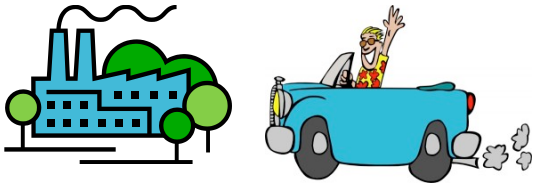
Biogenic, Fire, Lightning Emissions and Chemical Boundary Conditions

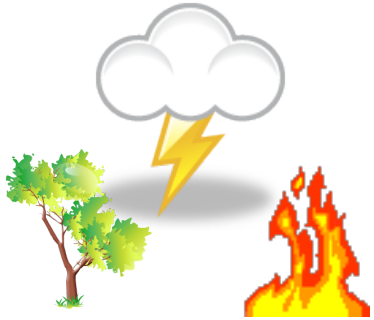
Mary Barth, Gabriele Pfister, Christine Wiedinmyer,
Louisa Emmons, Rajesh Kumar

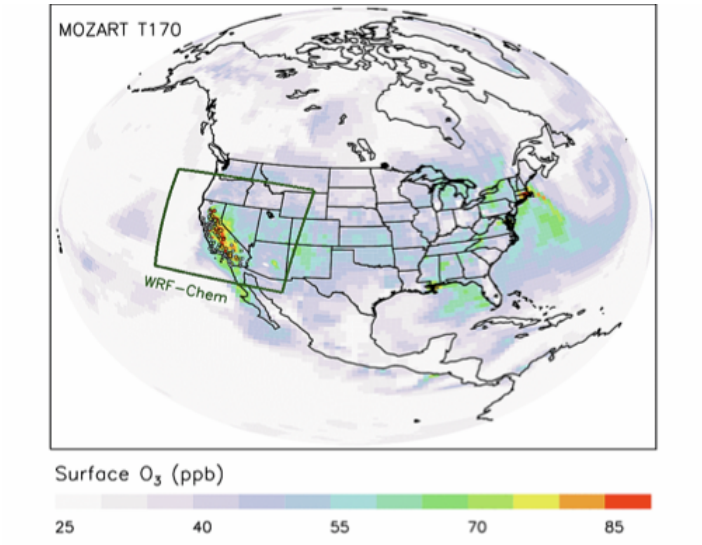
Emissions for Chemical Transport Models

- Anthropogenic
  - Point, Area, Mobile



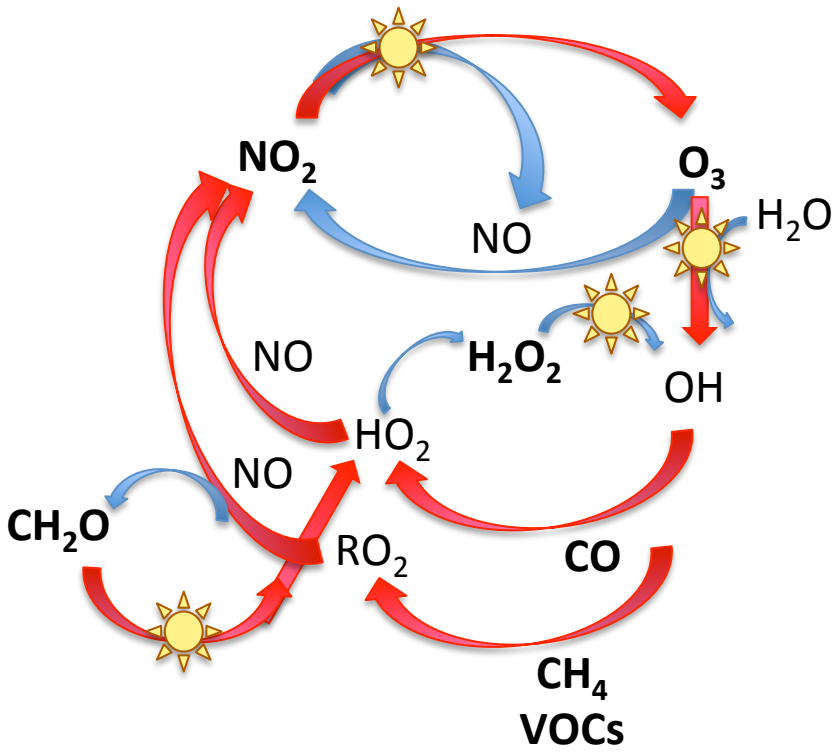
- Biogenic
- Biomass Burning
- Lightning
- Volcanoes





Chemical Production of Ozone

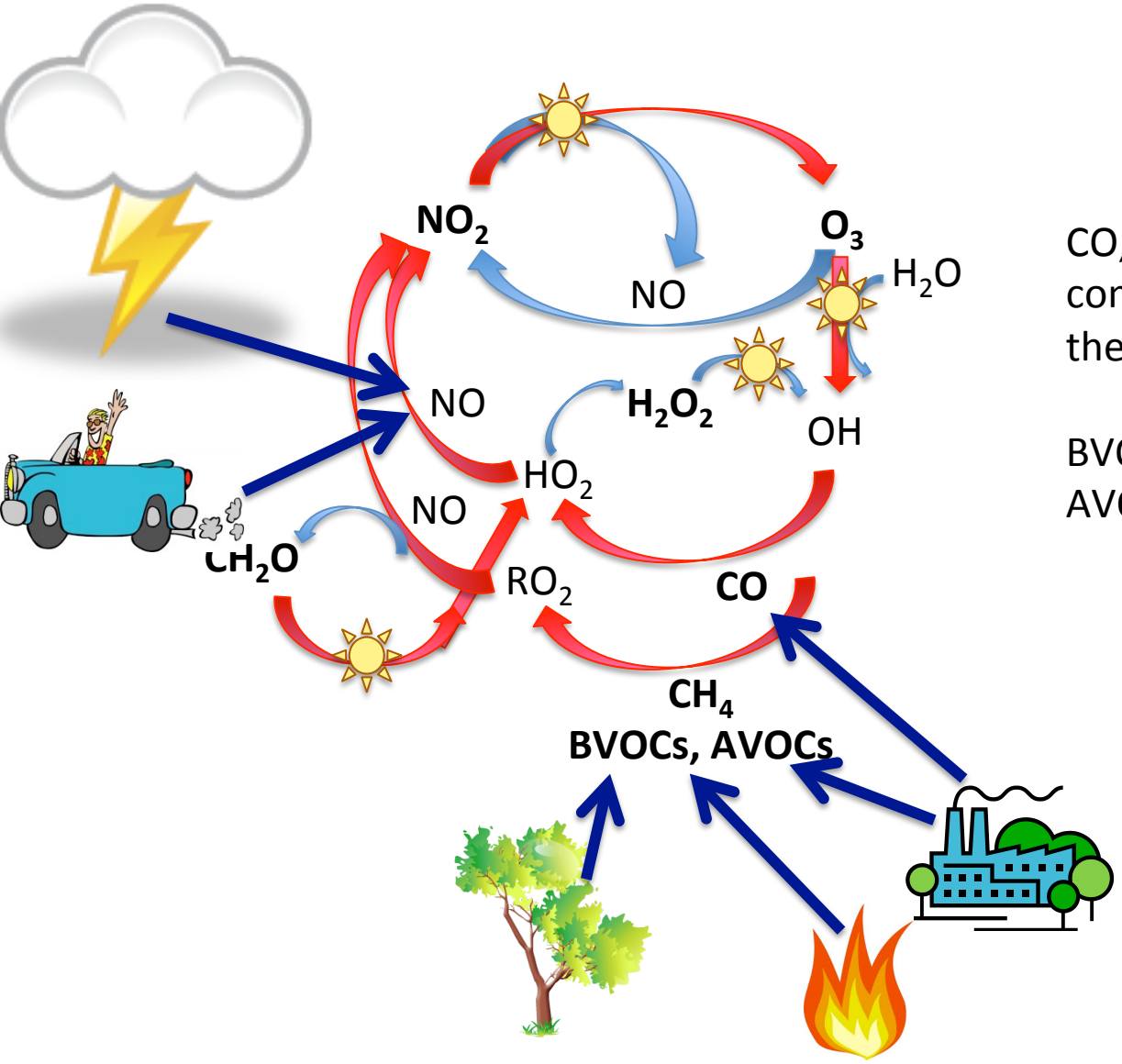
(Atmospheric Chemistry 101)



To make ozone, need
sunlight
$NO_x = NO + NO_2$
$HO_x = OH + HO_2$

HO_x precursors are CO, CH_4, and volatile organic compounds (VOCs)

Emissions and the Chemical Production of Ozone



CO, CH_4, and volatile organic compounds (VOCs) are the fuel for the chemistry

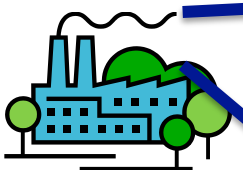
BVOC = biogenic VOC
AVOC = anthropogenic VOC

Emissions and Aerosols

Oceans

DMS

SO_2 → **SO_4**

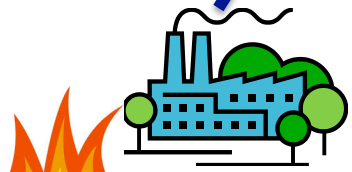


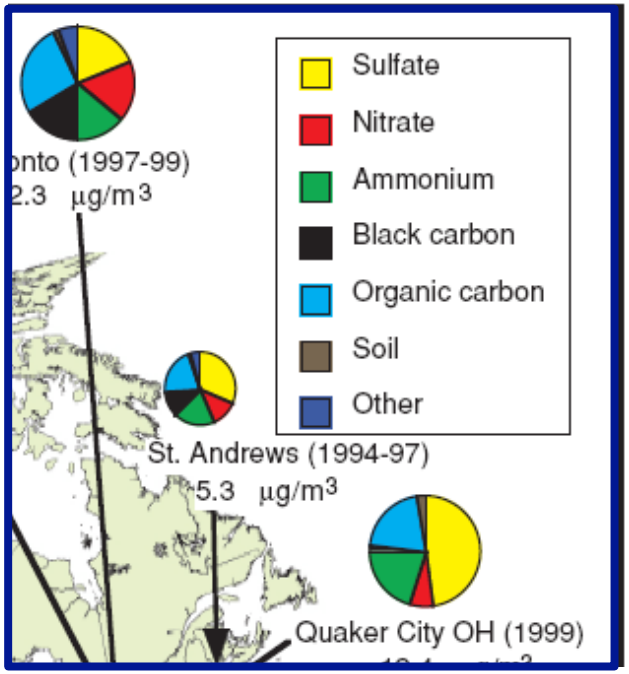
NO

$HNO_3 – NH_3 – SO_4$ equilibrium → **$(NH_4)_2SO_4$, NH_4HSO_4, NH_4NO_3** aerosols

VOC + O_3 → SVOC

SVOC + O_3 → **SOA**





(NARSTO, 2004)

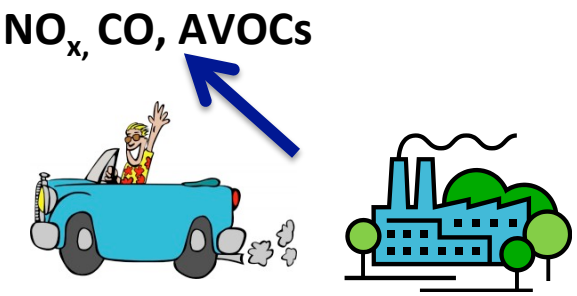
Dust, Sea salt

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

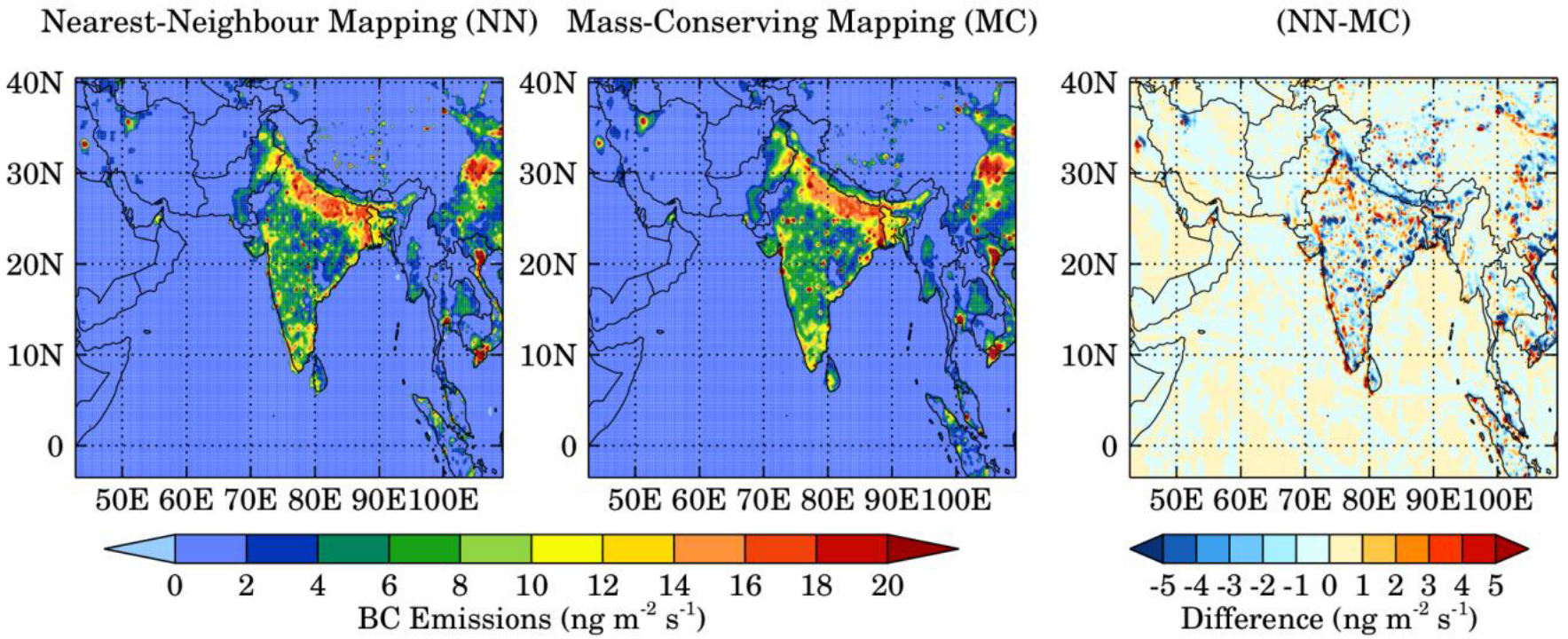
Mass conserving anthropogenic emissions preprocessor

anthro_emis: creates WRF-Chem gridded anthropogenic emission files from latitude-longitude gridded input anthropogenic emission files

- Both diurnal (wrfchemi_00z_d<nn>) and serial (wrfchemi_d<nn>_<date>) files can be created
- Capable of handling both regional and global input datasets
- Tested with MACCity, EDGAR-HTAP and SEAC4RS emission inventory
- Package includes a sample namelist file mozcart.inp
- Creates wrfchemi* files in anthro_emis directory



Benefit of Mass Conservation



The spatial patterns look similar with both the nearest neighbor and mass conserving mapping but total emissions can be different by about 10%.

Domain total emissions:

Original Inventory : 203 Gg/year

Nearest-neighbor mapping : 229 Gg/year.

Mass Conserving Anthropogenic Emissions Preprocessor

- To compile: *make_anthro*
- To run: *anthro_emis < anthro_emis.inp > anthro_emis.out*
- Example namelist "mozcart.inp" (included in download)

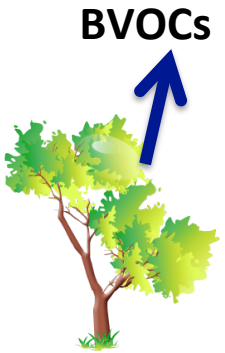
```
&CONTROL
 anthro_dir =  ' '
 src_file_prefix = 'IPCC_emissions_'
 src_file_suffix = '_surface_1850-2000_1.9x2.5.nc'
 src_names = 'CO(28)','NO(30)','BIGALK(72)','BIGENE(56)','C2H4(28)','C2H5OH(46)',
          'C2H6(30)','C3H6(42)','C3H8(44)','CH2O(30)','CH3CHO(44)','CH3COCH3(58)',
          'CH3OH(32)','MEK(72)','SO2(64)','TOLUENE(92)','NH3(17)',
          'OC(12)','BC(12)','CH3COOH(60)'
 sub_categories = 'anthro'
 emis_map = 'CO->CO','NO->NO','BIGALK->BIGALK','C2H4->C2H4','C2H5OH->C2H5OH',
         'C2H6->C2H6','C3H6->C3H6','C3H8->C3H8','CH2O->CH2O','CH3CHO->CH3CHO',
         'CH3COCH3->CH3COCH3','CH3OH->CH3OH','MEK->MEK','SO2->SO2','TOLUENE->TOLUENE',
         'NH3->NH3','OC(a)->OC','BC(a)->BC','CH3COOH->CH3COOH'
 sub_categories = 'anthro'
 serial_output     = .true.
 start_output_time = '2010-05-01_00:00:00'
 stop_output_time  = '2010-10-31_00:00:00'
 output_interval   = 86400
/
```

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 km^2 resolution



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

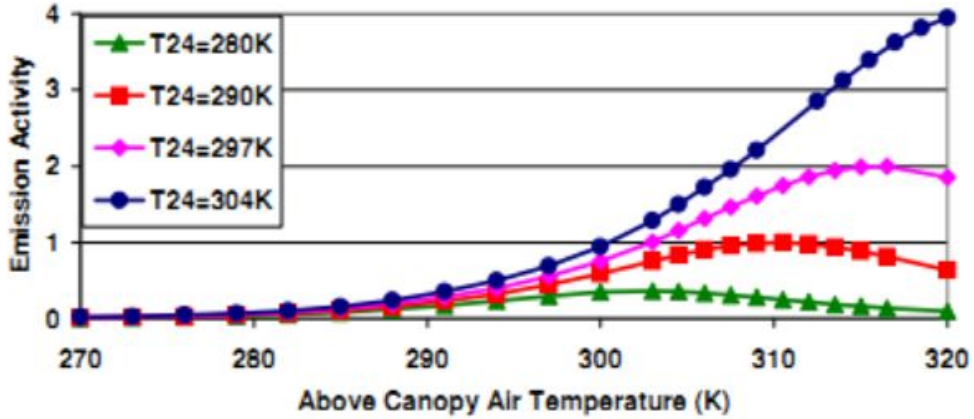
MEGAN Framework: Calculation of emissions

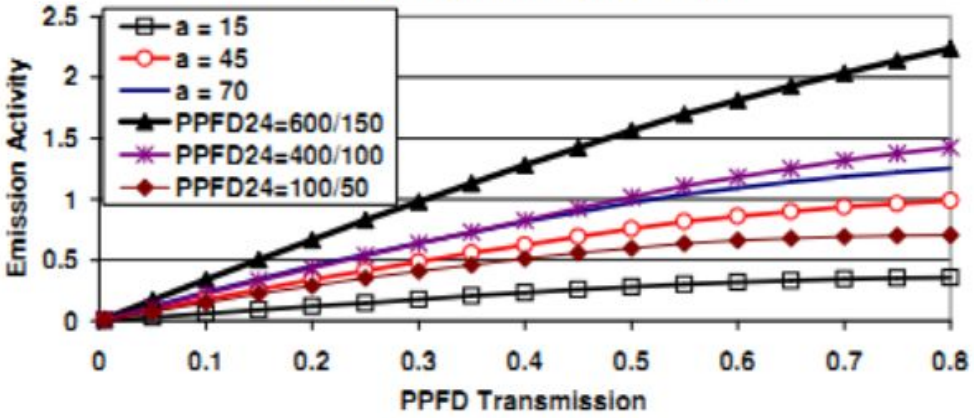
$$EM = \varepsilon \bullet \gamma_{CE} \bullet \gamma_{age} \bullet \gamma_{SM} \bullet \rho$$

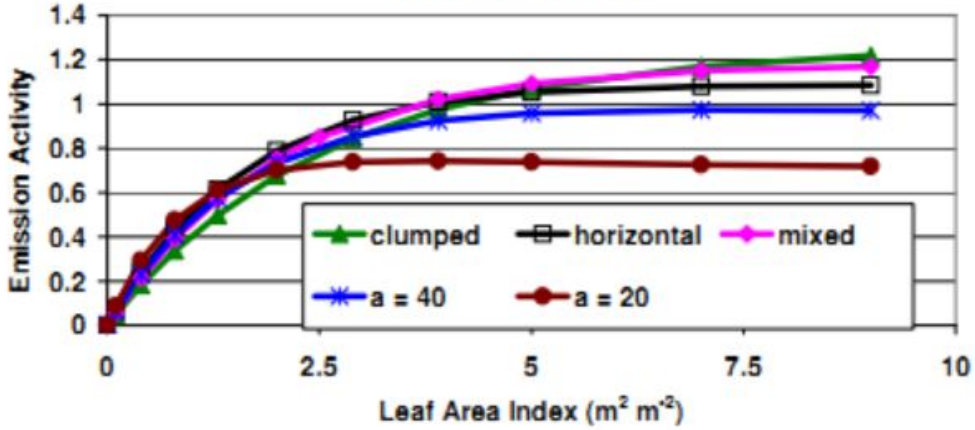
$$\gamma_{CE} = \gamma_{LAI} \bullet \gamma_{P} \bullet \gamma_{T}$$

EM: Emission (µg m^{-2} hr^{-1})
ε: Emission Factor (µg 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







Emissions increase as

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

Guenther et al., 2006, *ACP*

Emission Factors for Isoprene

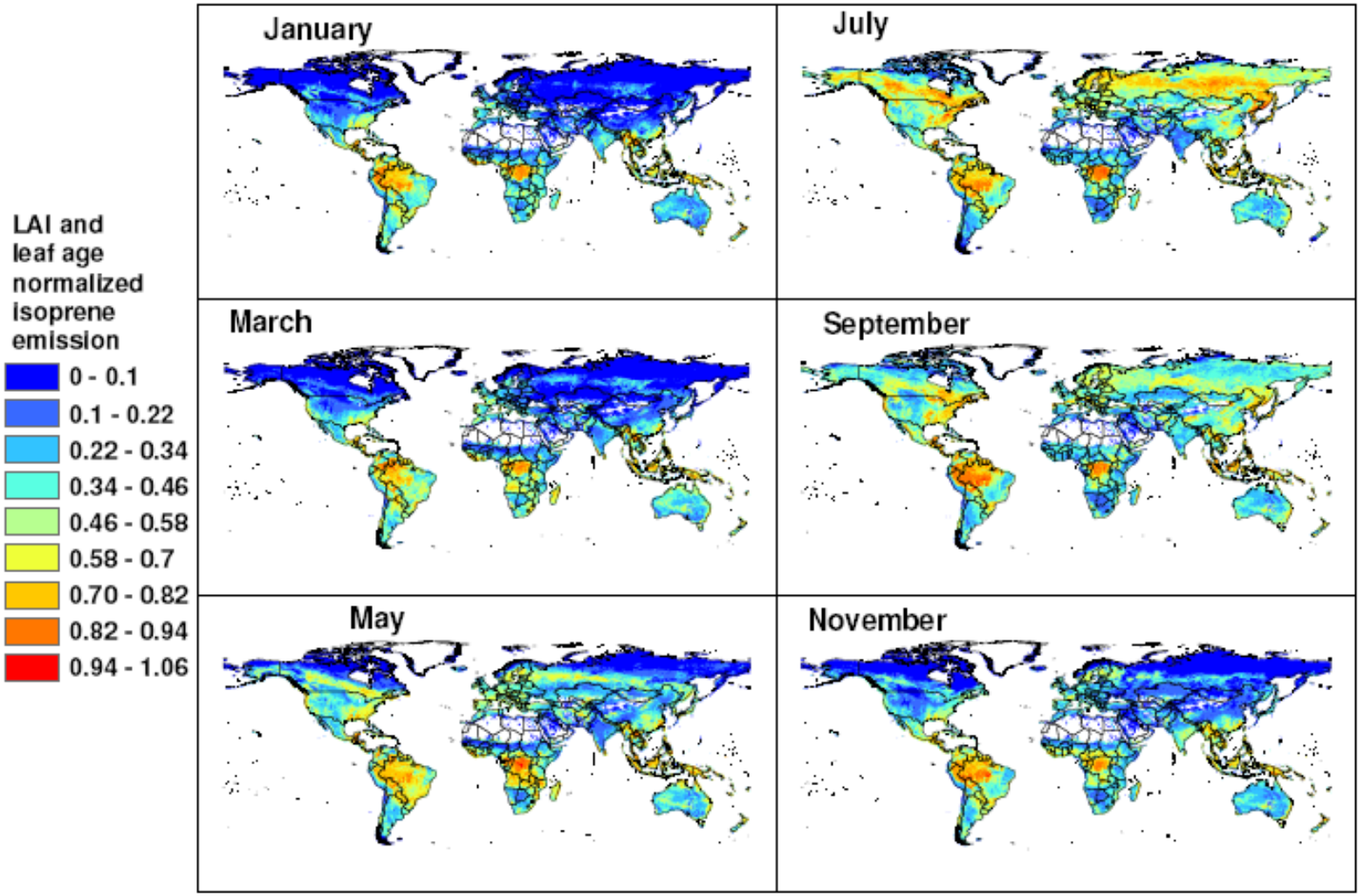
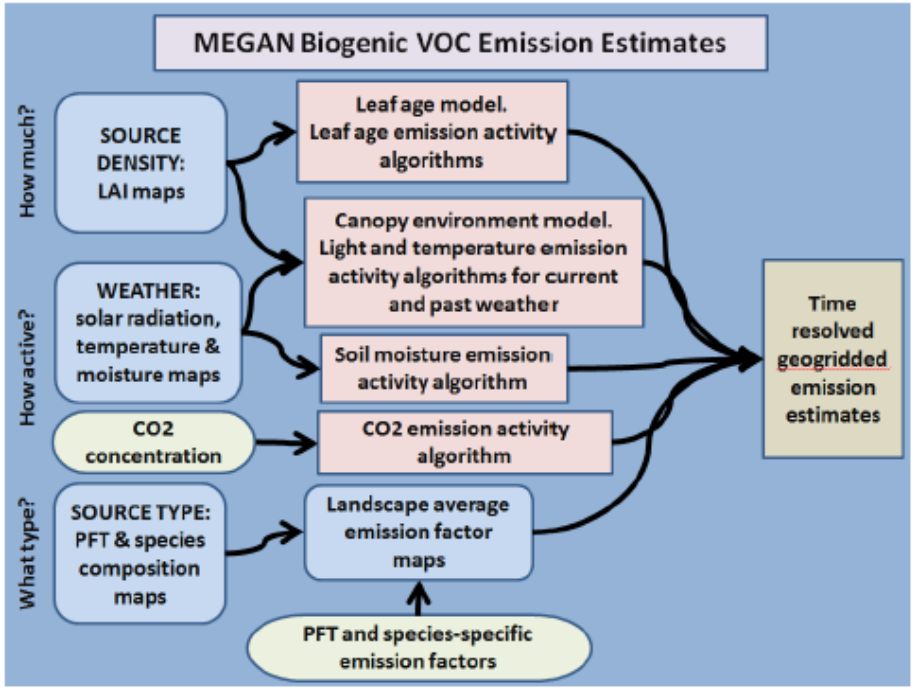


Fig. 5. Monthly normalized isoprene emission rates estimated with MEGAN for 2003. Rates are normalized by the emission estimated for standard LAI (=5 m^2 m^{-2}) and leaf age (80% mature leaves). These normalized rates illustrate the variations associated with changes in only LAI and leaf age; i.e. all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

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



from Guenther et al., 2012

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*

Read into WRF-chem simulation

Temp @ 2m
Downward Solar Radiation

Read in from model

Process 1:
Calculation of Gamma Values

Process 2:
Calculation of explicit emissions

Process 3:
Speciation of Emissions to pre-determined Mechanism:
Current Options include:
MOZART, CBMZ, SAPRC, RADM2, RACM

Return emissions to model

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

bio_emiss

Bio_emiss is a pre-processor for creating MEGAN input for WRF-Chem. To obtain bio_emiss, see the **Download** section below.

MEGAN preprocessor

- To compile:
  make_util megan_bio_emis - creates the executable *megan_bio_emiss*

- megan_bio_emiss is controlled by a namelist file (e.g. megan_bio_emiss.inp)

```
&control

domains = 3,                                  creates wrfbiochemi_dnn for three domains  (default: 1)
start_lai_mnth = 4,                           starting month for the monthly LAI (default: 1)
end_lai_mnth   = 6,                           ending month for the monthly LAI (default: 12)
wrf_dir   = '/home/me/megan/wrf_files',       path to wrfinput_dnn (default: current)
megan_dir = '/home/me/megan/30sec'              path to MEGAN input files (default: current)
/
```

- To run : *megan_bio_emiss < megan_bio_emiss.inp > megan_bio_emiss.out*

Running WRF-Chem with MEGAN

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

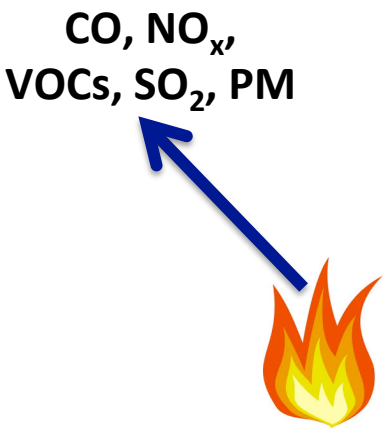
```
&time_control   (activate settings only either during real.exe or initial wrf.exe)
   auxinput6_interval_h      = 24
   auxinput6_inname          = 'wrfbiochemi_d01',
   io_form_auxinput6         = 2,

&chem
   bio_emiss_opt = 3
   bioemdt = your choice     (minutes)
```

Fire Emissions: Fire INventory from NCAR (FINN)

Daily fire emissions calculated with FINNv1

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$_i$ /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.

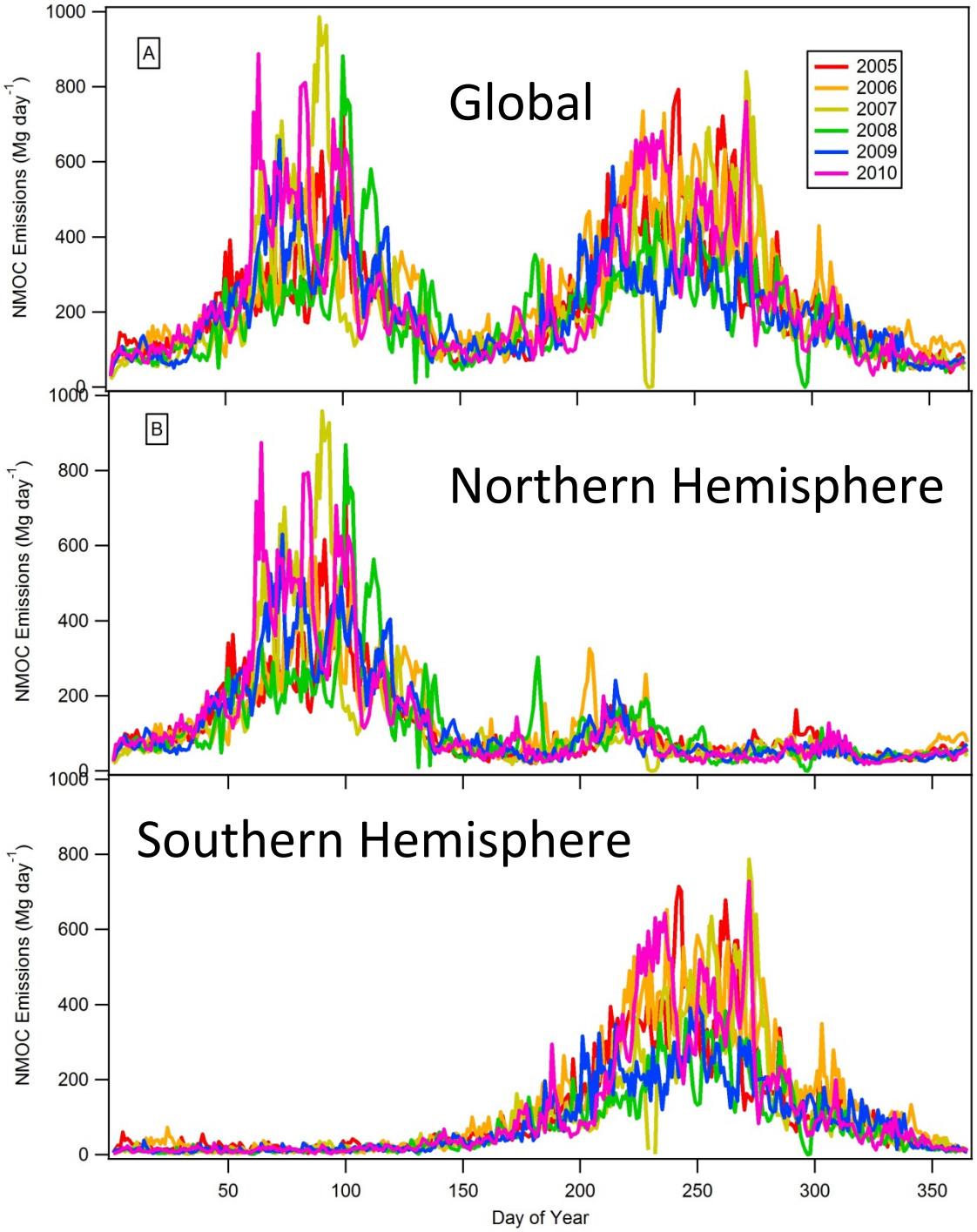
Speciation of VOCs provided for MOZART-4, SAPRC99, GEOS-Chem

Plume rise option available- *but requires additional inputs*

Global Daily Emissions

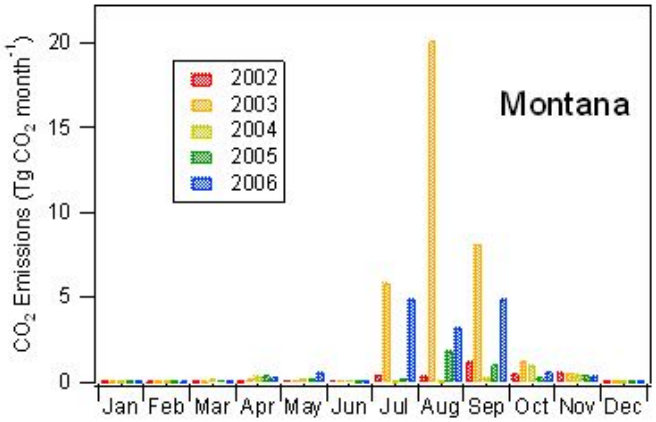
Emissions highly variable

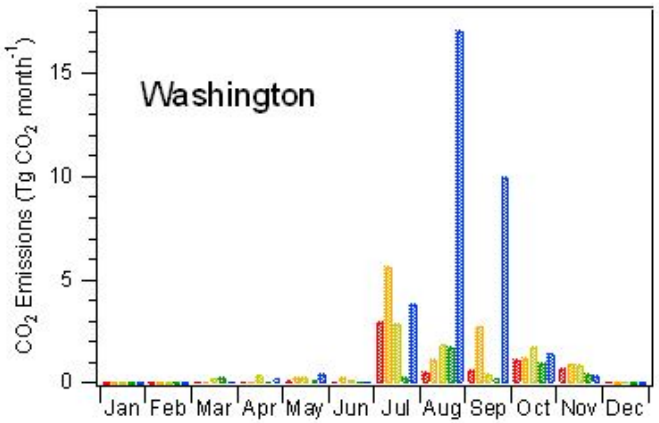
- Daily
- Season
- Spatial

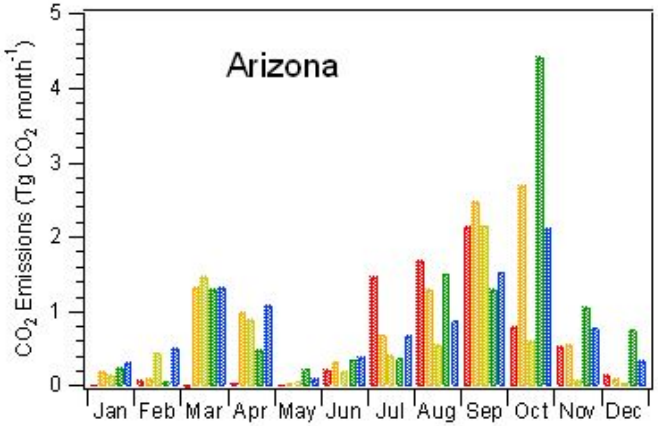


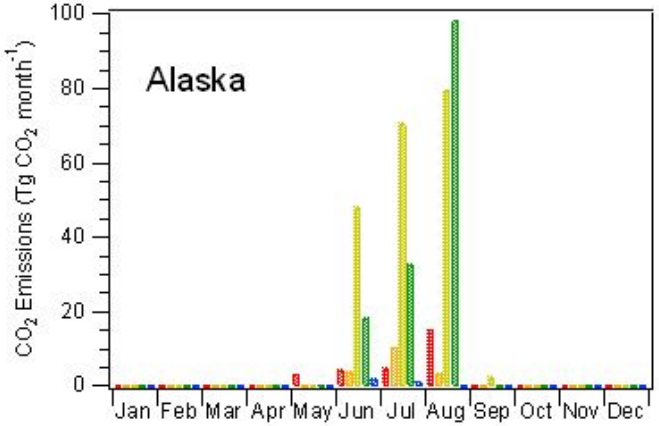
Wiedinmyer et al., *GMD*, 2011

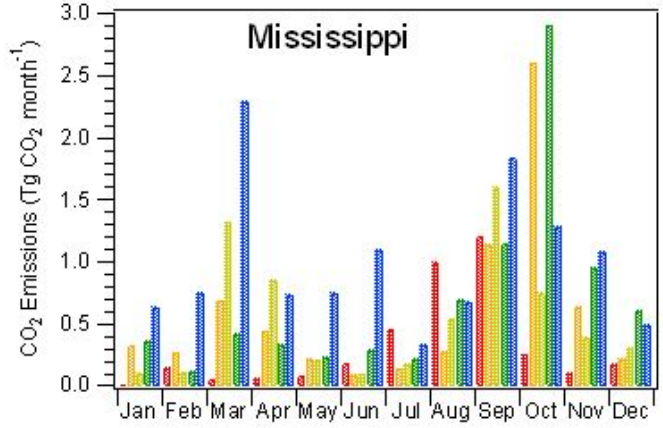
Fire Emissions Variability:
-Spatial
-Temporal

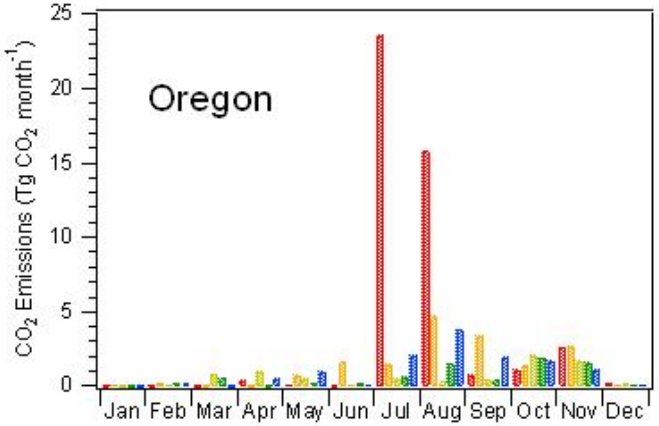












Wiedinmyer and Neff,
Carbon Balance and Management,
2007

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 compile: *make_fire_emis*
- To run: *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.
```

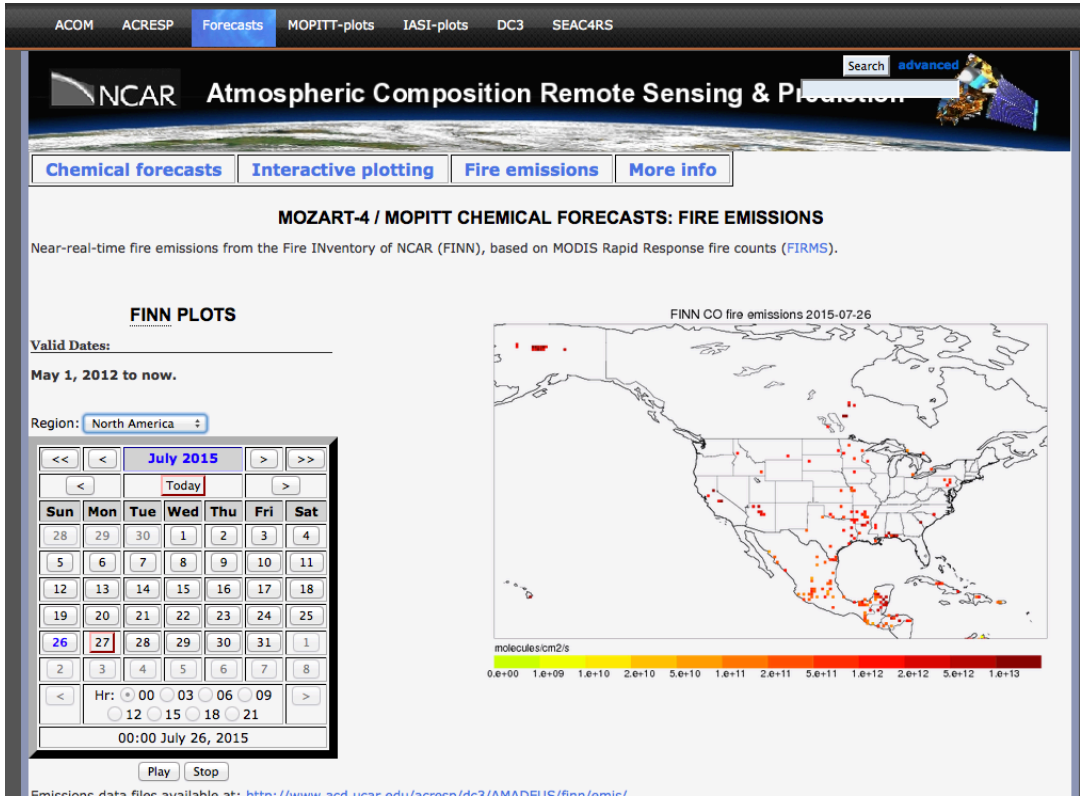
Fire INventory from NCAR (FINN)

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/



Lightning-NO_x Emissions

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

When lightning is triggered,

- Temperature increases to 1000s degrees
- This splits many molecules including N_2 and O_2

When temperature drops to normal,

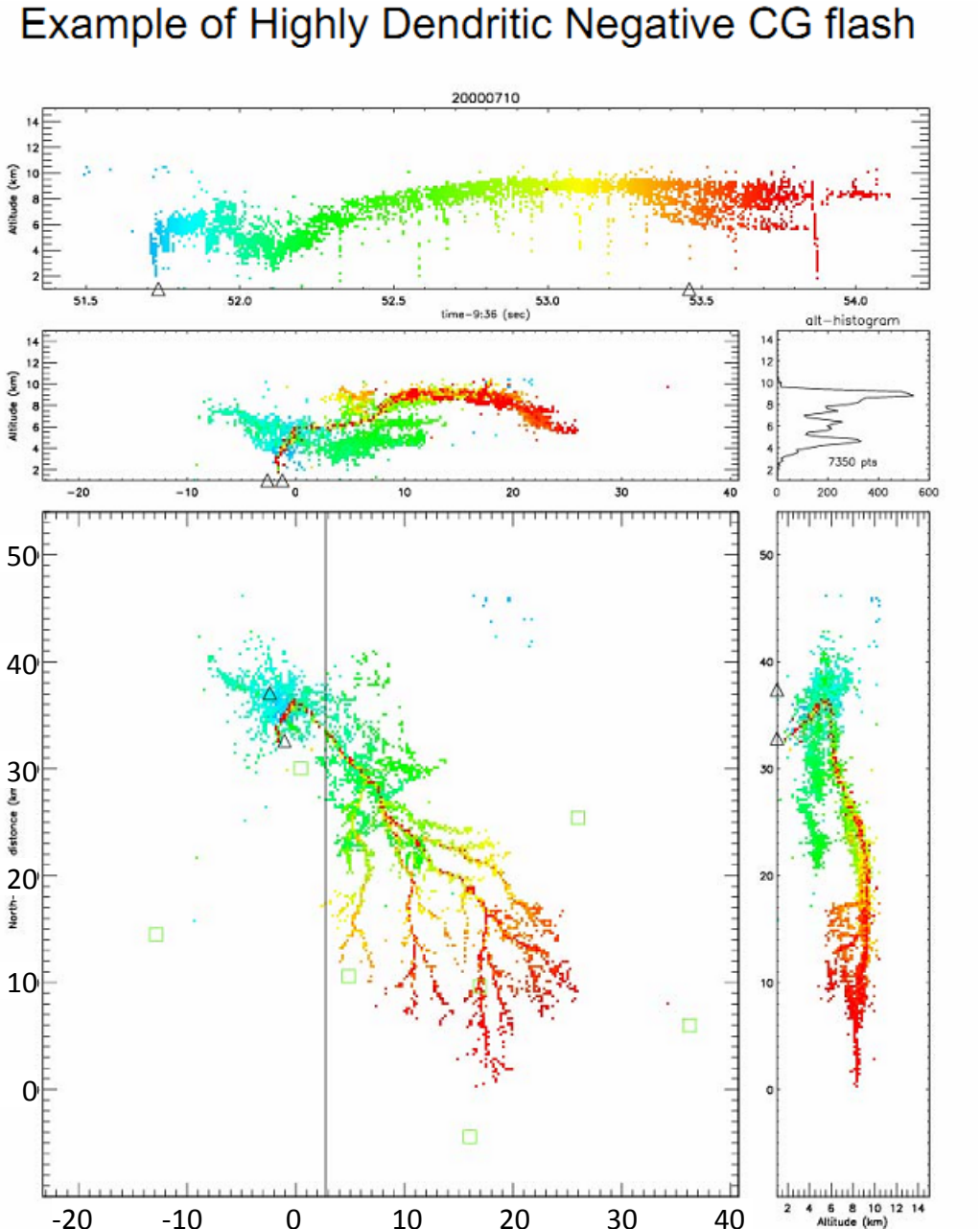
- Some of the N and O atoms recombine with each other

→ 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



- 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)	cloud top height
– Price and Rind (1993)	maximum vertical velocity
– Deierling (2006);	precipitation ice mass
– Wiens et al. (2005)	updraft volume
– Deierling et al. (2008)	ice mass flux product
– Petersen et al. (2005)	ice water path

Precipitating Ice = mostly graupel and hail but includes snow

Ice mass flux product

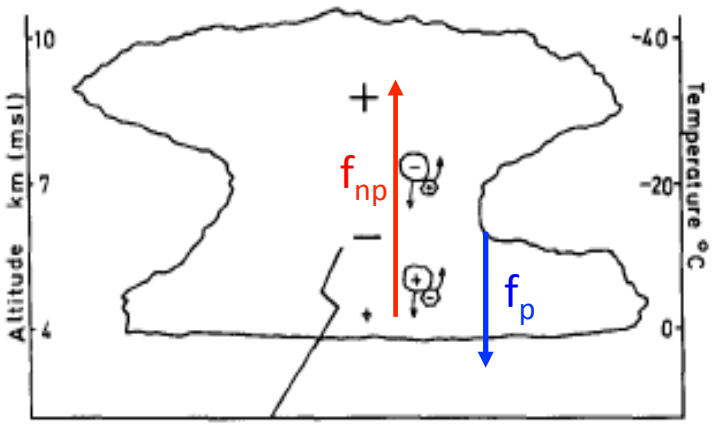


FIG. 2. A schematic of graupel–ice-crystal charge transfer above and below the reversal temperature level in a thunderstorm.

1) Predicting Lightning Flashrate

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

  Flashrate = $5.7 \times 10^{-6}\ w_{max}^{4.5}$ (option 1)

  Flashrate = $3.44 \times 10^{-5}\ H^{4.9}$ (option 2)

  H = cloud top height of the 20 dBZ contour

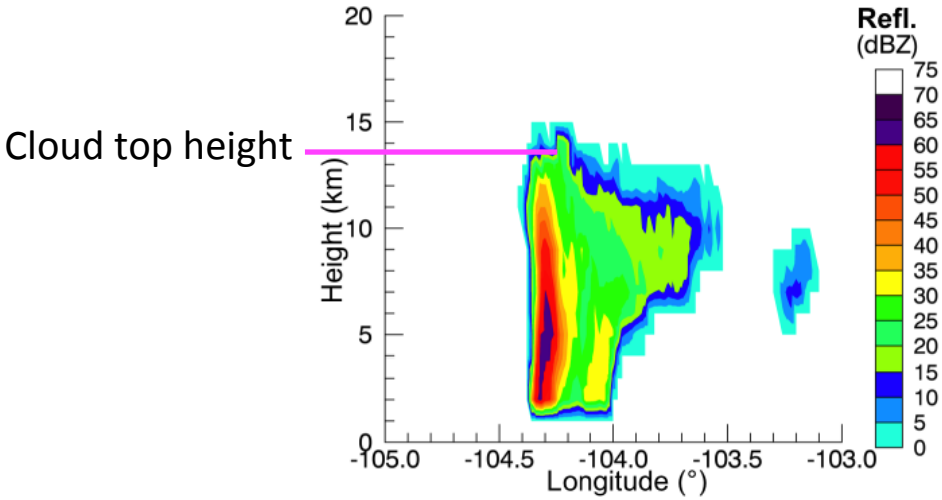
- Convective-parameterized parameterization: Wong et al., GMD,

  Flashrate = $3.44 \times 10^{-5}\ H^{4.9}$ (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

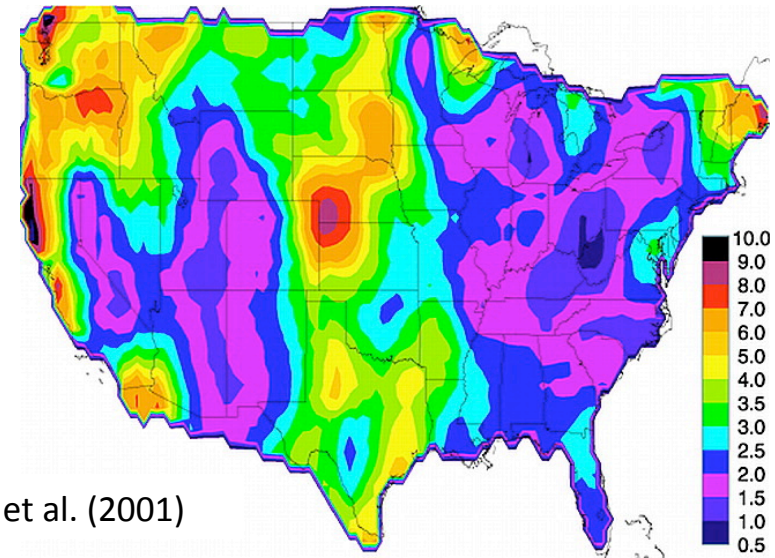
- Prescribed Values
  - 1) Set to a specified value everywhere
  - 2) Set to a very coarsely prescribed climatology (Boccippio et al., 2001)
  - 3) Gridded input – need to provide input

- 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



Boccippio et al. (2001)

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

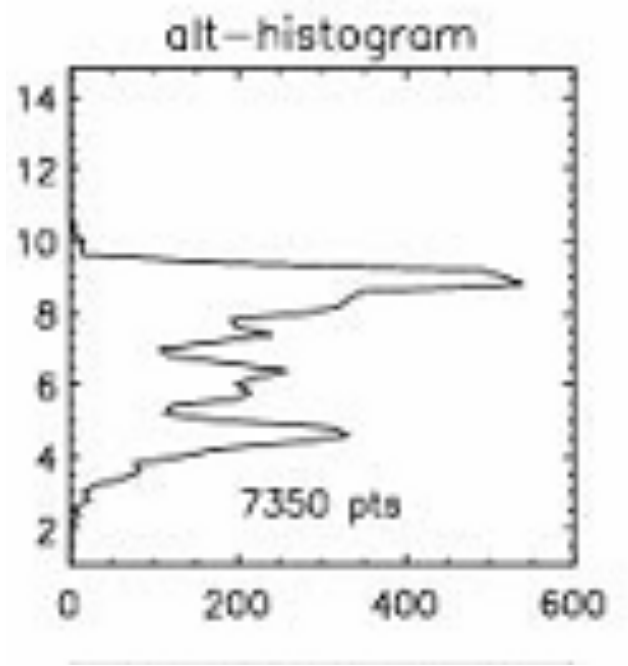
  → looks pretty good for Colorado storms, but 10 dBZ may be a better number elsewhere

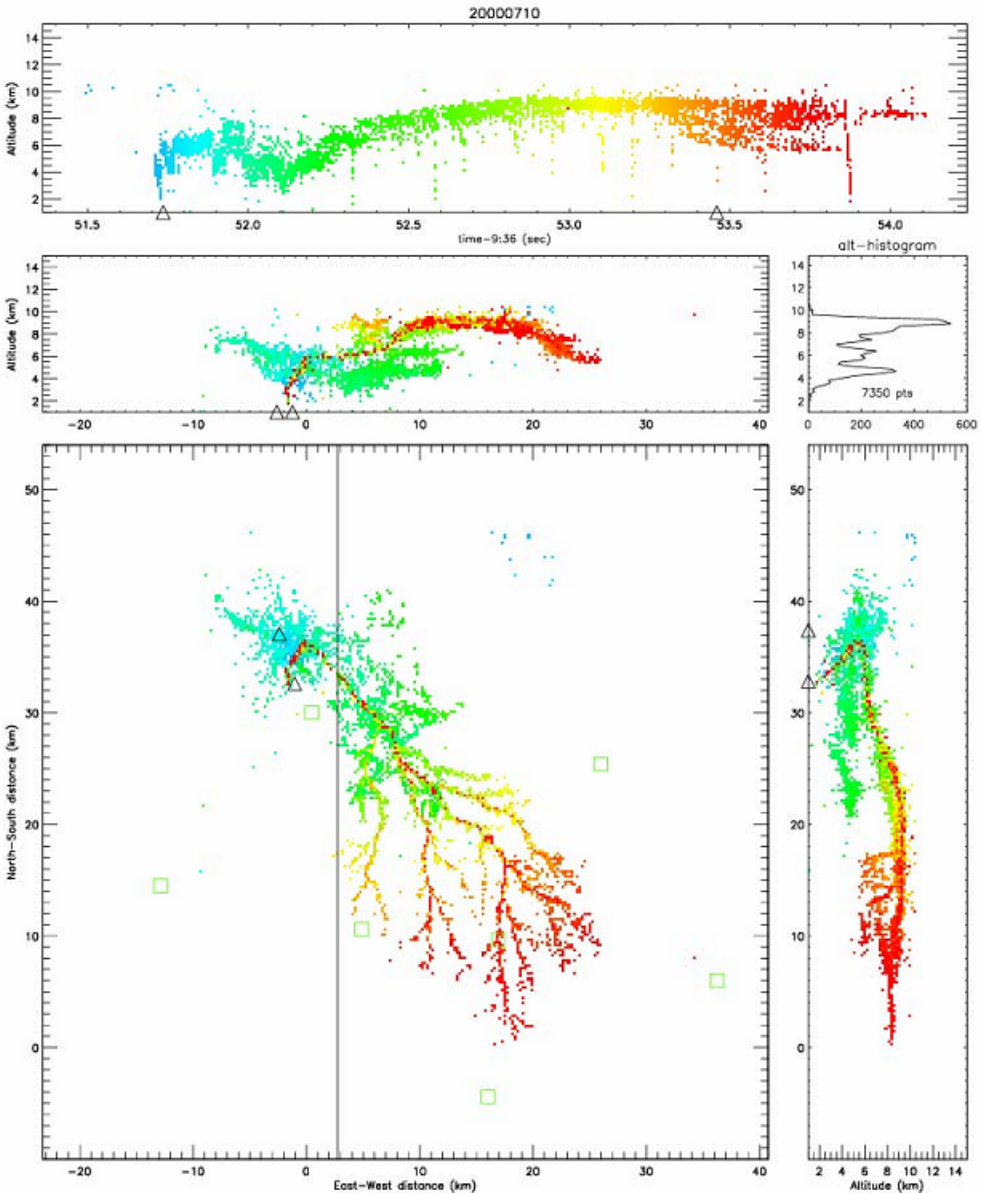
- Convective-parameterized parameterization: Wong et al., 2012

  Placed throughout the grid cell

3) Determine where to put the NO emissions

Vertical Placement





3) Determine where to put the NO emissions

Vertical Placement

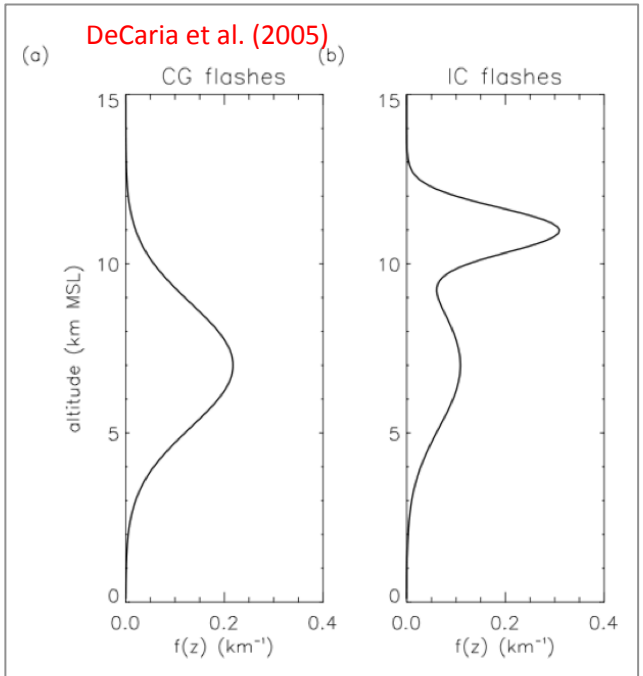
- Cloud-resolving parameterization: Barth et al., ACP, 2012

  Uses DeCaria et al. (2005) curves

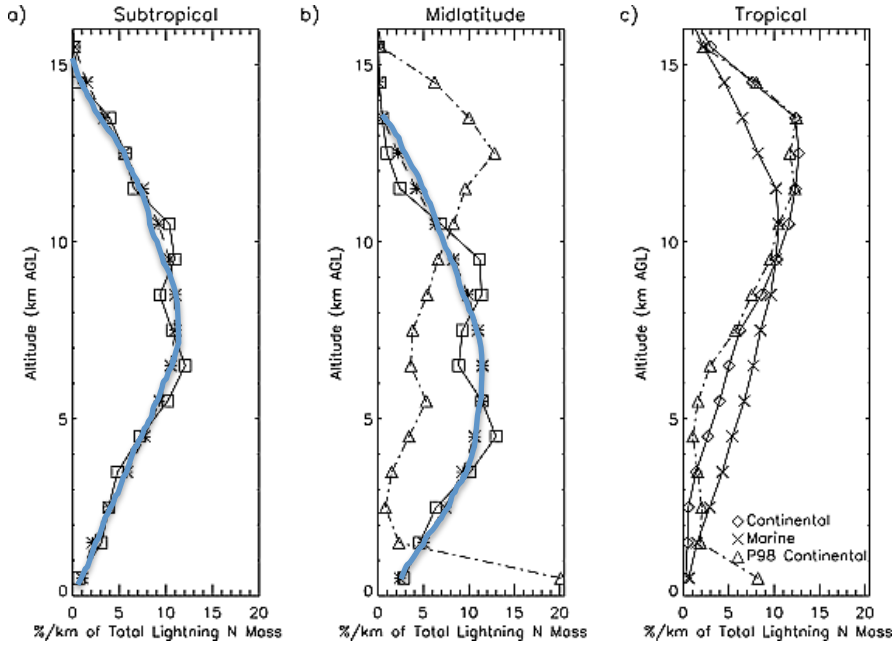
- Convective-parameterized parameterization: Wong et al., GMD,

  Uses Ott et al. (2010) curves

DeCaria et al. (2005)



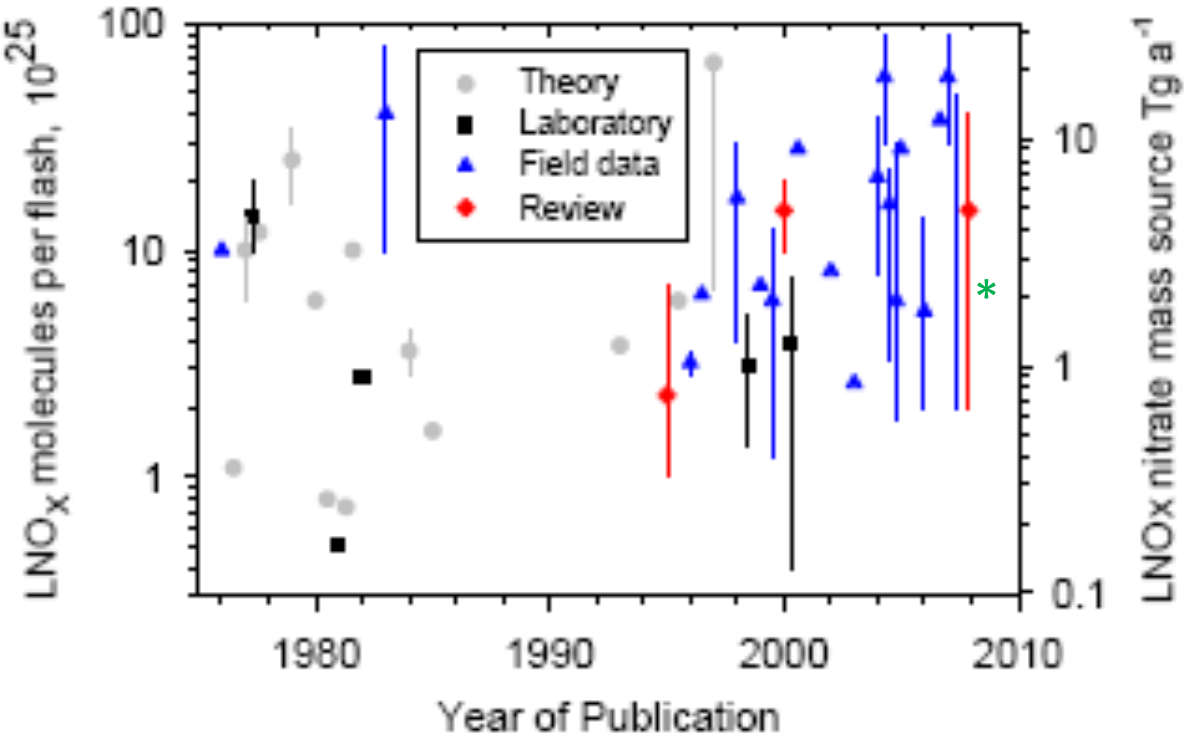
Ott et al. (2010)



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



107 – 291 moles/flash

Pollack et al. (2015, submitted)

Note:
Ongoing research to find "a good number" to use.
This number is often adjusted when evaluating model results with observations.

Running WRF-Chem with Lightning-NOx emissions

```
&physics
      lightning_option                    = 11,   1,
      iccg_method                         = 2,    2,
      lightning_dt                        = 75,   75,
      cellcount_method                    = 0,    1,
      lightning_start_seconds             = 600,  600,
      flashrate_factor                    = 20.,  1.,
      cldtop_adjustment                   = 0,    0,

&chem
      lnox_opt                            = 1,    2,
      N_IC                                = 125., 500.,
      N_CG                                = 125., 500.,
```

parameterized convection

cloud resolving convection

See WRF-Chem Users Guide for option choices

Chemical Boundary Conditions

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.

Chemical Boundary Conditions

mozbc – set chemical initial and lateral boundary conditions

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

Chemical Boundary Conditions

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 }
met_file_suffix   = '.nc'                 suffix string for the WRF meterological files (default: '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)

Chemical Boundary Conditions

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. O_3 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

Download input files for running WRF-Chem V3.3.1 with Chemical Upper Boundary Conditions: UBC_inputs.tar

Contact the following people with your questions

NCAR Preprocessors: Stacy Walters stacy@ucar.edu
Gabriele Pfister pfister@ucar.edu
FINN emissions: Christine Wiedinmyer christin@ucar.edu
MOZART data files: Louisa Emmons emmons@ucar.edu
Lightning emissions: Mary Barth barthm@ucar.edu

NO

BVOCs

CO, NO_x, VOCs, SO_2, PM