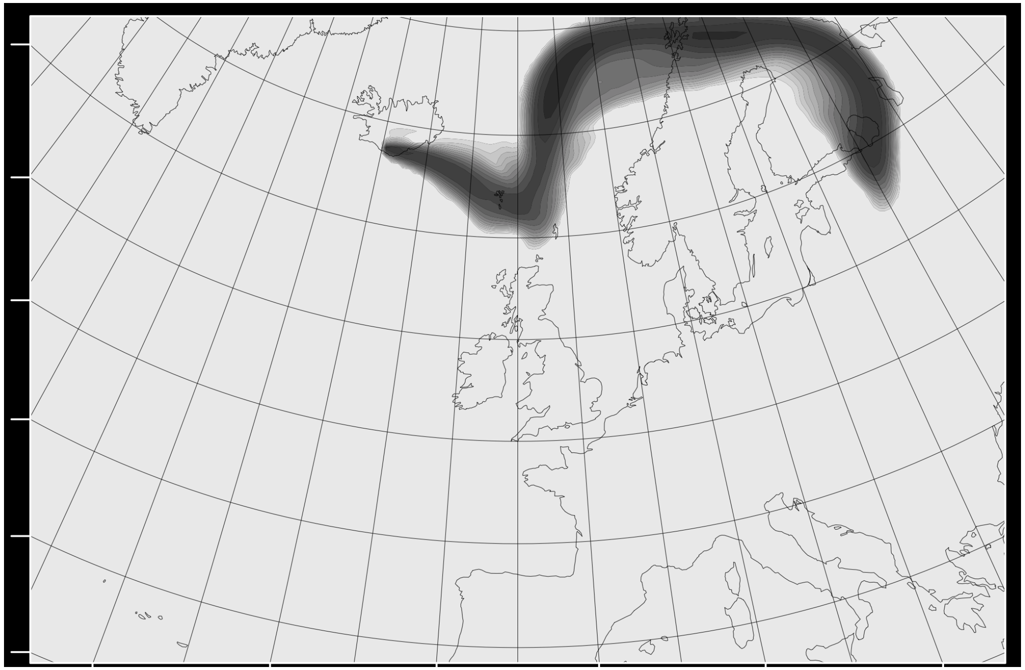
First WRF-Chem runs for “Big E”

- 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

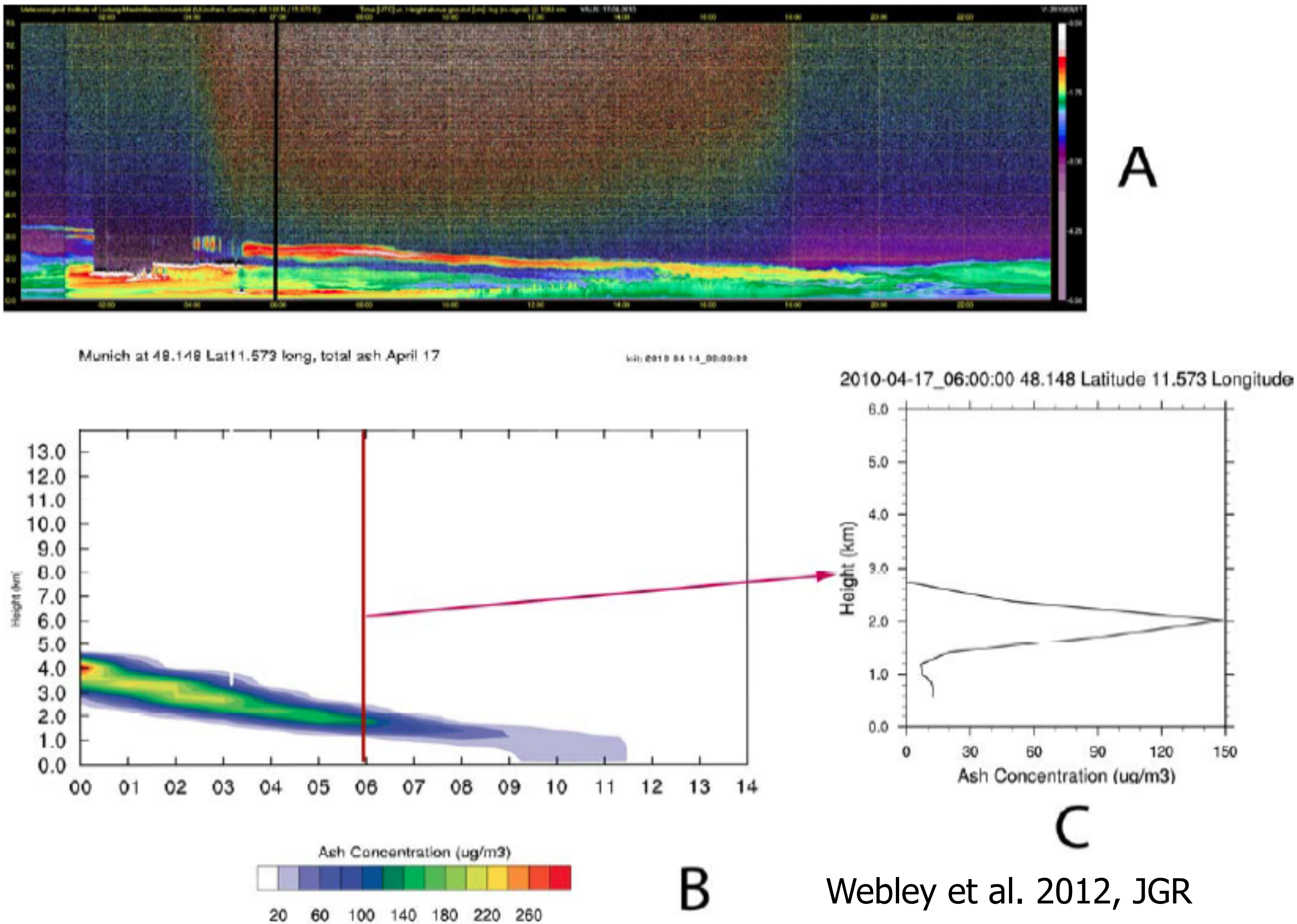


VA advisory from London



WRF-Chem

Forecast compared to Munich Lidar, April 17, 06Z



Webley et al. 2012, JGR

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

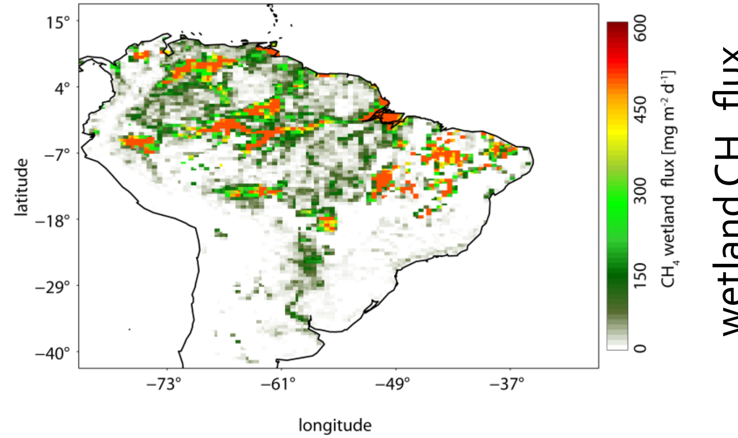
- **Online calculation of biospheric CH_4 fluxes**
  wetland – Kaplan (2002)
  termite – Sanderson (1996)
  soil uptake – Ridgwell et al. (1999)

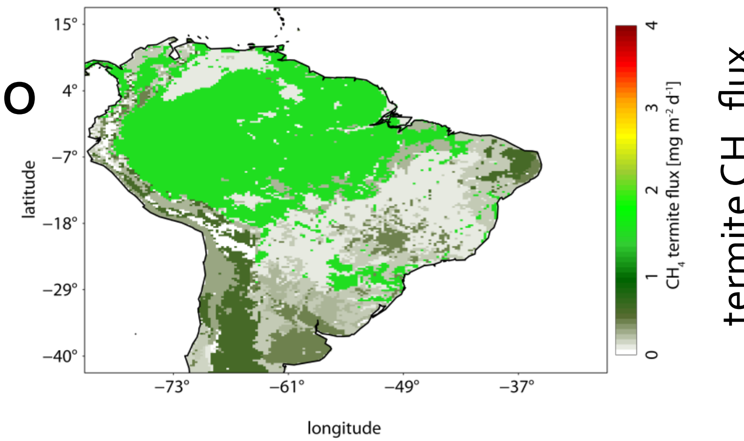
- **Passive tracer simulations for CO_2, CH_4, and CO**
  (including all options of CO_2 tracer package, chem_opt=16)

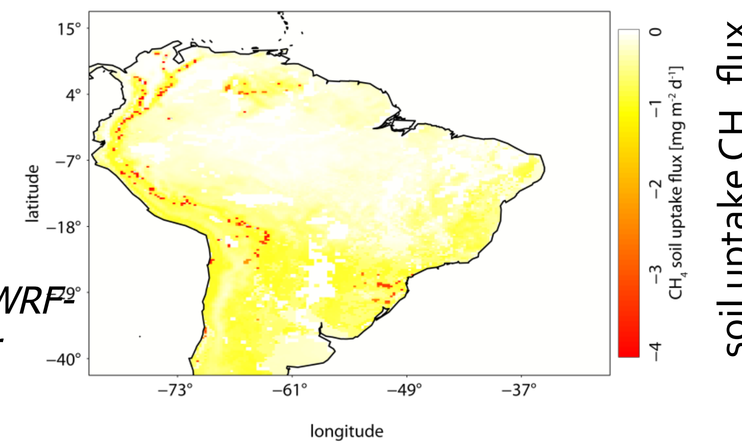
- **Tuning of wetland fluxes** through namelist options wpeat and wflood possible

- **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



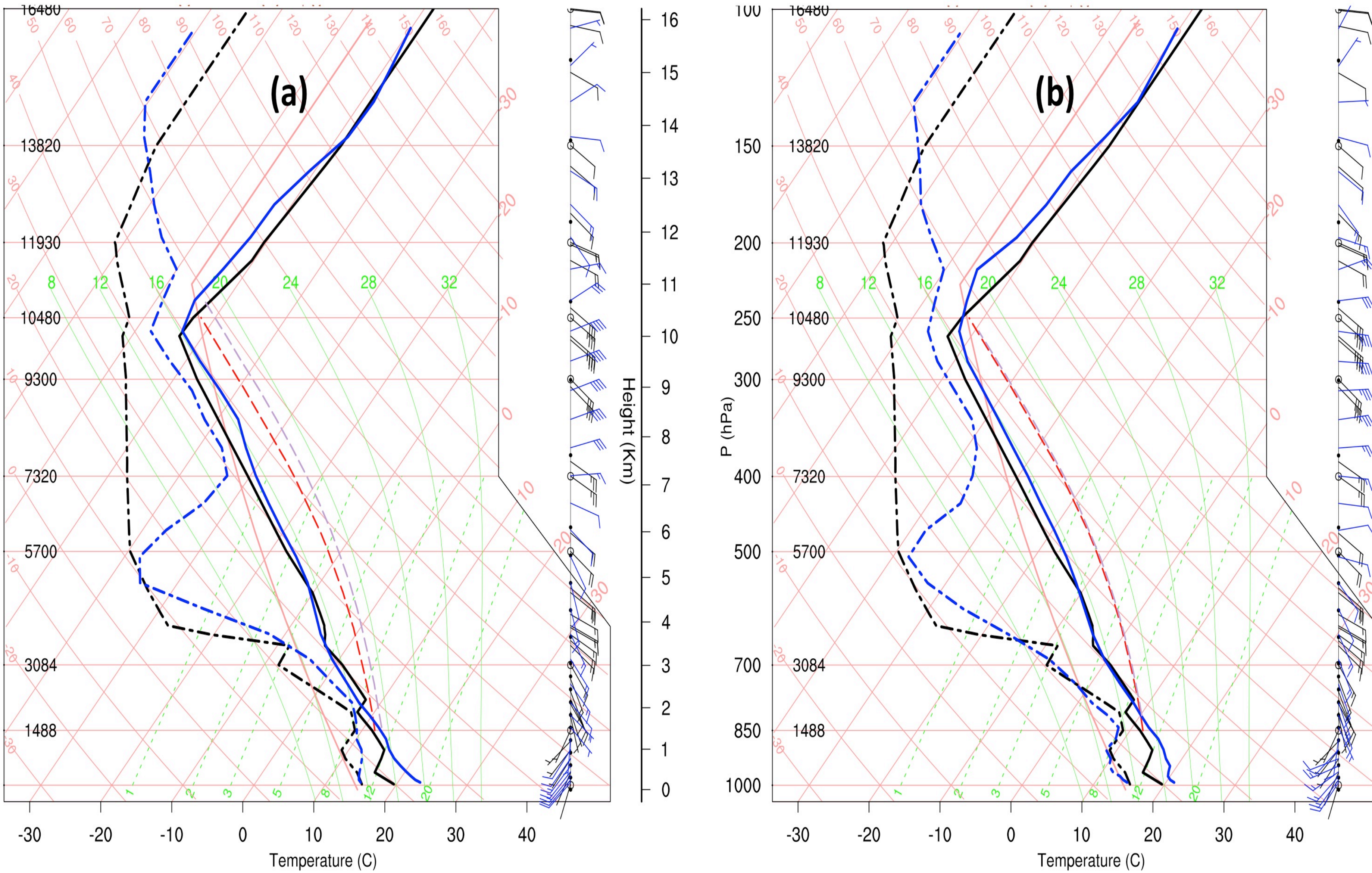




How is the meteorological forecast affected by aerosol?

- 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 chemistry may positively influence forecasts when strong signals exist
  - Influence on meteorological data assimilation

No fires **24-hr forecast** **With fires**

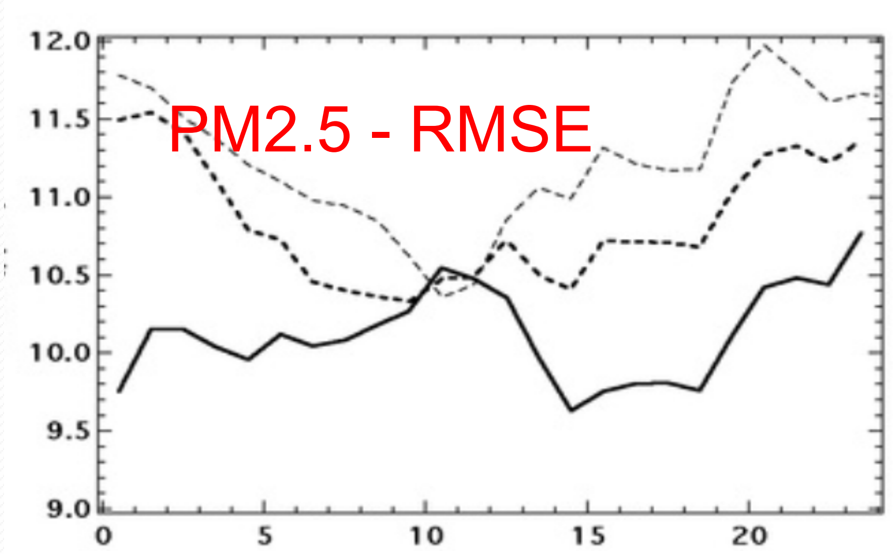


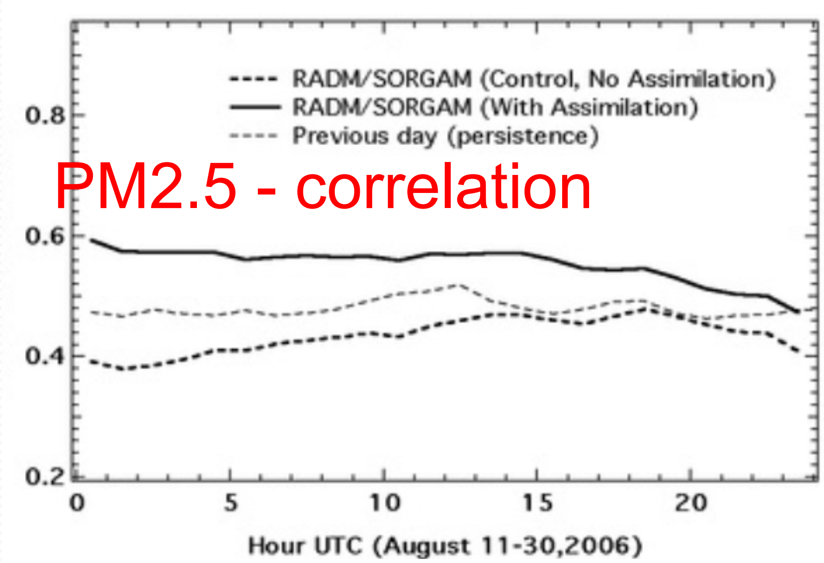
Observed (black) and predicted (blue) sounding for Fairbanks, Alaska, on July 4, 0000UTC.

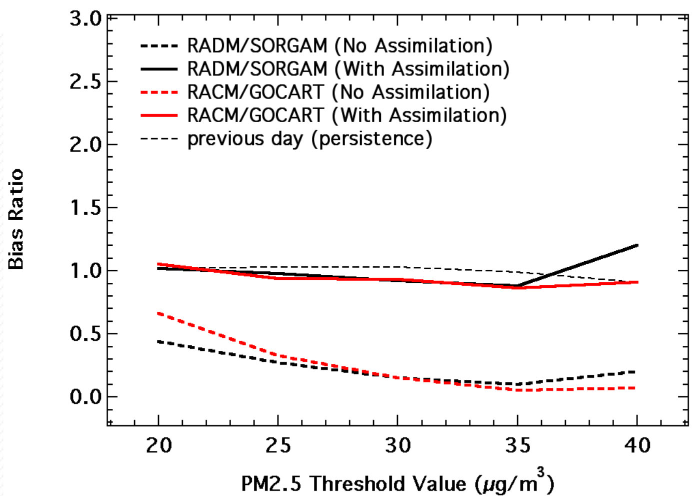
Chemical data assimilation: WRF-Chem and Grid Point Statistical Interpolation package (GSI)

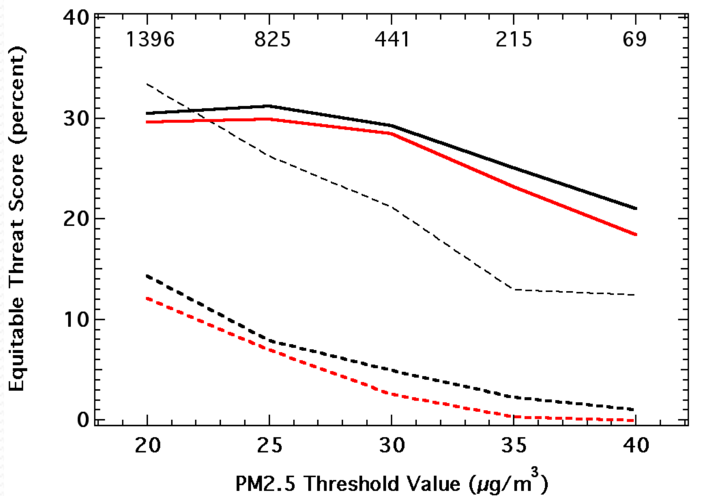
2 months worth of WRF-Chem runs:

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









Chemical data assimilation: ARW-WRF/Chem

Much work in progress

- at ESRL (EnKF)
- at NCAR (AOD assimilation with GSI)
- EnKF as well as 4DVAR at Universities in collaboration with NCAR (WRFPLUS, and WRFDART groups), and ESRL

These approaches are not released to community yet

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

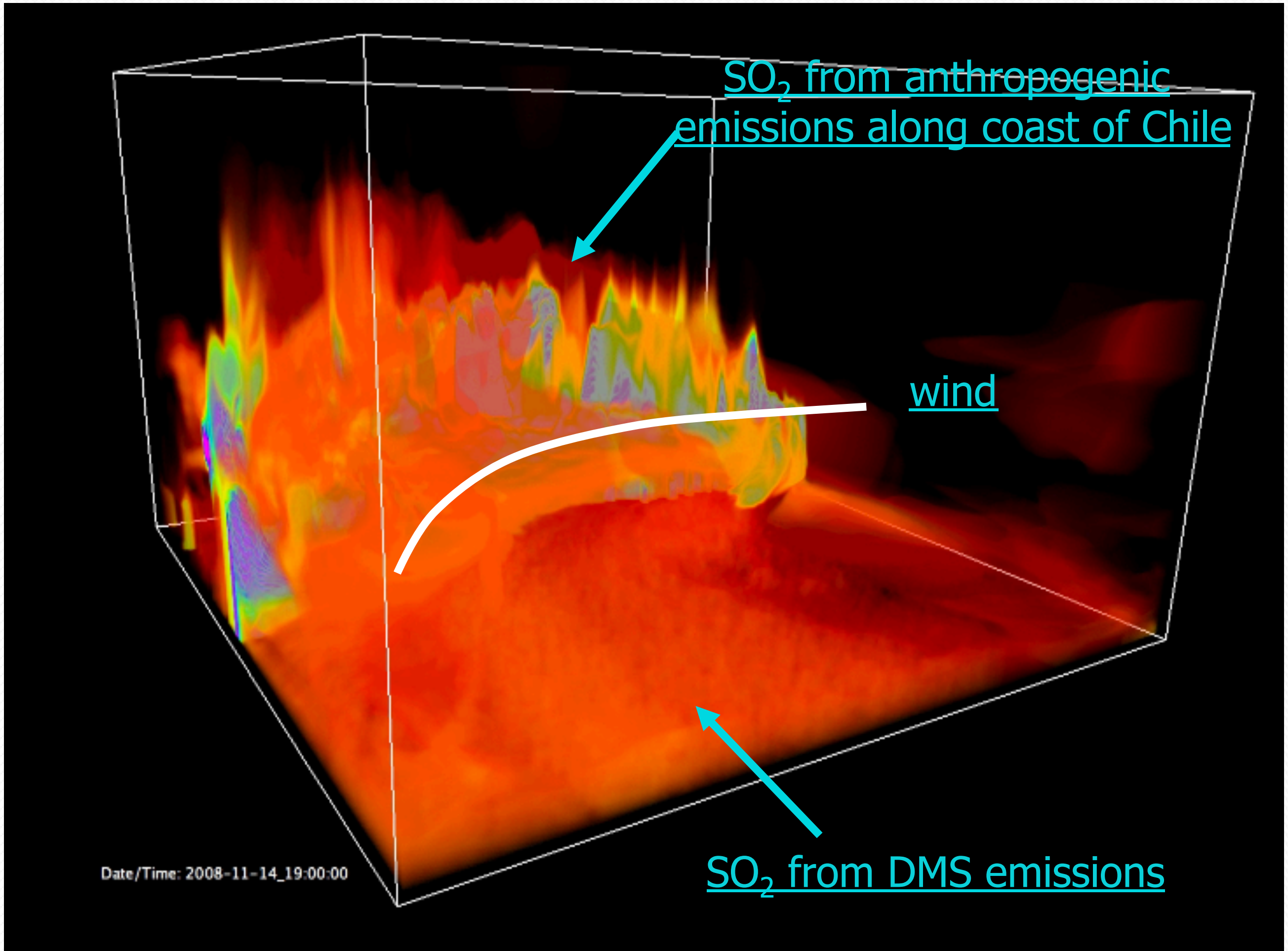
Resources

- 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

DMS and Sea-Salt Emissions

- DMS chemistry now included in GOCART and MOSAIC

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



GEOPHYSICAL RESEARCH LETTERS, VOL. 34, L13801, doi:10.1029/2007GL029979, 2007

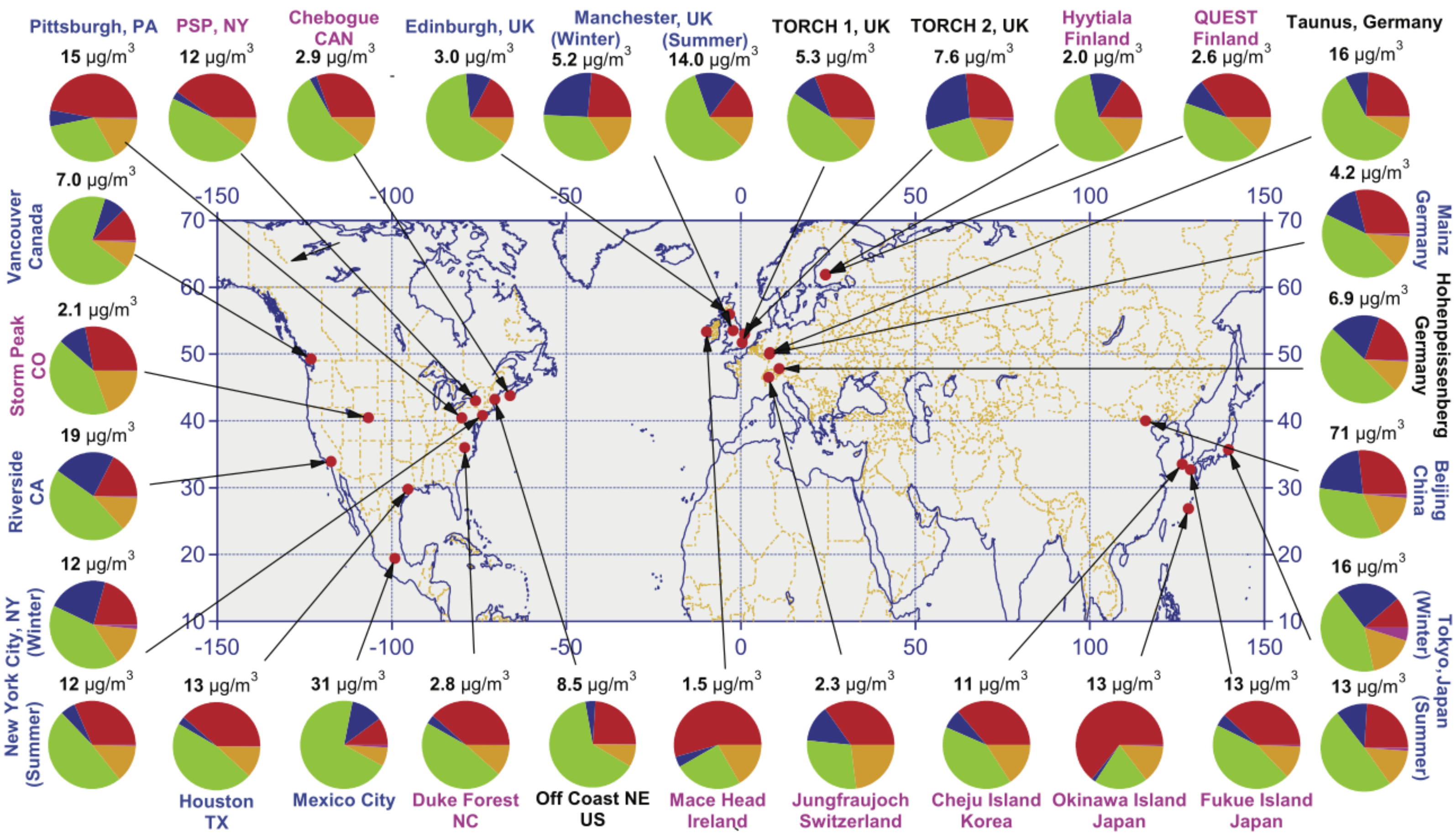


Figure 1. Location of the AMS datasets analyzed here (data shown in Table S1 in the auxiliary material). Colors for the study labels indicate the type of sampling location: urban areas (blue), <100 miles downwind of major cites (black), and rural/remote areas >100 miles downwind (pink). Pie charts show the average mass concentration and chemical composition: organics (green), sulfate (red), nitrate (blue), ammonium (orange), and chloride (purple), of NR-PM$_1$.