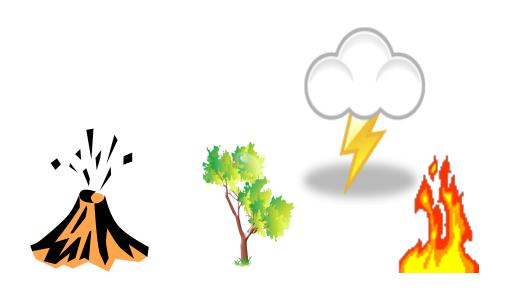
Biogenic, Wildfire, Lightning, and Volcano Emissions in WRF-Chem

Megan Bela (NOAA-ESRL, <u>megan.bela@noaa.gov</u>)

Stuart McKeen (NOAA-ESRL)

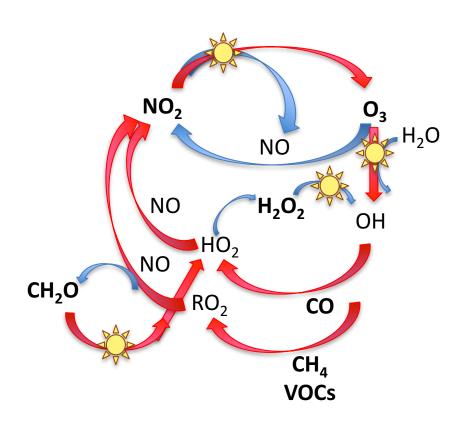
Mary Barth, Gabriele Pfister, Christine Wiedinmyer, Louisa Emmons (NCAR-ACOM)



WRF-Chem Tutorial – Boulder, CO - February 2017

Chemical Production of Ozone

(Atmospheric Chemistry 101)

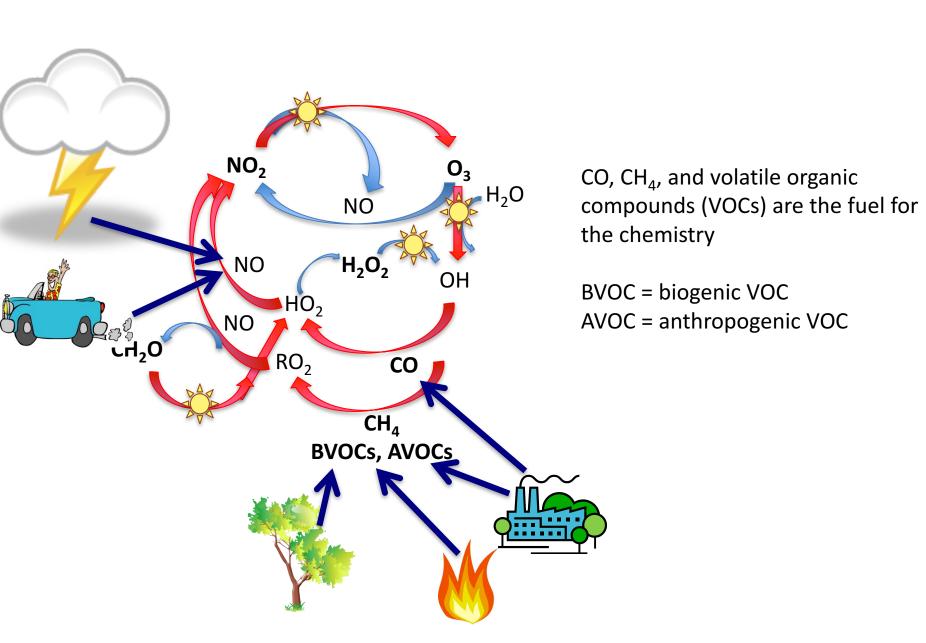


To make ozone, need sunlight $NO_x = NO + NO_2$

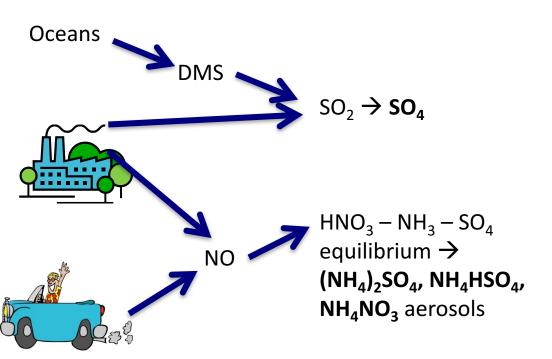
 $HO_x = OH + HO_2^2$

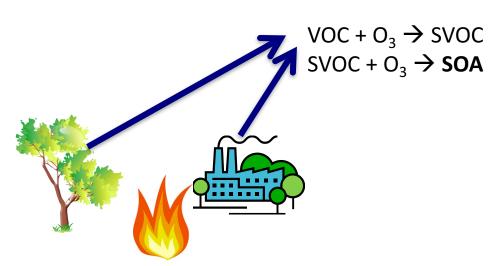
HO_x precursors are CO, CH₄, and volatile organic compounds (VOCs)

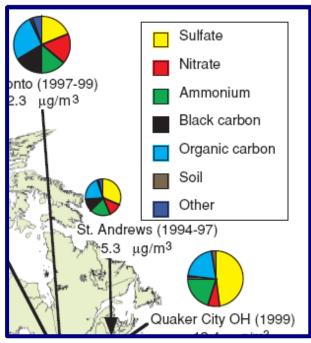
Emissions and the Chemical Production of Ozone



Emissions and Aerosols







(NARSTO, 2004)

Dust, Sea salt

Emissions calculated in WRF-Chem based on wind speed and land cover / use information

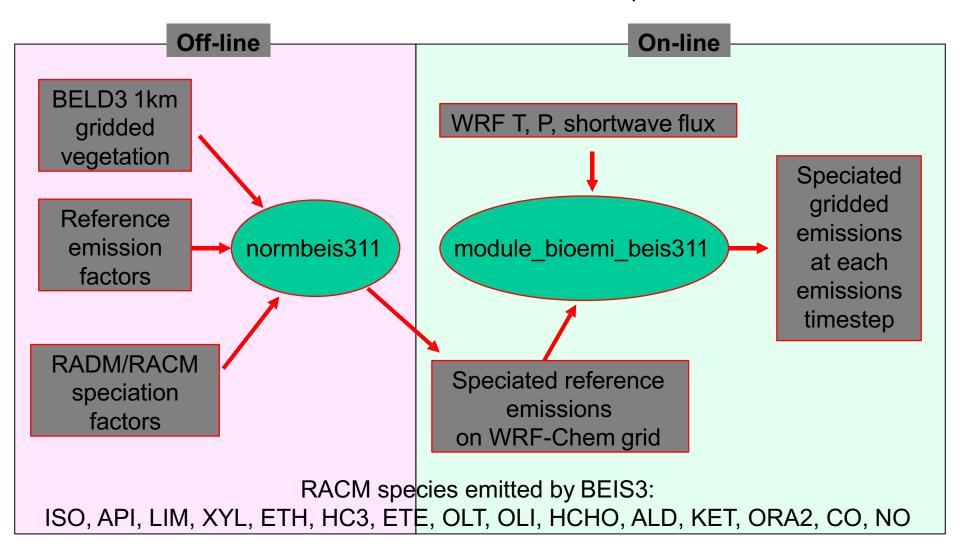
WRF-Chem Biogenic Emissions

4 choices for Biogenic emissions

- **No additional biogenic emission files** (bio_emiss_opt = 0):
 - Provide biogenic emissions through anthropogenic input (monthly GEIA 2002 1 deg x 1 deg or MEGAN 2000 0.5 deg x 0.5 deg)
- **Simple Guenther approach** (bio_emiss_opt = 1):
 - Landuse based emissions following Guenther et al (1993, 1994), Simpson et al. (1995). Emissions depends on both temperature and photosynthetic active radiation.
 - No additional input data files.
- **EPA BEIS-3.14/BELD** biogenic emissions (bio_emiss_opt=2):
 - Biogenic Emissions Inventory System (BEIS) version 3.14 [Schwede et al., 2013] with land-use from the Biogenic Emissions Landuse Database version 3 (BELD3) [Pierce et al., 1998].
 - Static 2-D surface reference data provided in input data file (wrfbiochemi_d01)
 - Biogenic emissions are modified according to the meteorology (T, shortwave radiation)
- **MEGAN version 2 biogenic emissions** (bio_emiss_opt=3):
 - Model of Emissions of Gases and Aerosol from Nature [*Guenther et al.*, 2006]. MEGAN Preprocessor available at http://www.acom.ucar.edu/wrf-chem/download.shtml
 - Static 2-D surface reference data provided in input data file (wrfbiochemi_d01)
 - Static biogenic fields are modified according to the meteorological conditions

Implementation of BEIS3 in WRF/Chem

Based on EPA BEIS3 v14 for SMOKE processor



Biogenic Emissions Modeling: MEGAN

MEGAN:

Model of Emissions of Gases and Aerosols from Nature

- Guenther et. al., Atmospheric Chemistry and Physics, 2006
 - Version 2.1 is in preparation for WRF-Chem
- 134 emitted chemical species
 - Isoprene
 - Monoterpenes
 - Oxygenated compounds
 - Sesquiterpenes
 - Nitrogen oxide
- 1 km² resolution

Online version of MEGAN in WRF-CHEM currently same as offline version 2.04

BVOCs

MEGAN Framework: Calculation of emissions

$$EM = \varepsilon \bullet \gamma_{CE} \bullet \gamma_{age} \bullet \gamma_{SM} \bullet \rho$$
$$\gamma_{CE} = \gamma_{LAI} \bullet \gamma_{P} \bullet \gamma_{T}$$

EM: Emission (μg m⁻² hr⁻¹)

ε: Emission Factor (μ g m⁻² hr⁻¹)

γ_{CE}: Canopy Factor

 γ_{age} : Leaf Age Factor

 γ_{SM} : Soil Moisture Factor

ρ: Loss and Production within plant canopy

γ_{LAI}: Leaf Area Index Factor

 γ_P : PPFD Emission Activity Factor (light-dependence)

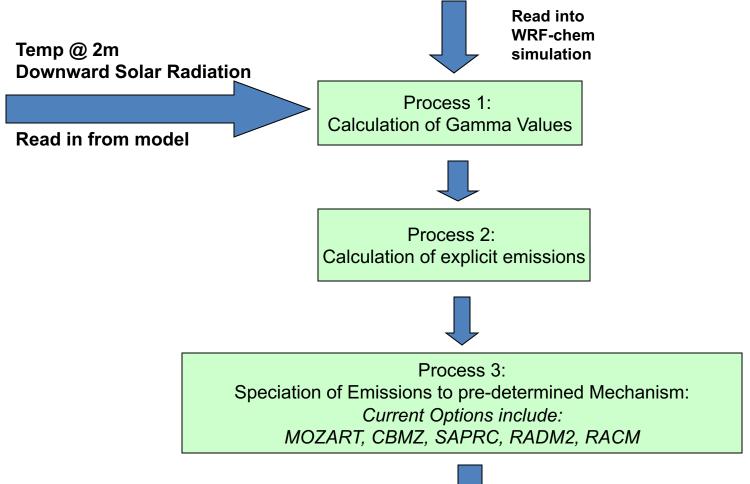
 γ_T : Temperature Response Factor



PREPROCESSOR: bio emiss

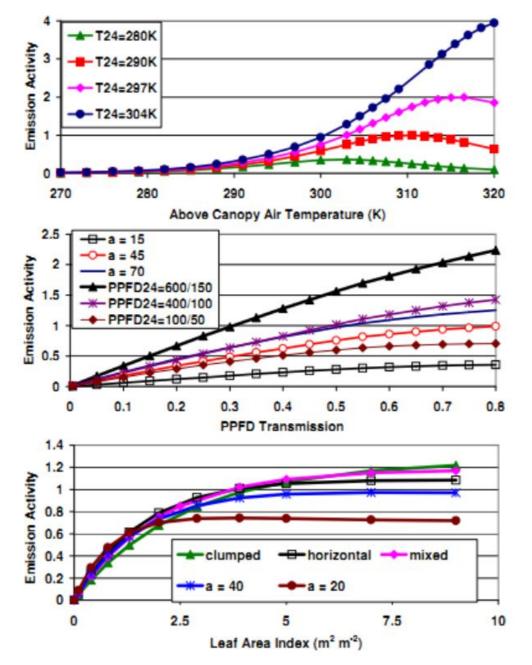
Includes isoprene emission factors, LAI, plant functional type fractions, and climatological temperature and solar radiation for each model grid cell

Preprocessed prior to WRF-chem simulation*





Return emissions to model



Emissions increase as

- Temperature increases
- PPFD transmission (light) increases
- Leaf area index increase

Guenther et al., 2006, ACP

Emission Factors for Isoprene

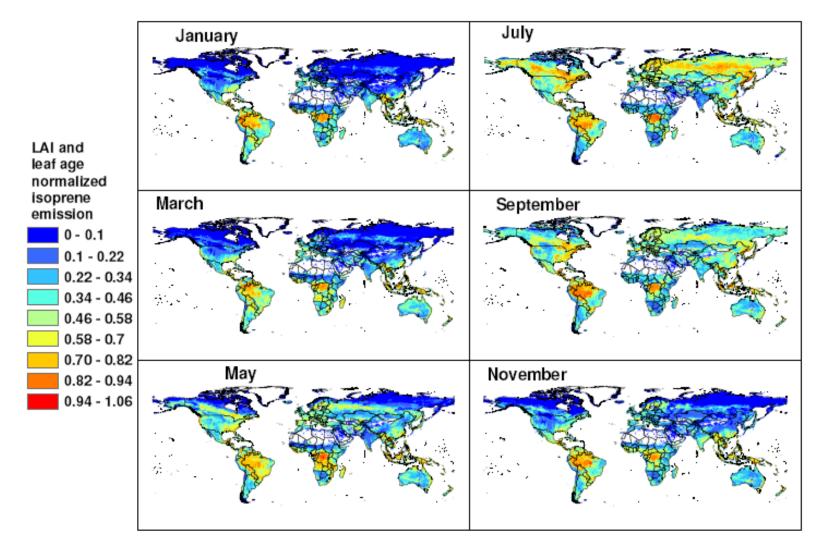
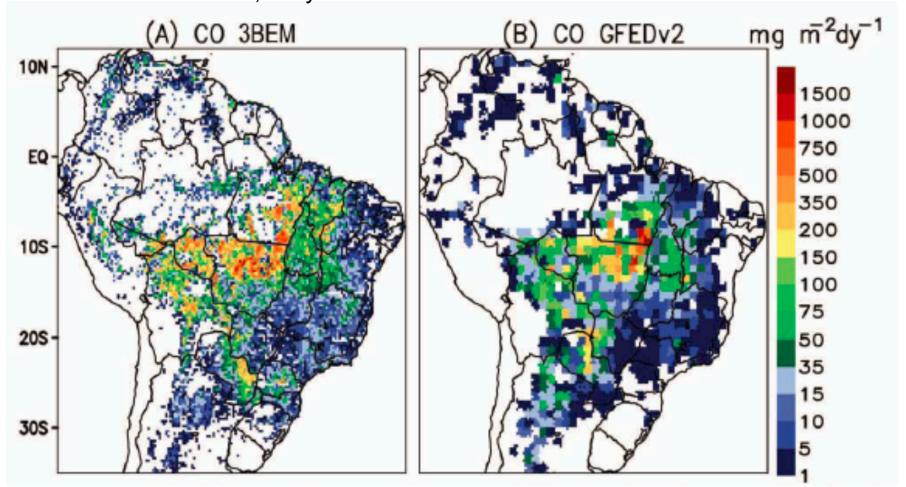


Fig. 5. Monthly normalized isoprene emission rates estimated with MEGAN for 2003. Rates are normalized by the emission estimated for standard LAI (= $5 \, \text{m}^2 \, \text{m}^{-2}$) and leaf age (80% mature leaves). These normalized rates illustrate the variations associated with changes in only LAI and leaf age; i.e. all other model drivers are held constant.

Biomass burning emissions

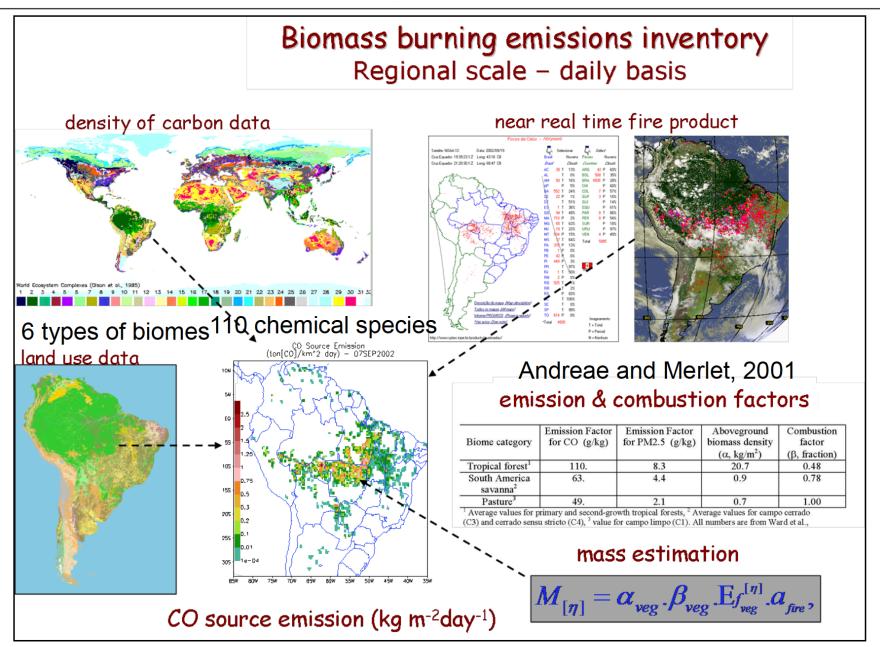
Brazilian Biomass Burning Emission Model (**3BEM**) Model resolution, daily Global Fire Emissions Database (**GFEDv2**) 10 x 10, 8-day or monthly, 1997 - 2004



Average daily CO emissions, Aug.-Oct. 2002, 35 km

Freitas et al. (2011)

3BEM



Freitas et al., 2005; Longo et al., 2007

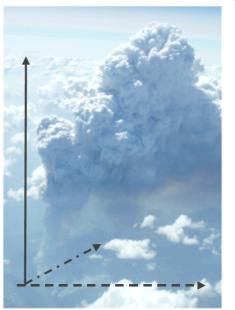
3BEM Plume Rise

Biomass burning and wildfires

Smoldering: mostly surface emission.

Flaming: mostly direct injection in the PBL,

free troposphere or stratosphere.

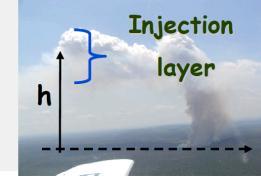


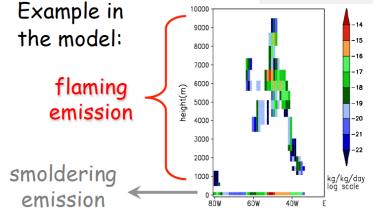
Plume rise model

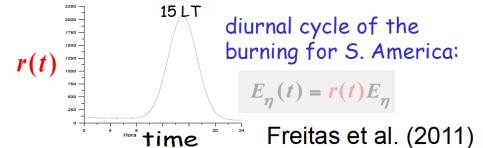
total emission flux: F_{η} being λ the smoldering fraction

smoldering term :
$$E_{\eta} = \frac{\lambda F_{\eta}}{\rho_{air} \Delta z_{\text{first phys.}}}$$

flaming term:
$$E_{\eta} = \frac{(1-\lambda)F_{\eta}}{\rho_{air}\Delta z_{injection}}$$





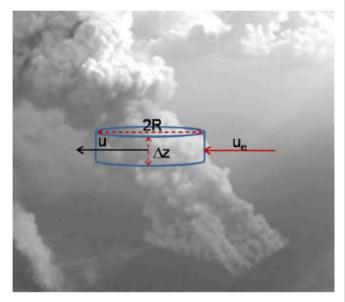


Environmental Wind Effects on Plume Rise



Biomass burning plumes in the Amazon region without (left) and with (right) environmental wind shear Photos: M.O. Andreae, M. Welling

Environmental Wind Effects on Plume Rise



$$\lambda_{\text{entr}} = \frac{2\alpha}{R} |w|$$

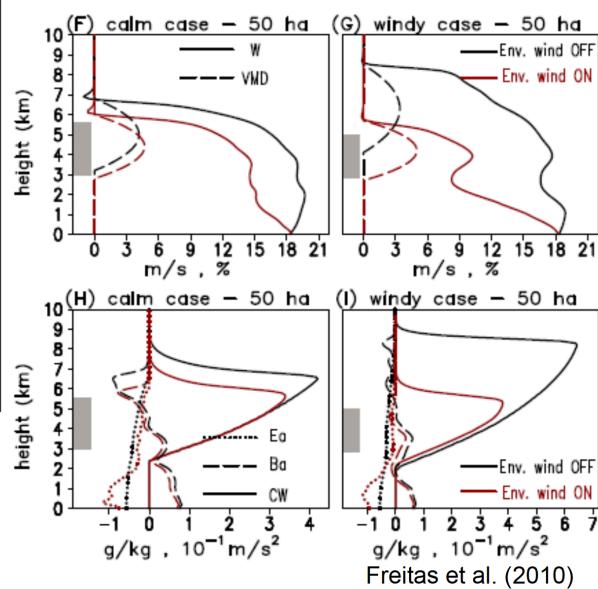
$$\delta_{\text{entr}} = \frac{2}{\pi R} (u_e - u)$$

W: vertical velocity
VMD: vertical mass distribution
Ea: Entrainment acceleration

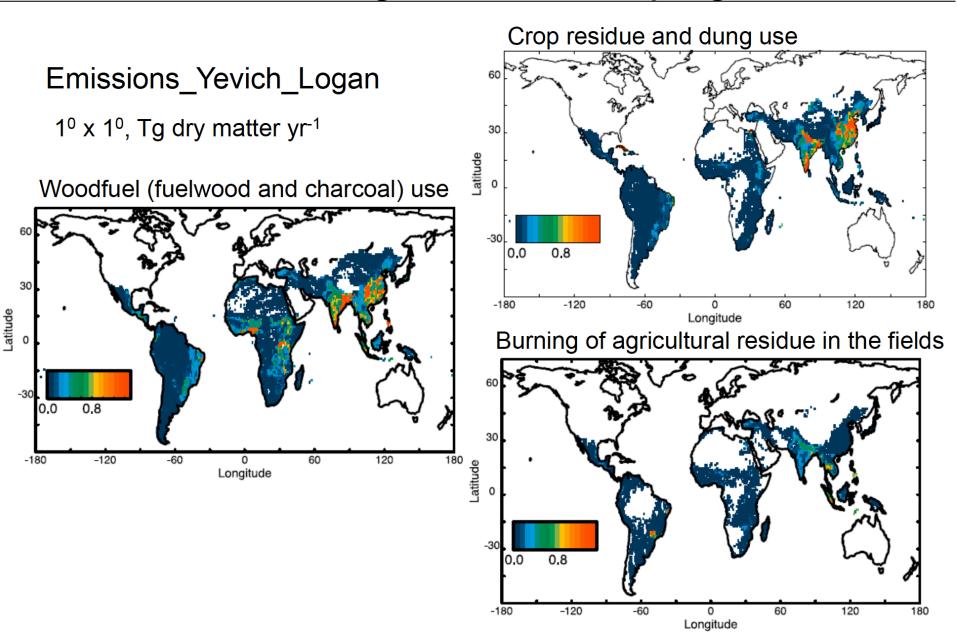
Ba: buoyancy acceleration

CW: total condensate water

1-D PRM results for a 50 ha fire, calm and windy conditions



Biofuel burning in the developing world

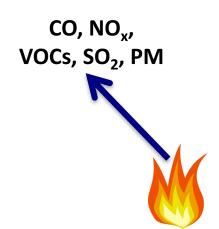


Yevich and Logan, 2003

Fire Emissions: Fire INventory from NCAR (FINN)

<u>Daily fire emissions calculated with FINNv1</u> Wiedinmyer et al., *Geoscientific Model Development*, 2011

- Daily, 1 km resolution, global estimates of the trace gas and particle emissions from open burning of biomass
- Uses satellite observations of active fires and land cover, together with emission factors and estimated fuel loadings
- Available for hindsight and forecast model applications



Modeling Fire Emissions

$$Emissions_i = f(A(x,t), B(x,t), E_{f_i})$$

A(x,t): Area burned

B(x): Biomass burned (biomass burned/area)

- type of vegetation (ecology)
- fuel characteristics:
 - amounts of woody biomass, leaf biomass, litter, ...
- fuel condition
 - moisture content

E_{fi}: Emission factor (mass emission, /biomass burned)

- fuel characteristics
- fuel condition

Version 1 Model Drivers:

MODIS Rapid Response fire detections

MODIS Vegetation Continuous Fields and Land Cover Type

Emission factors from Akagi et al., ACP, 2011.

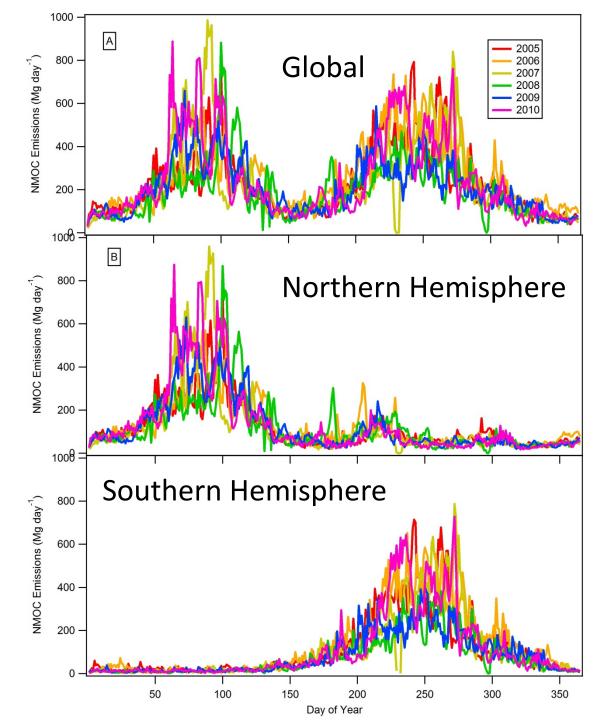
Speciation of VOCs provided for MOZART-4, SAPRC99, GEOS-Chem

Plume rise option available- but requires additional inputs

Global Daily Emissions

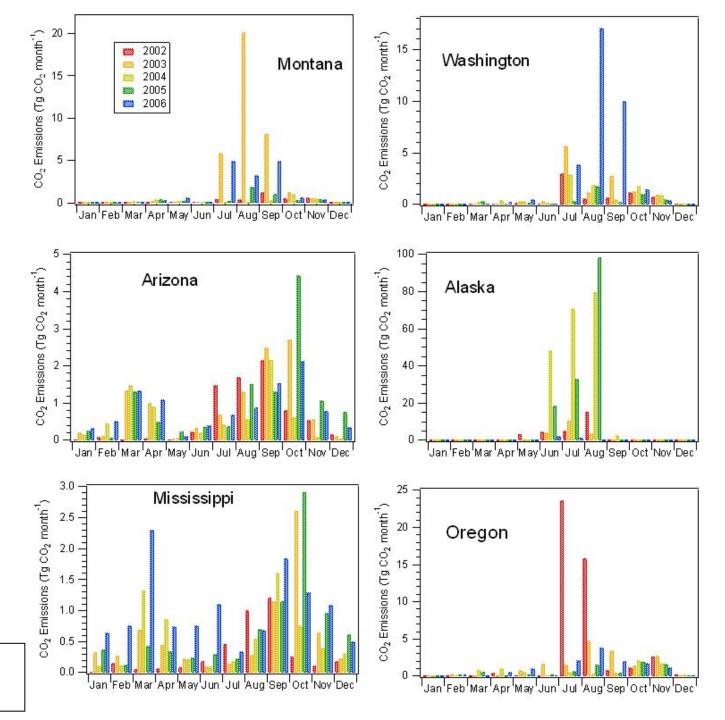
Emissions highly variable

- Daily
- Season
- Spatial



Fire Emissions Variability:

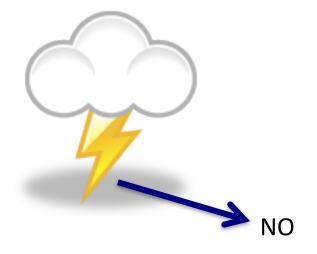
- -Spatial
- -Temporal



Wiedinmyer and Neff, Carbon Balance and Management, 2007

Lightning-NO_x Emissions

- Cloud-resolving parameterization: Barth et al., ACP, 2012
- Convective-parameterized parameterization: Wong et al., GMD, 2013





When lightning is triggered,

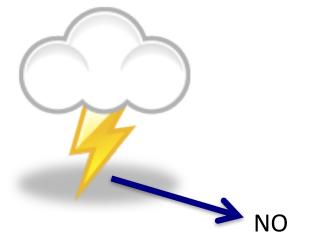
- Temperature increases to 1000s degrees
- This splits many molecules including N₂ and O₂

When temperature drops to normal,

- Some of the N and O atoms recombine with each other
- \rightarrow NO (nitric oxide)

4 Steps in Predicting NOx Production from Lightning

- 1) Predict lightning flashrate
- 2) Determine intracloud to cloud-to-ground lightning ratio
- 3) Determine where to put the NO emissions
- 4) Prescribe how much NO is emitted per flash

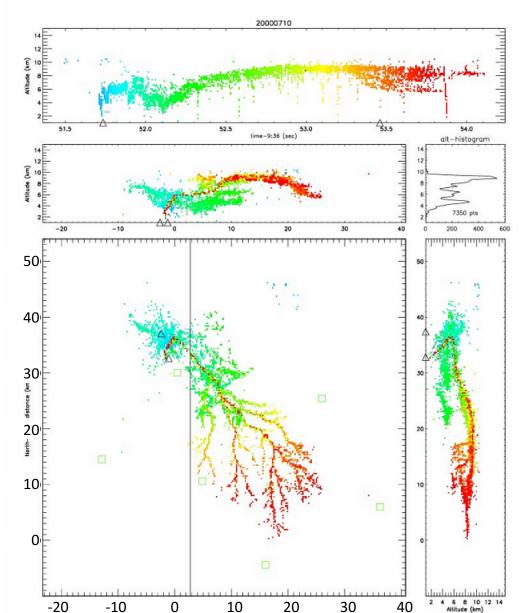






Example Lightning Flash

Example of Highly Dendritic Negative CG flash



- Lightning can be very long in length, with many branches
- Lightning can cover a broad altitude range
- Some places (like Colorado)
 have many, many more IC
 flashes than CG flashes

1) Predicting Lightning Flashrate

Parameterized prediction:

Williams (1985)

Price and Rind (1993)

Deierling (2006);

Wiens et al. (2005)

Deierling et al. (2008)

Petersen et al. (2005)

cloud top height

maximum vertical velocity

precipitation ice mass

updraft volume

ice mass flux product

ice water path

Precipitating Ice = mostly graupel and hail but includes snow

Ice mass flux product

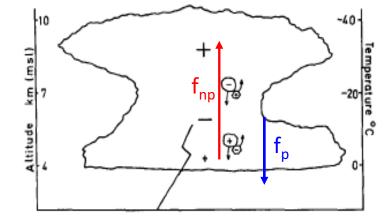


Fig. 2. A schematic of graupel-ice-crystal charge transfer above and below the reversal temperature level in a thunderstorm.

1) Predicting Lightning Flashrate

Cloud-resolving parameterization: Barth et al., ACP, 2012

Flashrate = $5.7x10^{-6} w_{\text{max}}^{4.5}$ (option 1)

Flashrate = $3.44x10^{-5} H^{4.9}$ (option 2)

H = cloud top height of the 20 dBZ contour

Convective-parameterized parameterization: Wong et al., GMD,
 Flashrate = 3.44x10⁻⁵ H^{4.9} (only option)

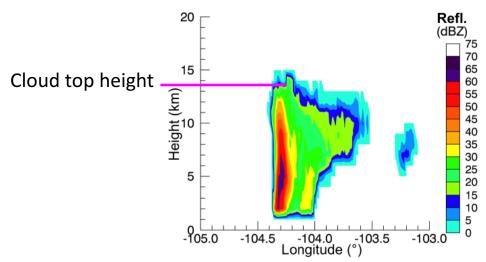
H = level of neutral buoyancy (from Grell convective parameterization)

Can adjust H in namelist.input

Note:

These are highly non-linear estimates and are often wrong.

- → **flashrate_factor** for adjusting
- → Active research for improving these equations

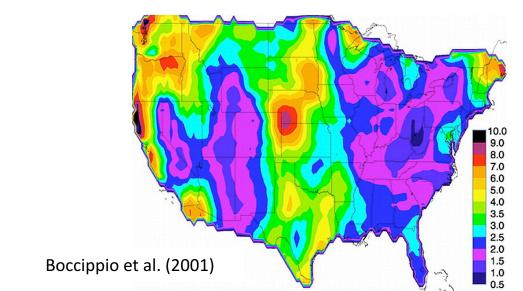


2) Determine Intracloud to Cloud-to-Ground Flash Ratio

- Prescribed Values
 - 1) Set to a specified value everywhere
 - 2) Set to a very coarsely prescribed climatology (Boccippio et al., 2001)
 - 3) Gridded input need to provide input
- Predict IC:CG (Price and Rind, 1993) $IC/CG = 0.021 d^4 0.648 d^3 + 7.49 d^2 36.54 d + 63.09$ d = depth of the "cold cloud", from T=0°C to cloud top

Note:

Recommend using a prescribed IC:CG ratio



3) Determine where to put the NO emissions

Horizontal Placement

Cloud-resolving parameterization: Barth et al., ACP, 2012
 Placed within 20 dBZ reflectivity region

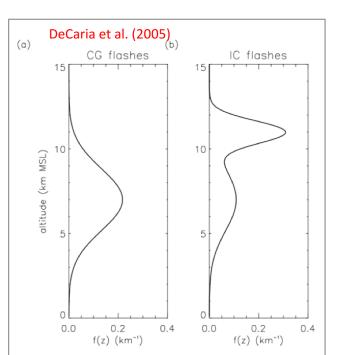
Current research is evaluating how good this assumption is

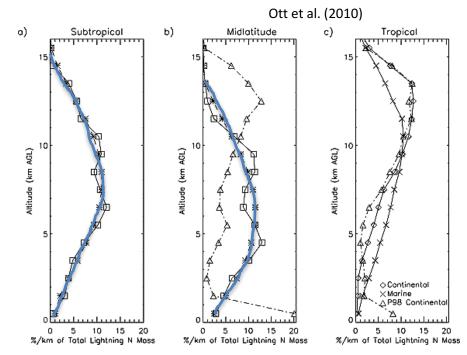
- → looks pretty good for Colorado storms, but 10 dBZ may be a better number elsewhere
- Convective-parameterized parameterization: Wong et al., GMD,
 Placed throughout the grid cell

3) Determine where to put the NO emissions

Vertical Placement

- Cloud-resolving parameterization: Barth et al., ACP, 2012
 Uses DeCaria et al. (2005) curves
- Convective-parameterized parameterization: Wong et al., GMD,
 Uses Ott et al. (2010) curves

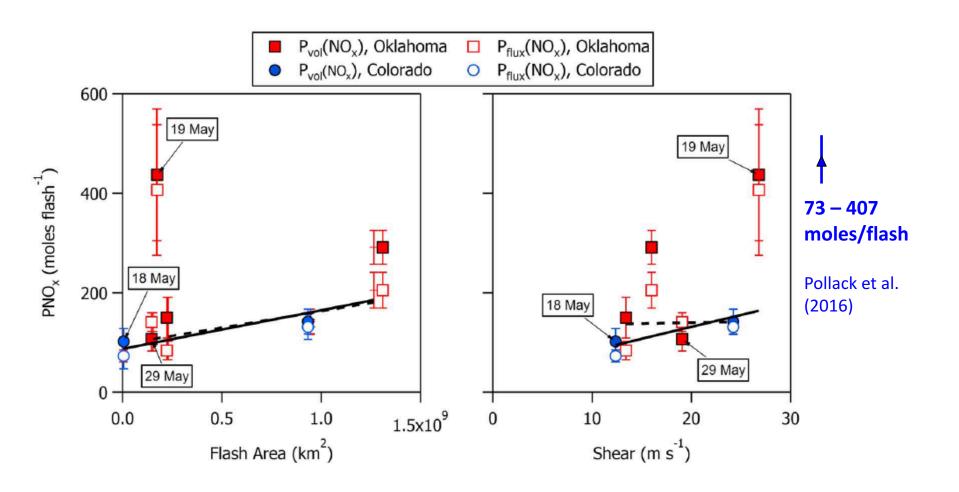




4) Prescribe how much NO is emitted per flash

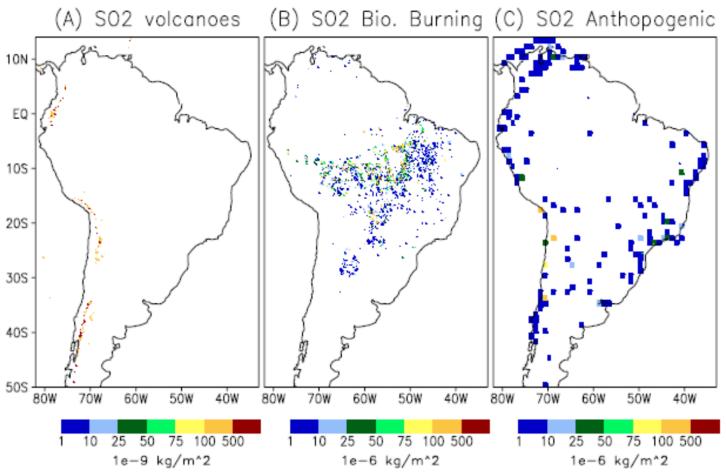
Review of LNOx production rates (Schumann and Huntrieser, 2007)

• 3-8 Tg N/year = 50-500 moles NO/flash



Volcano emissions

Based on Mastin et al. (2009) database of 1535 volcanoes Mass eruption rate, plume height and time duration SO₂ from AEROCOM program, 1979 – 2007 (Diehl, 2009)



SO₂ emissions on 27 August 2002 on a 0.2° rectangular projection grid: (A) Diehl (2009), (B) 3BEM, (C) EDGAR Freitas et al. (2011)

Contact the following people with your questions

Megan Bela (megan.bela@noaa.gov)

NCAR Preprocessors: Stacy Walters stacy@ucar.edu

Gabriele Pfister <u>pfister@ucar.edu</u>

FINN emissions: Christine Wiedinmyer christin@ucar.edu

MOZART data files: Louisa Emmons emmons@ucar.edu

Lightning emissions: Mary Barth barthm@ucar.edu

PREP-CHEM-SRC brams_help@cptec.inpe.br





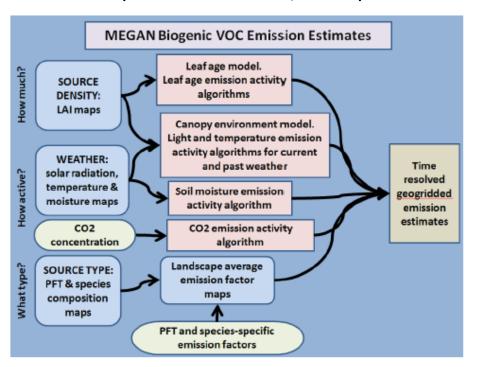
CO, NO_x, VOCs, SO₂, PM



MEGAN online biogenic emissions

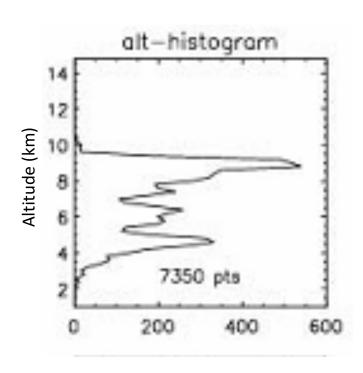
In Summary:

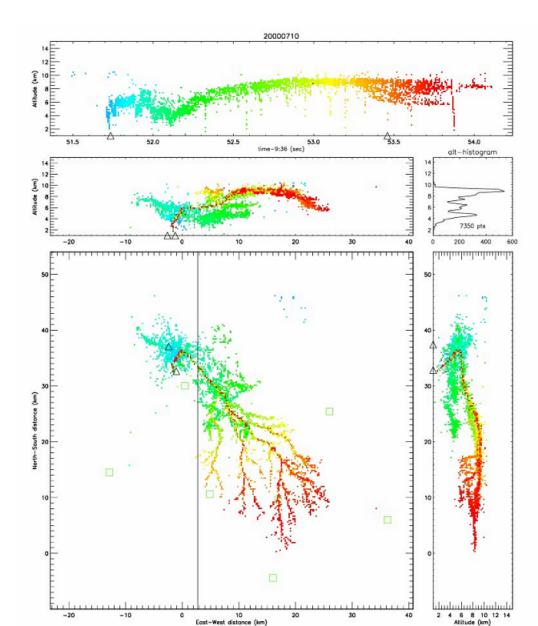
- Estimate emissions of VOCs, NO_x and CO from vegetation
- Driving variables include landcover, weather, and atmospheric chemical composition
- Note: currently land cover used in MEGAN differs from that used within WRF-Chem
- Plan: Update to MEGAN 2.1 (Guenther et al., 2012) and link to CLM land cover



3) Determine where to put the NO emissions

Vertical Placement





WRF/Chem Biogenic Emissions

(BEIS3.14/BELD option)

Edit **namelist.input** file in the WRFV2/test/em_real directory:

- · chem_opt=1, (need to turn on chemistry)
- bio_emiss_opt=2.

If necessary, modify the med_read_bio_chem_emiss routine in WRFV2/chem/module_input_chem_bioemiss.F to read your data set.

%> compile bio_conv

convert_bioemiss.exe placed in chem directory

Run convert_bioemiss.exe to make wrfbiochemi_d01 data file.

Run real.exe to create wrfinput data file - the biogenic emissions should now be included in the wrfinput data file.

MEGAN preprocessor

- Static input fields needed to run with online MEGAN biogenic emissions:
 Isoprene Emissions Factors, monthly LAI, Solar Radiation & Temperature,
 Fractional coverage of broadleaf and needeleaf trees, shrubs and herbaceous
- Compatible with MOZART, CBMZ, RADM, RACM, SAPRC (see module_data_mgn2mech.F for species mapping)
- Download source code (megan_bio_emiss.tar) and global input data (megan.data.tar.gz)
- megan_bio_emiss is a single cpu code, which
 - ✓ reads global MEGAN input data
 - ✓ maps them on the WRF-Chem domain
 - ✓ creates wrfbiochemi_d<domain> file

https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community

MEGAN preprocessor

• To <u>compile</u>:

```
make_util megan_bio_emis - creates the executable megan_bio_emiss
```

megan_bio_emiss is controlled by a <u>namelist</u> file (e.g. megan_bio_emiss.inp)

• To <u>run</u>: megan_bio_emiss < megan_bio_emiss.inp > megan_bio_emiss.out

Running WRF-Chem with MEGAN

- WRF-Chem output variables: EBIO_<species>
- namelist.input:

Compiling PREP-SRC-CHEM

Install libraries: netCDF, Zlib, HDF5
Set library paths in:

PREP-CHEM-SRC-1.x/bin/build/include.mk.<compiler> make OPT=<compiler>.wrf CHEM=RADM_WRF_FIM



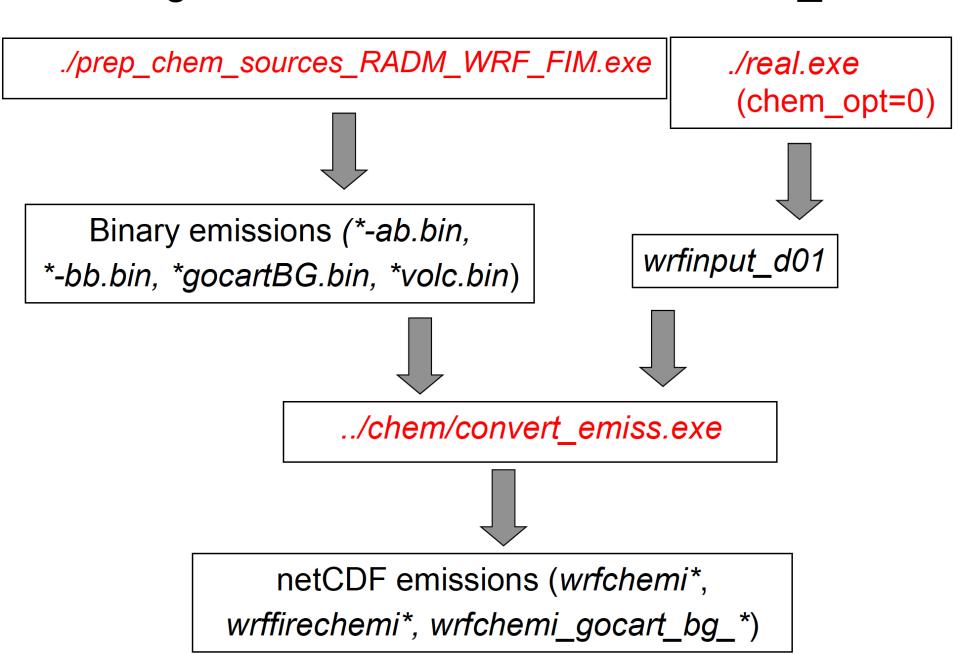
Executable: prep_chem_sources_RADM_WRF_FIM.exe

```
$RP INPUT
!----- grid type
grid_type= 'lambert',
                           ! 'polar' = polar stereo. grid output
                            ! 'II' = lat/lon grid output
                            ! 'lambert' = lambert grid output
                            ! 'mercator' = mercator grid output
 ----- date of emission
 ihour=0.
 iday=12,
 imon=7,
 iyear=2004,
!----- select the sources datasets to be used: 1 = yes, 0 = not
 use retro=1,
 retro_data_dir='/import/archive/u1/uaf/freitas/Emission_data/RETRO/anthro',
 use edgar = 1, ! 0 - not, 1 - Version 3, 2 - Version 4 for some species
 use qocart=1.
 user_data_dir='/home/poluicao/EMISSION_DATA/SouthAmerica_Megacities',
 use bioge =2, ! 1 - GEIA, 2 - MEGAN
 use fwbawb=1.
 fwbawb data dir='/import/archive/u1/uaf/freitas/Emission data/Emissions Yevich Logan',
 use gfedv2=0,
 use bbem=1,
 use bbem plumerise=1,
```

```
!----- if the merging of gfedv2 with bbem is desired (=1, yes, 0 = no)
 merge GFEDv2 bbem =0,
!----- Fire product for 3BEM/3BEM-plumerise emission models
bbem wfabba data dir='/import/archive/u1/uaf/freitas/Emission data/fires data/WF ABBA/filt/f,
bbem_modis_data_dir ='/import/archive/u1/uaf/freitas/Emission_data/fires_data/MODIS/Fires.',
bbem_inpe_data_dir ='/import/archive/u1/uaf/freitas/Emission_data/fires_data/DSA/Focos',
bbem extra data dir ='/import/archive/u1/uaf/freitas/Emission data/fires data/xxxxx,
!----- gocart background
 use gocart bg=1,
!----- volcanoes emissions
 use_volcanoes=0,
 volcano index=0, !REDOUBT
 use these values='NONE',
! define a text file for using external values for INJ HEIGHT, DURATION,
! MASS ASH (units are meters - seconds - kilograms) and the format for
! a file 'values.txt' is like this: 11000, 10800, 1.5e10
! use_these_values='values.txt',
 begin eruption='198912141930', !begin time UTC of eruption YYYYMMDDhhmm
!----- degassing volcanoes emissions
 use degass volcanoes=0,
 degass_volc_data_dir='/home/poluicao/EMISSION_DATA/VOLC_SO2',
```

```
!----- For regional grids (polar, Lambert, Mercator)
 NGRIDS = 3, ! Number of grids to run
 NNXP = 391,463,499, ! Number of x gridpoints
 NNYP = 271,454,478, ! Number of y gridpoints
 NXTNEST = 0, 1, 2, ! Grid number which is the next coarser grid
 DELTAX = 18000,
 DELTAY = 18000, ! X and Y grid spacing
 ! Nest ratios between this grid and the next coarser grid.
 NSTRATX = 1, 3, 3, ! x-direction
 NSTRATY = 1, 3, 3, ! y-direction
 NINEST = 1, 78, 128, ! Grid point on the next coarser
 NJNEST = 1, 30, 153, ! nest where the lower southwest
! NKNEST = 1, 1, 1, ! nest where the lower southwest
                ! corner of this nest will start.
                ! If NINEST or NJNEST = 0, use CENTLAT/LON
 POLELAT = 15., ! If polar, latitude/longitude of pole point
 POLELON = 10., ! If lambert, lat/lon of grid origin (x=y=0.)
 STDLAT1 = 0., ! If polar, unused
 STDLAT2 = 15., ! If lambert, standard latitudes of projection (truelat2/truelat1 from
   namelist.wps, STDLAT1 < STDLAT2)
 CENTLAT = 15.0
 CENTLON = 10.0
```

Running PREP-CHEM-SRC and convert_emiss



FINN Fire Emissions Preprocessor

- create WRF-Chem ready fire emissions from FINN inventory wrffirechemi_d<domain>_<date> for use with online plume rise
 (can also be merged into wrfchemi files)
 note: fire_emis also works to create global emission files for MOZART-4/CAM-Chem
- Works for different chemical schemes (namelist controlled)
- WRAP diurnal emission profile applied
- Processor and FINN inputs available on Web
- FINN inputs in MOZART-4, SAPRC99, and GEOS-Chem speciation

https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community

Fire_Emis

Fortran based preprocessor for creating fire emission inputs for WRF-Chem when running with plumerise and also for creating fire emission inputs for the MOZART-4 and CAM-Chem global models. The fire emissions inventory is based on the Fire Inventory from NCAR (FINN). Both software (fire_emis.tgz) and required FINN input data sets are available at the download page.

The fire_emis.tgz file when uncompressed {tar -zxf fire_emis.tgz} yields three directories {data_files, src, and test} and two readme files {README.WRF.fire and README.GLB.fire }. The data_files directory is empty and is where users should put the FINN files and the wrfinput_d<domain> file(s). The test directory contains two test namelist input files, one for creating WRF inputs and another for creating global inputs. Users are highly advised to read the README files before using the fire emission utility.

FINN Fire Emissions Preprocessor

- To <u>compile</u>: *make_fire_emis*
- To <u>run</u>: fire_emis < fire_emis.inp > fire_emis.out
- Example namelist "fire_emis.inp" for MOZCART

```
&control
domains
            = 1.
fire directory = ",
fire filename = 'GLOB2012a_MOZ4_07242012.txt',
wrf directory = ",
start date = '2012-06-01',
end date = '2012-06-10',
diag level = 1,
wrf2fire map = 'co -> CO', 'no -> NO', 'so2 -> SO2', 'bigalk -> BIGALK', 'bigene -> BIGENE', 'c2h4 -> C2H4',
                 'c2h5oh - C2H5OH', 'c2h6 -> C2H6', 'c3h8 -> C3H8', 'c3h6 -> C3H6', 'ch2o -> CH2O',
                 'ch3cho -> CH3CHO', 'ch3coch3 -> CH3COCH3', 'ch3oh -> CH3OH', 'mek -> MEK',
                 'toluene -> TOLUENE','nh3 -> NH3','no2 -> NO2','open -> BIGALD','c10h16 -> C10H16',
                 'ch3cooh -> CH3COOH', 'cres -> CRESOL', 'glyald -> GLYALD', 'mgly -> CH3COCHO',
                 'gly -> CH3COCHO', 'acetol -> HYAC', 'isop -> ISOP', 'macr -> MACR', 'mvk -> MVK',
                 'oc -> 0.24*PM25 + 0.3*PM10;aerosol', 'bc -> 0.01*PM25 + 0.08*PM10;aerosol',
                 'pm10 raw -> PM10;aerosol', 'pm25 raw -> PM25;aerosol',
                 'sulf -> -0.01*PM25 + 0.02*PM10;aerosol',
                 'pm25 -> 0.36*PM25;aerosol', 'pm10 -> -0.61*PM25 + 0.61*PM10;aerosol'
```

FINN Fire Emissions Preprocessor

Running WRF-Chem with FINN emissions and plumerise:

```
&time_control
    auxinput7 inname
                                  = 'wrffirechemi d<domain> <date>',
    auxinput7_interval_m
                                  = 60, 60, 60,
    io_form_auxinput7
                                  = 2,
    frames per auxinput7
                                  = 1, 1, 1,
&chem
    biomass_burn_opt
                                  = your choice
    plumerisefire_frq
                                  = your choice
    scale_fire_emiss
                                  = .true.
```

Fire INventory from NCAR (FINN)

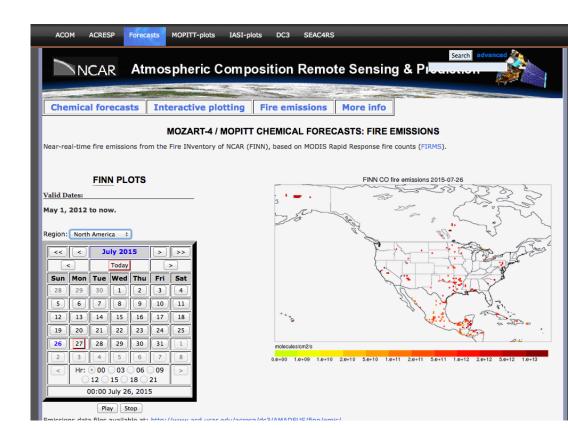
Daily global emissions available from 01 January 2002 – 30 June

2014 https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community

Also available at:

http://www.acom.ucar.edu/acresp/forecast/fire-emissions.shtml

http://www.acom.ucar.edu/acresp/dc3/AMADEUS/finn/emis/



Running WRF-Chem with Lightning-NOx emissions

```
&physics
     lightning option
                                        = 11, 1,
     iccg method
                                        = 2, 2,
     lightning dt
                                        = 75, 75,
                                        = 0, 1,
     cellcount method
                                        = 600, 600,
     lightning start seconds
     flashrate_factor
                                        = 20., 1.,
                                        = 0. 0.
     cldtop adjustment
&chem
                                        = 1, 2,
     lnox opt
                                        = 125., 500.,
     N IC
                                        = 125., 500.,
     N CG
                                 parameterized cloud resolving
                                    convection convection
```

See WRF-Chem Users Guide for option choices

mozbc – set chemical initial and lateral boundary conditions

- chemical initial and boundary conditions are needed to account for initial concentrations and inflow
- fills the chemical fields in wrfinput_d<domain> and wrfbdy_d<domain> with global model output
- set-up for MOZART-4 and CAM-Chem global model output
- controlled by namelist file (e.g. define species mapping; mappings available for MOZART to RACM, RADM, CBMZ, MADE/SORGAM, MOSAIC, GOCART)
- Interpolation in time and space
- MOZART-4 output for past years and forecasts available on Web

https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community

mozbc: Create lateral boundary and initial conditions from a global chemistry model NCAR/ACD has developed a program to create time-varying chemical lateral boundary conditions for WRF-Chem from MOZART-4 output. For questions about running mozbc please contact: Stacy Walters (stacy at ucar . edu), Mary Barth (barthm at ucar . edu), or Gabriele Pfister (pfister at ucar . edu). For technical details please refer to this document: Conversion of MOZART species to WRF-Chem. To obtain mozbc, see the **Download** section below.

mozbc – set chemical initial and lateral boundary conditions

- mozbc operates on the most common map projections in WRF (Lambert, Mercator, Polar, Lat/Lon)
- To <u>compile</u>: make_mozbc -> will create the executable mozbc
- Package includes example namelist files ("mozbc.inp")
- To <u>run</u>: mozbc < mozbc.inp > mozbc.out
- to enable chemical IC and BC when running WRF-Chem set in namelist.input: have_bcs_chem = .true

Example namelist file for mozbc:

```
&control
do bc = .true.
                                     defines if BC are set (default: .false.)
do ic = .true.
                                     defines if IC are set (default: .false.)
domain = 2
                                     number of domains to work on (default: 1);
                                     e.g. d=2 sets BC for d01 and IC for d01 and d02
dir_wrf = '/ptmp/me/WRF chem/'
                                     path to WRF-Chem files (met em*, wrfinp*, wrfbdy*)
dir_moz = '/ptmp/me/MOZBC/'
                                     path to MOZART/CAM-Chem input files
fn_moz = 'h0040.nc'
                                 initial MOZART/CAM-Chem file; mozbc increments filenames,
                                filenames must be of the form prefix<nnn>.nc
moz_var_suffix = '_VMR_avrg'
                               suffix string for MOZART/CAM-Chem variables (default: 'VMR inst')
met file prefix = 'met em'
                                prefix string for the WRF meterological files (default: 'met em')
                                {standard WRF names: met em.d<nn>.<yyyy-mm-dd hh:mm:ss>.nc }
                                suffix string for the WRF meterological files (default: 'nc')
met file suffix = '.nc'
met file separator = '.'
                                separator character for WRF meterological files (default: '.')
spc map = 'o3 -> O3', 'o -> O', 'o1d cb4 -> O1D', 'n2o -> N2O', 'no -> NO',
          'DUST 4 -> .2348*[DUST3]+.5869*[DUST4];1.e9', 'DUST 5 -> .5869*[DUST4];1.e9'
```

Note: Sometimes a species is not in the MOZART output. Just remove that species from the spc_map namelist. (unless it is really important to include)

ubc - upper chemical boundary conditions

- WRF-Chem does not have a stratosphere –possible issues when looking at UTLS or comparing to some satellite products (e.g. trop. O₃ retrievals)
- o3,no,no2,hno3,ch4,co,n2o, n2o5 are set to climatology above certain pressure level and relaxed to tropopause level below
- Same scheme as used in the global models, MOZART-4 and CAM-Chem
- Climatologies available for present and future times
- download climatologies from Web
- namelist.input (&chem):

```
have_bcs_upper = .true.
fixed_upper_bc = 50.
fixed_ubc_inname = "ubvals_b40.20th.track1_1996-2005.nc"
```

https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community

Upper Boundary Conditions