Emissions Data Tools for Use with WRF-Chem

Steven Peckham

Emissions Data

- Several tools are available to help generate emissions
  - **Prep_chem_sources**
    - Anthropogenic
    - Biogenic (included in anthropogenic)
    - Biomass Burning
    - GOCART Background fields
    - Volcano
  - Anthro_emiss (NCAR/ACD) – limited testing (MOZART & CAM)
  - **MEGAN** (NCAR/ACD)
    - Biogenic emissions
  - FINN (NCAR/ACD)
    - Biomass Burning (retrospective simulation)
  - Emiss_v03 (NOAA)
    - Anthropogenic (USA only)
  - Others
    - SMOKE (US EPA)

Generating Emissions Fields for WRF-Chem with PREP-CHEM-SRC

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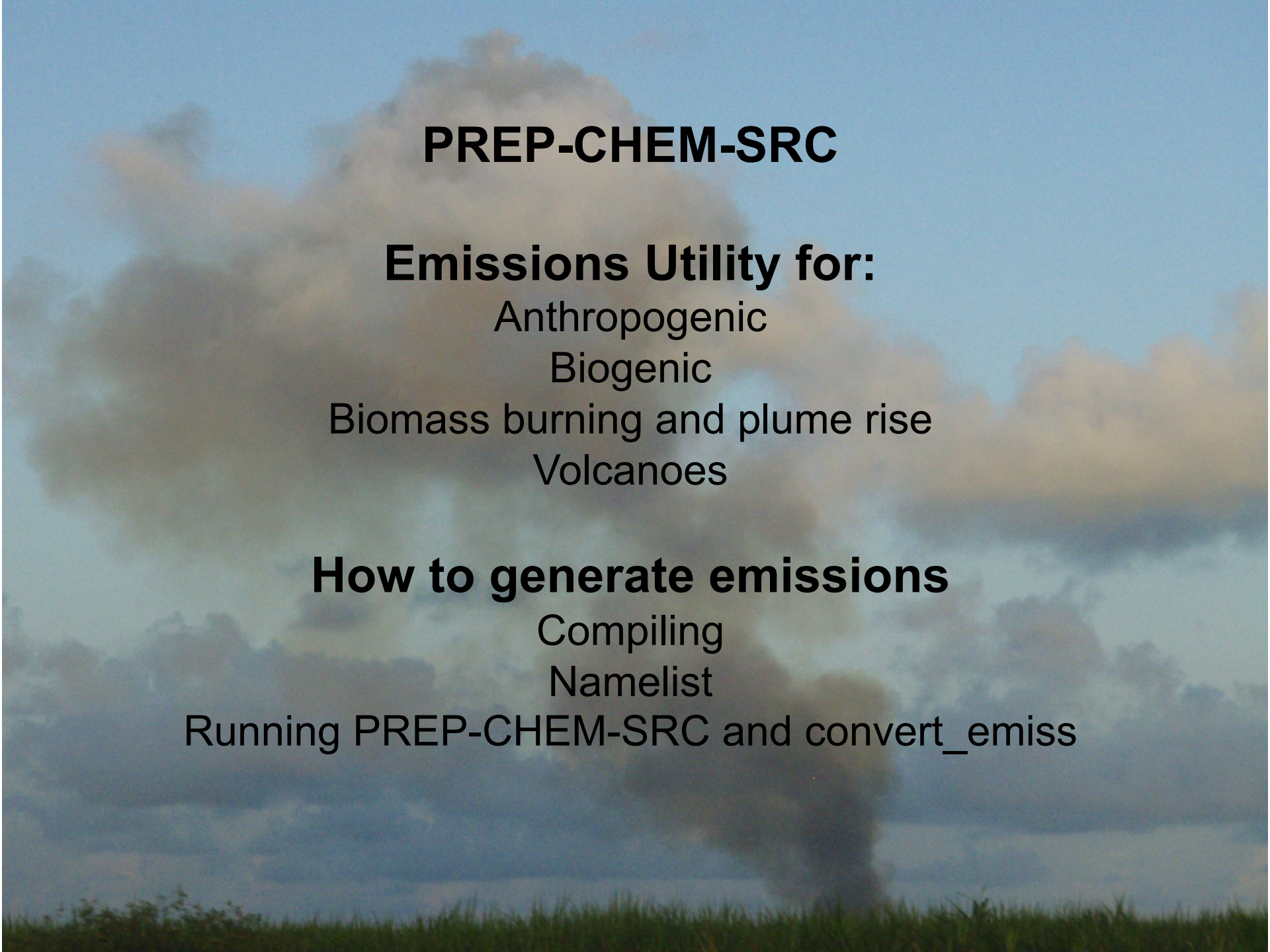

PREP-CHEM-SRC
Emissions Utility for:
Anthropogenic
Biogenic
Biomass burning and plume rise
Volcanoes
How to generate emissions
Compiling
Namelist
Running PREP-CHEM-SRC and convert_emiss

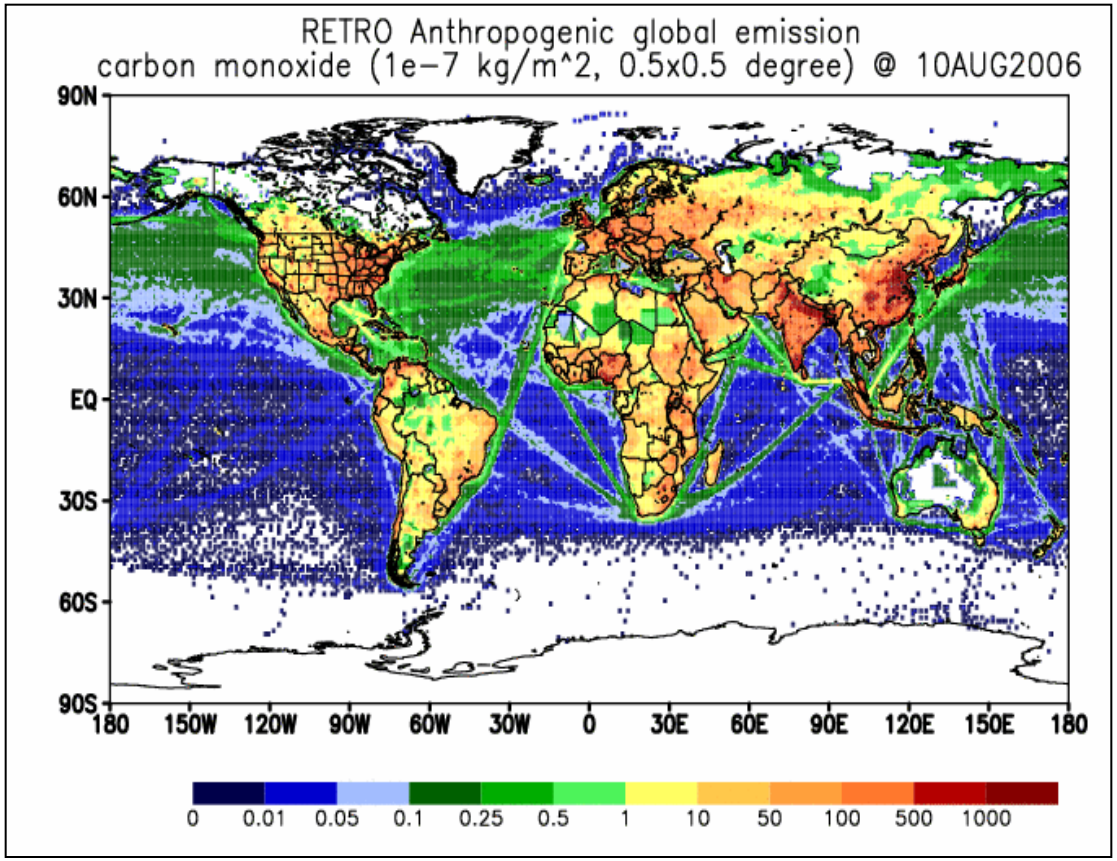
Anthropogenic emissions

Global Inventories

RETRO (0.5^0 x 0.5^0, monthly, 1960-2000)

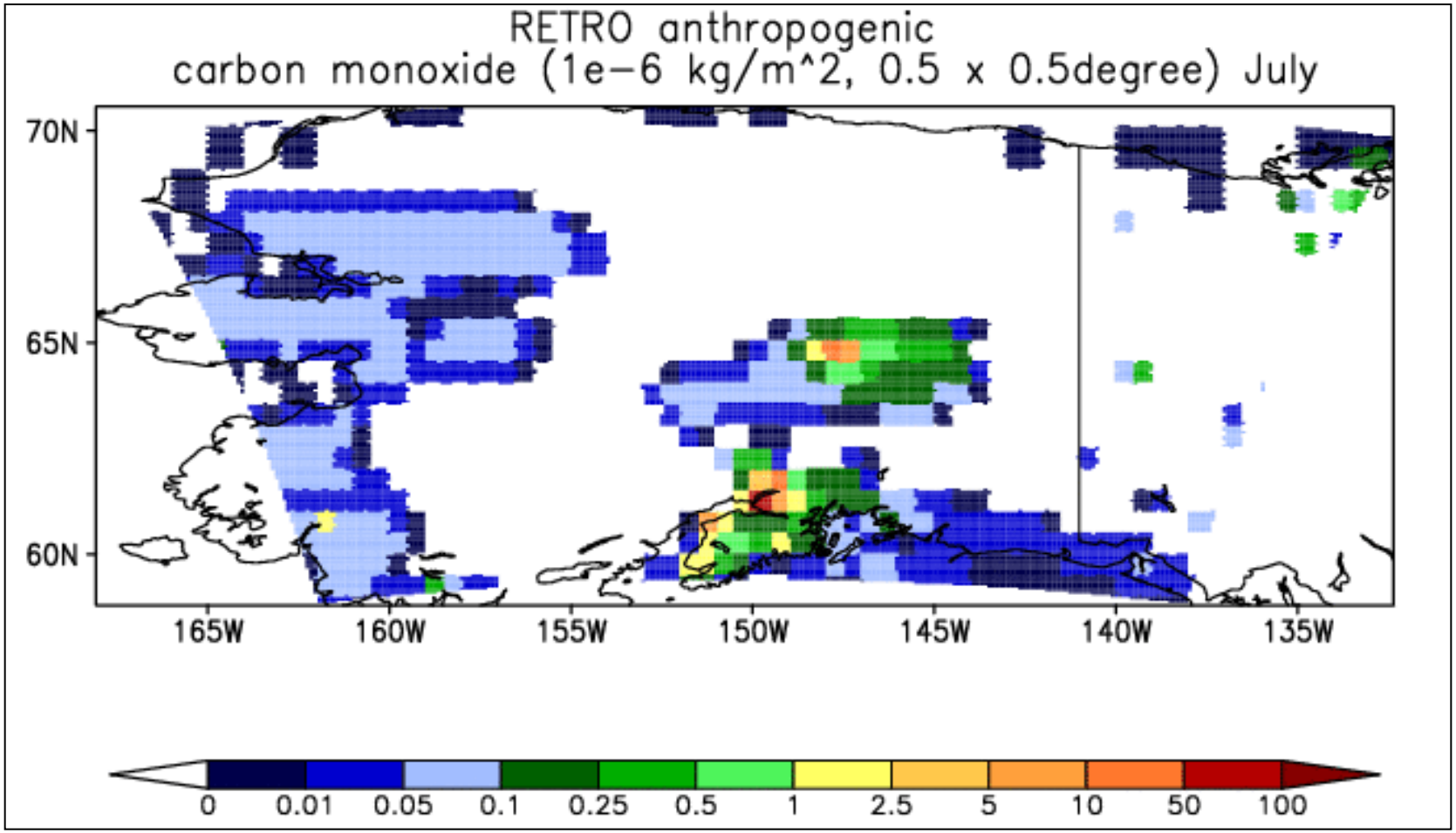
EDGAR v4.2 (0.1^0 x 0.1^0, annual,1970-2008)
CO_2, CH_4, N_2O, HFCs, PFCs, SF_6

GOCART
OC, BC and SO_2 (1^0 x 1^0, annual, 2006)
DMS (1^0 x 1.25^0, monthly)
NO_3, H_2O_2 and OH (3D, 1^0 x 1.25^0 monthly, 2006)



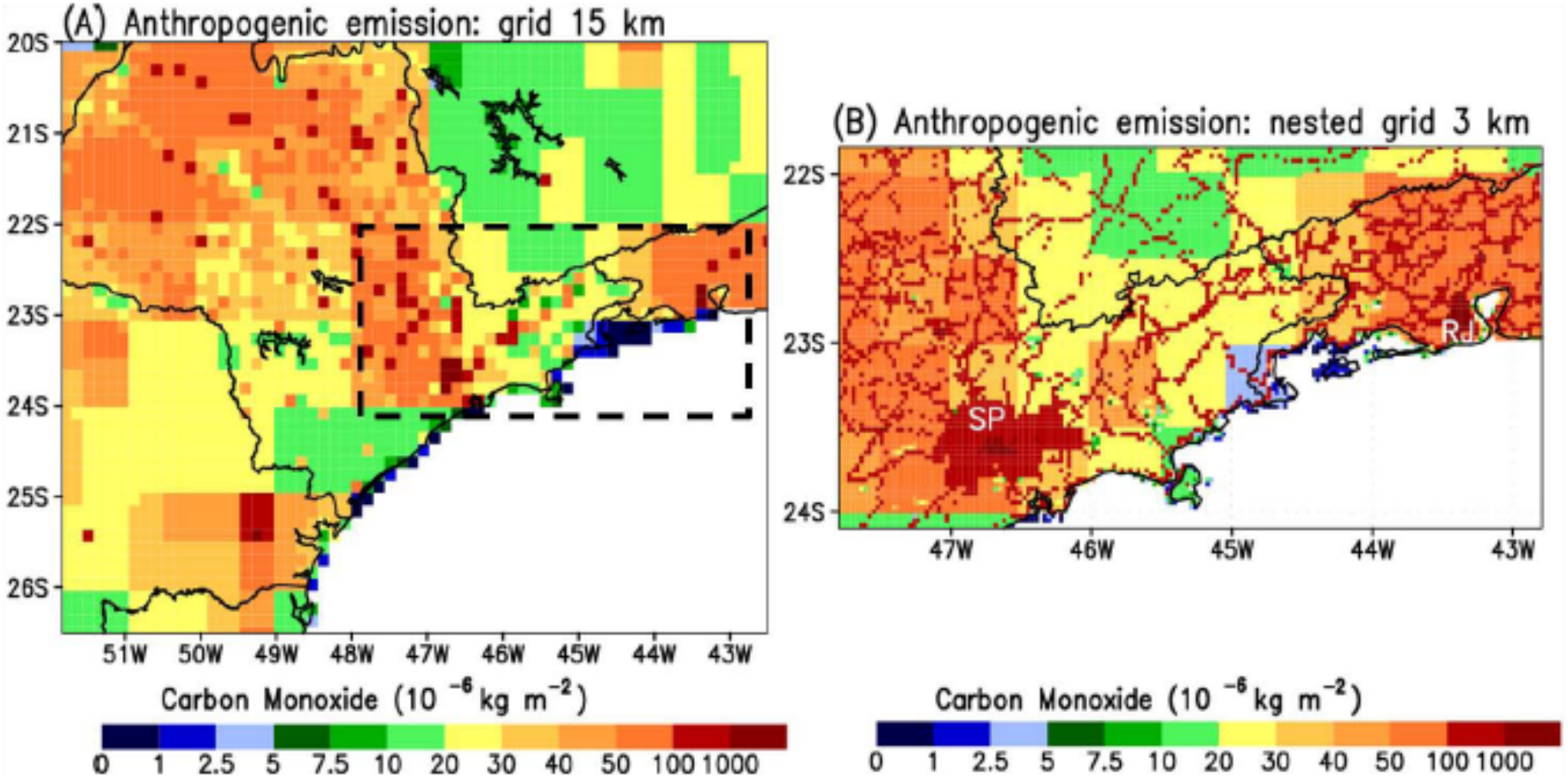
Anthropogenic emissions

Example for Alaska



Anthropogenic emissions

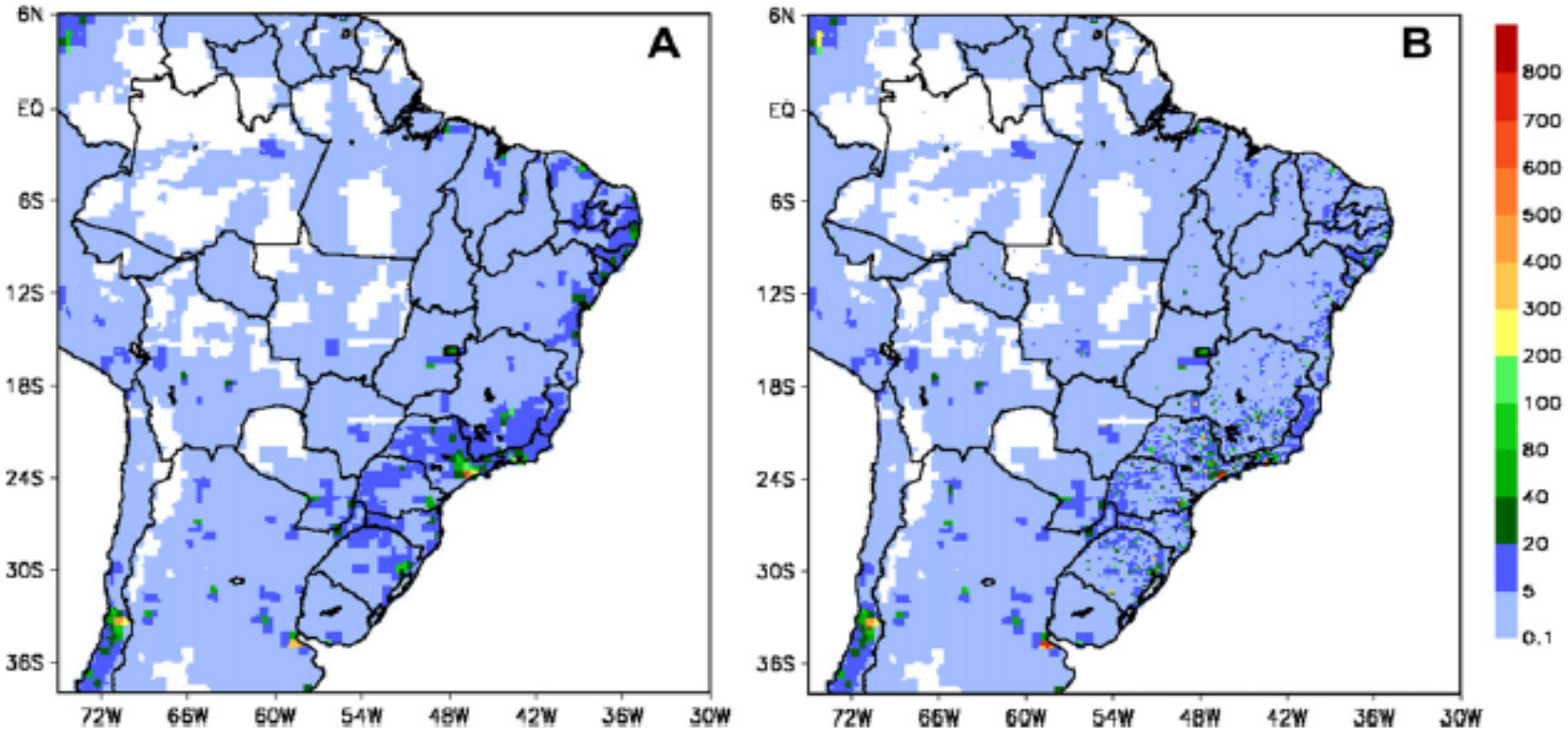
AREA DELIMITER algorithm distributes emissions on high resolution grids



Alonso et al. (2010)

Anthropogenic emissions

South America: Updated local inventories and extrapolation to cities without inventories based on socioeconomic data



CO emissions (x10^6 kg m^2 day^{-1})) on a 20 km grid covering South America without (A) and with (B) updated inventories

Alonso et al. (2010)

Biogenic emissions (if bio_emiss_opt=0)

1) GEIA

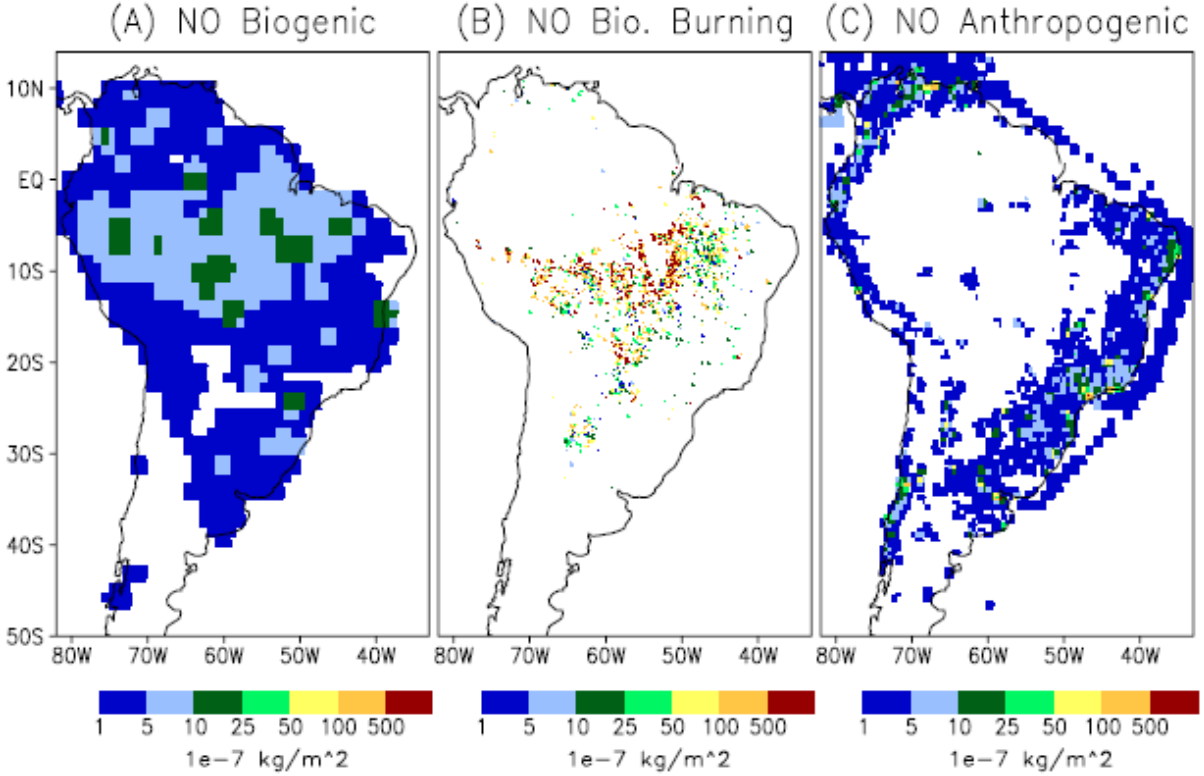
1^0 x 1^0, monthly, 2002

Acetone, C_2H_4, C_2H_6, C_3H_6, C_3H_8, CO, CH_3OH, DMS, NO, Isoprene, Terpenes and NVOC

2) MEGAN 2000 climatology

0.5^0 x 0.5^0, monthly, 2000

CO, CH_4, C_2H_4, C_2H_6, C_3H_6, C_3H_8, CH_3OH, Formaldehyde, Acetaldehyde, Acetone, other Ketones, Toluene, Isoprene, Monoterpenes and Sesquiterpenes



Daily emissions from (A) GEIA (B) 3BEM (C) RETRO for 27 August 2002 on a 0.2^0 grid

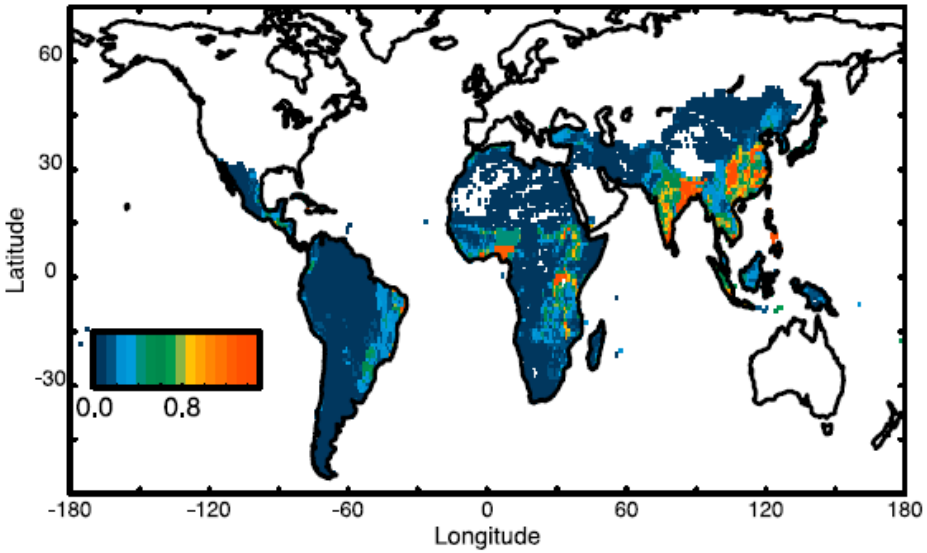
Alonso et al. (2010)

Biomass burning in the developing world

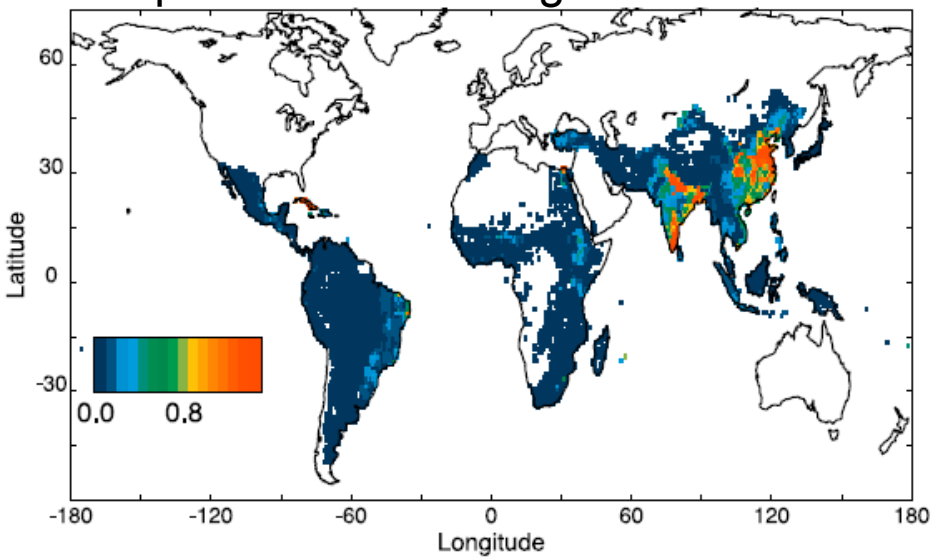
Emissions_Yevich_Logan

$1^0 \times 1^0$, Tg dry matter yr^{-1}

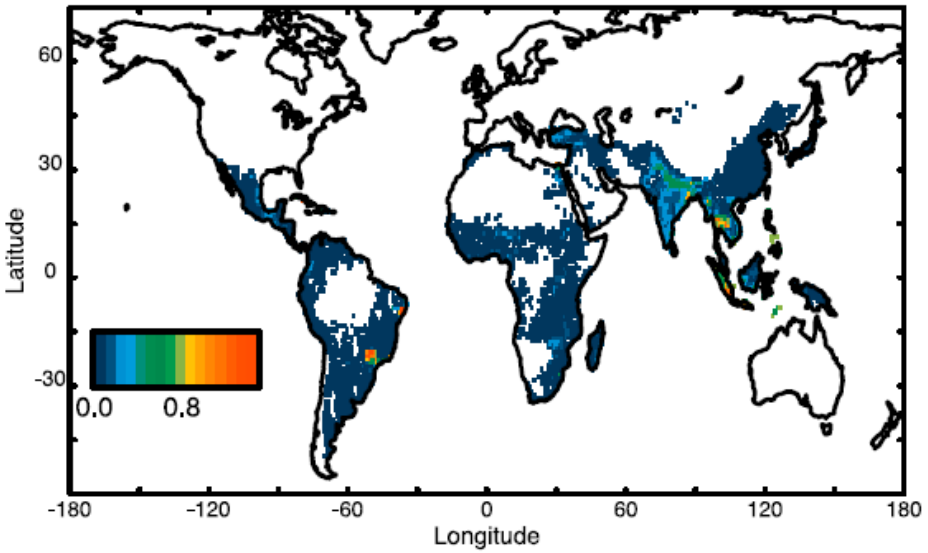
Woodfuel (fuelwood and charcoal) use



Crop residue and dung use



Burning of agricultural residue in the fields

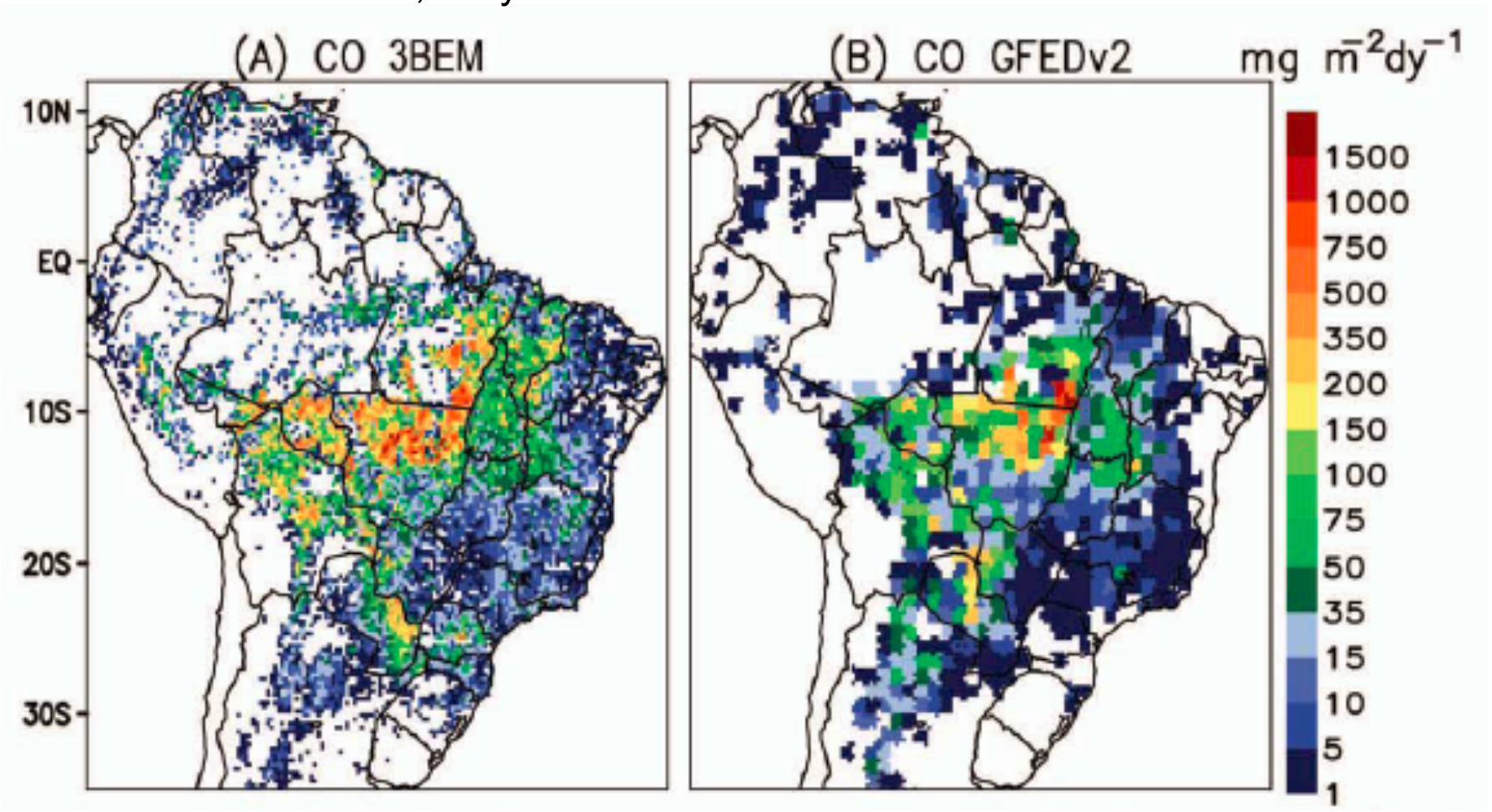


Yevich and Logan, 2003

Biomass burning emissions

Brazilian Biomass Burning Emission Model (**3BEM**)
Model resolution, daily

Global Fire Emissions Database (**GFEDv2**)
1^0 x 1^0, 8-day or monthly, 1997 - 2004

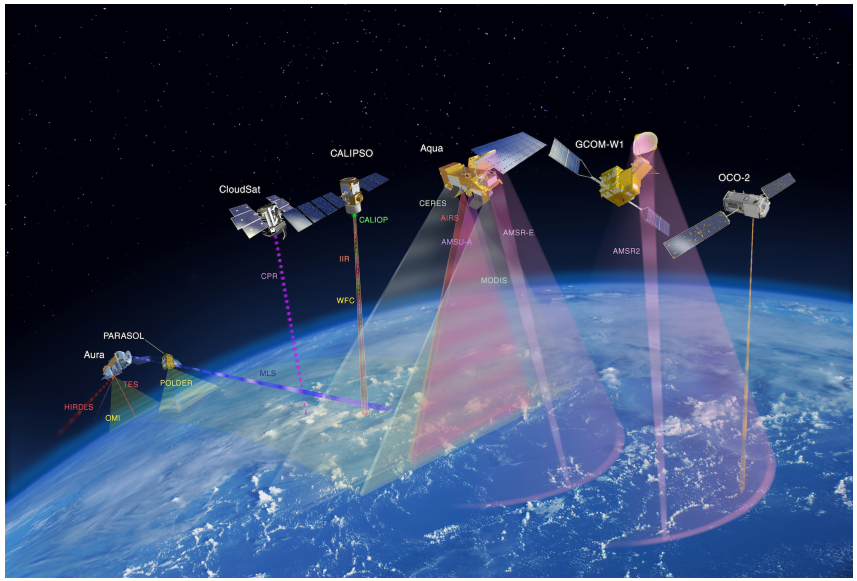


Average daily CO emissions, Aug.-Oct. 2002, 35 km

Freitas et al. (2011)

Wildfire Satellite Data

- Moderate-Resolution Imaging Spectroradiometer (MODIS) instruments on NASA's Aqua and Terra satellites.
  - Daily global 1km fire data
  - Available in real-time
    - https://earthdata.nasa.gov/data/near-real-time-data/firms
  - Data archives can be found online
  - Reads text (.txt) data files

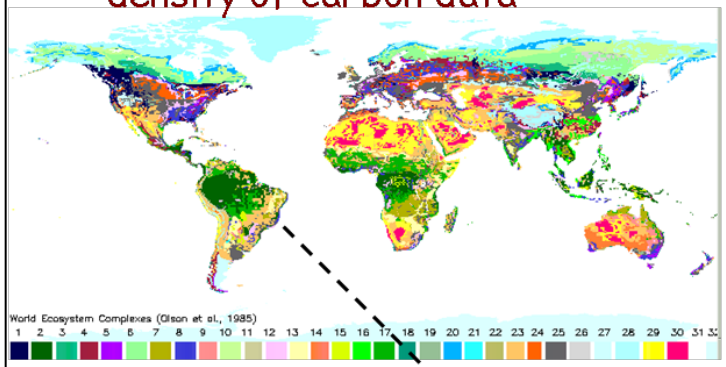


- GOES, MET, MTSAT
  - Automated Biomass Burning Algorithm (ABBA) fire products (http://wfabba.ssec.wisc.edu)
  - Derived from radiances from bands 1 (visible), 2 (3.9 micron), and 4 (11 micron)
  - Available in real time (GOES: North & South America domain, MET-9: Africa, MTSAT: Austrailia)

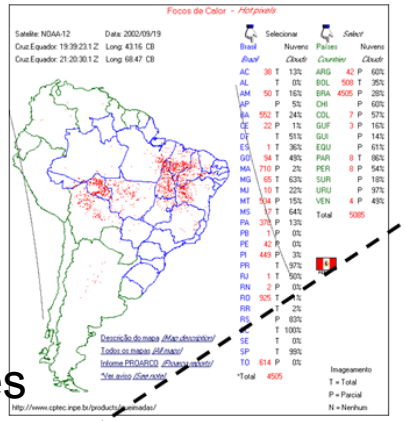
3BEM

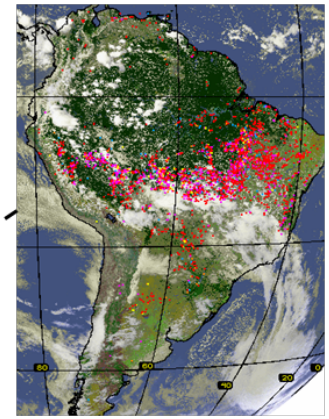
Biomass burning emissions inventory
Regional scale – daily basis

density of carbon data



near real time fire product

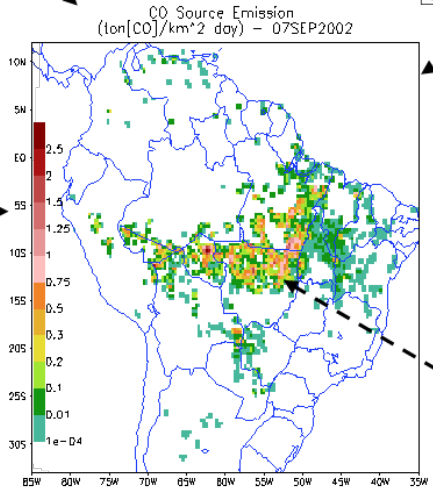




6 types of biomes

110 chemical species

land use data



Andreae and Merlet, 2001

emission & combustion factors

Biome category	Emission Factor for CO (g/kg)	Emission Factor for PM2.5 (g/kg)	Aboveground biomass density (α, kg/m^2)	Combustion factor (β, fraction)
Tropical forest[1]	110.	8.3	20.7	0.48
South America savanna[2]	63.	4.4	0.9	0.78
Pasture[3]	49.	2.1	0.7	1.00

[1] Average values for primary and second-growth tropical forests, [2] Average values for campo cerrado (C3) and cerrado sensu stricto (C4), [3] value for campo limpo (C1). All numbers are from Ward et al.,

mass estimation

$$M_{[\eta]} = \alpha_{veg} \cdot \beta_{veg} \cdot Ef_{veg}^{[\eta]} \cdot a_{fire},$$

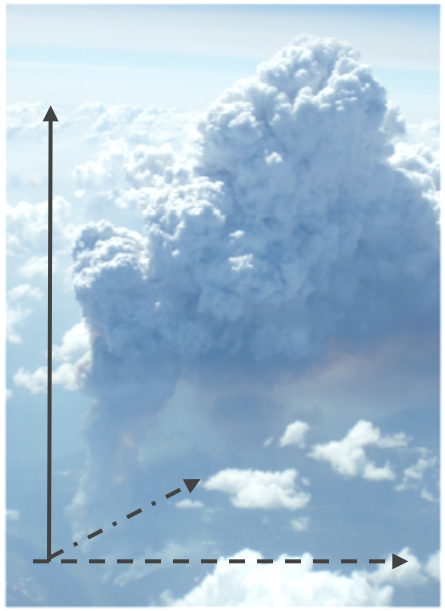
CO source emission (kg m^{-2}day^{-1})

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.

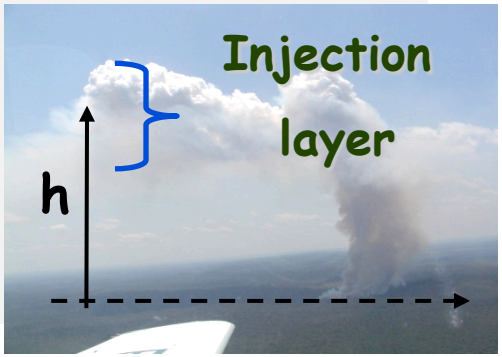


Plume rise model

total emission flux: F_η being λ the smoldering fraction

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

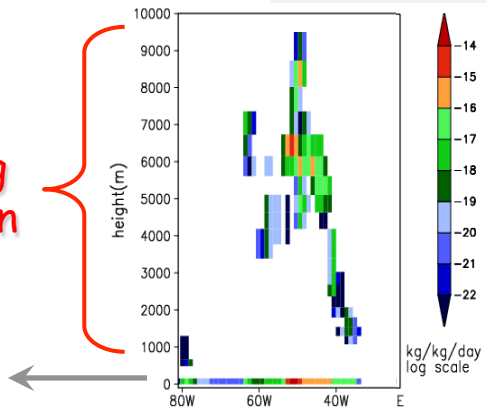
flaming term : $$E_\eta = \frac{(1-\lambda) F_\eta}{\rho_{air} \Delta z_{\text{injection layer}}}$$



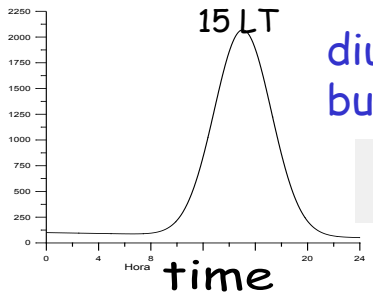
Example in the model:

flaming emission

smoldering emission



$r(t)$



diurnal cycle of the burning for S. America:

$$E_\eta(t) = r(t) E_\eta$$

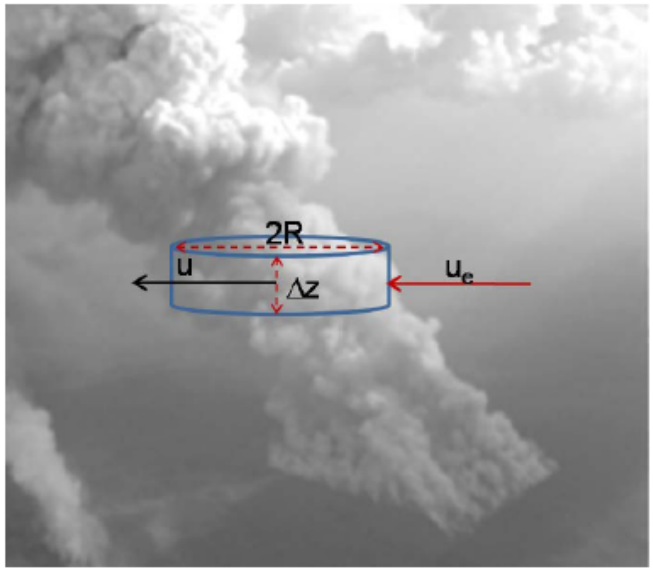
Freitas et al. (2011)

Recent Improvements: 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

Freitas et al. (2010)

Environmental Wind Effects on Plume Rise

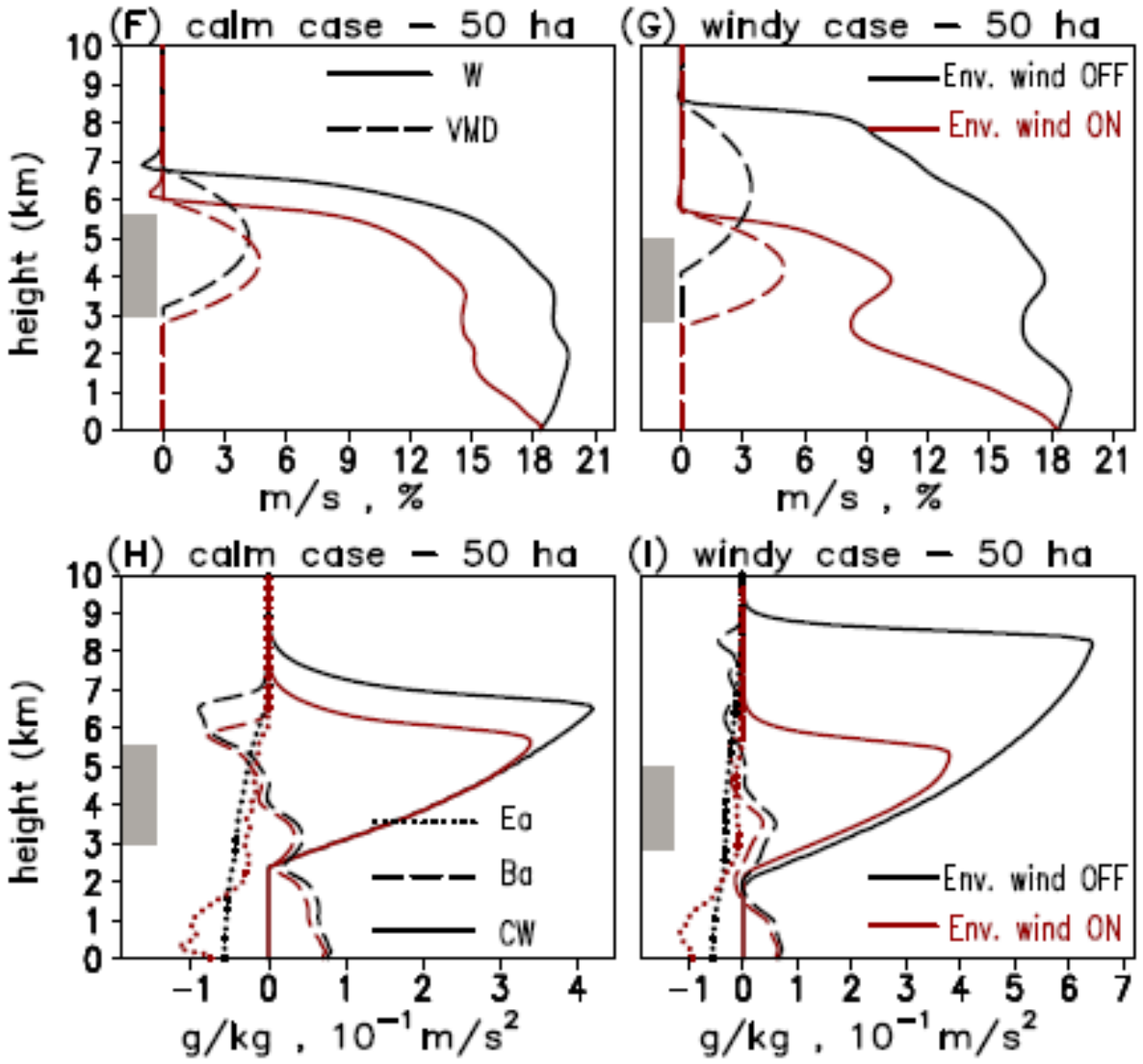


$$\lambda_{\text{entr}} = \frac{2\alpha}{R}|w|$$

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

W: vertical velocity
VMD: vertical mass distribution
Ea: Entrainment acceleration
Ba: buoyancy acceleration
CW: total condensate water

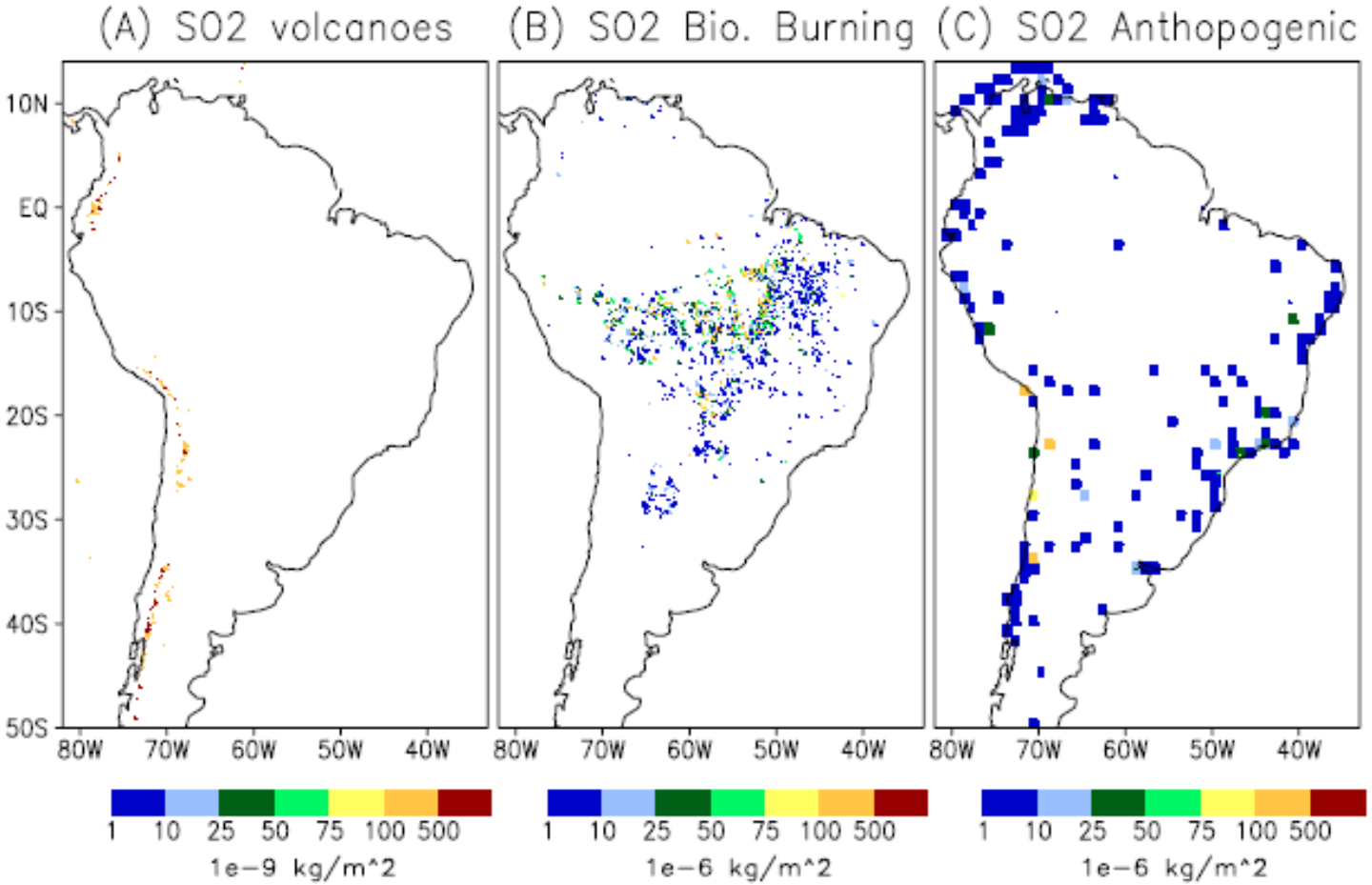
1-D PRM results for a 50 ha fire, calm and windy conditions



Freitas et al. (2010)

Volcano emissions

Based on Mastin et al. (2009) database of 1535 volcanoes
Mass eruption rate, plume height and time duration
SO_2 from AEROCOM program, 1979 – 2007 (Diehl, 2009)



SO_2 emissions on 27 August 2002 on a 0.2^0 rectangular projection grid: (A) Diehl (2009), (B) 3BEM, (C) EDGAR

Freitas et al. (2011)

Compiling PREP-SRC-CHEM

- Required libraries: HDF4/HDF5, zlib, jpeg, netCDF
- cd to:

  PREP-CHEM-SRC-1.4/bin/build
- Set library paths in:

  include.mk.<compiler>
- Compile

  make OPT=<compiler> CHEM=RADM_WRF_FIM

- cd to:

  PREP-CHEM-SRC-1.4/bin

Executable : *prep_chem_sources_RADM_WRF_FIM.exe*

Input file (namelist): prep_chem_sources.inp

Input file (namelist): prep_chem_sources.inp

```
$RP_INPUT
!---------------- grid_type
 grid_type=  'lambert',            !  'polar' = polar stereo. grid output
                                   !  'll'  = 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='/DATA/Emission_data/RETRO/anthro',
   use_edgar =2,  ! 0 - not, 1 - Version 3, 2 - Version 4 for some species
   use_seac4rs=1,
   ue_streets = 0,

   use_gocart=1,
   user_data_dir='/DATA/EMISSION_DATA/SouthAmerica_Megacities',

   use_bioge =2, ! 1 - GEIA, 2 – MEGAN
   use_fwbawb=1,
   fwbawb_data_dir='/DATA/Emission_data/Emissions_Yevich_Logan',
   use_gfedv2=0,
   use_bbem=1,
   use_bbem_plumerise=1,
```

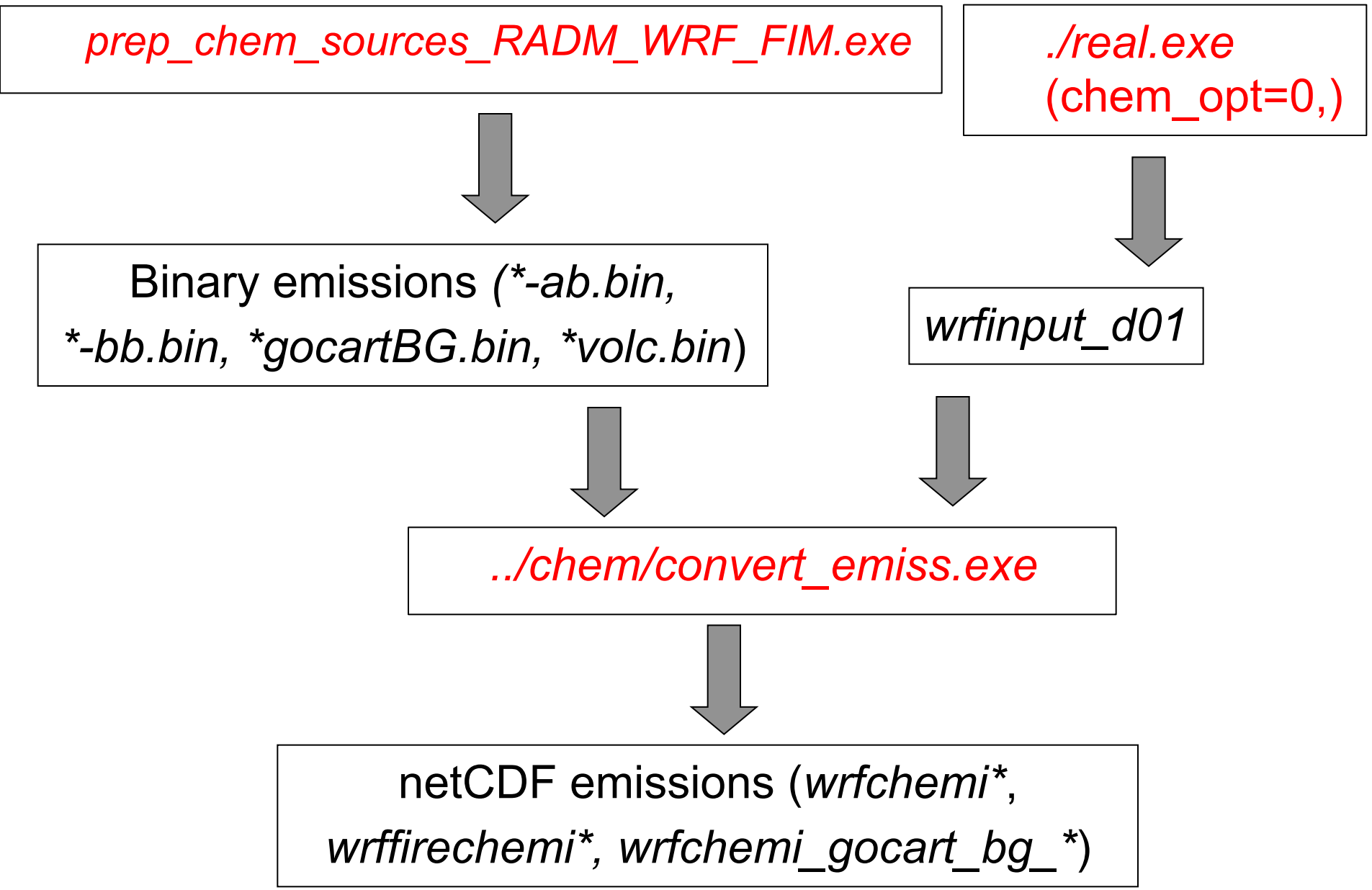
Input file (namelist): prep_chem_sources.inp

```
!---------------- 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='/DATA/Emission_data/fires_data/WF_ABBA/filt/f,
bbem_modis_data_dir   ='/DATA/Emission_data/fires_data/MODIS/Fires.',
bbem_inpe_data_dir    ='/DATA/Emission_data/fires_data/DSA/Focos',
bbem_extra_data_dir   ='/DATA/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='/DATA/EMISSION_DATA/VOLC_SO2',
```

Input file (namelist): prep_chem_sources.inp

```
!---------------- 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



References

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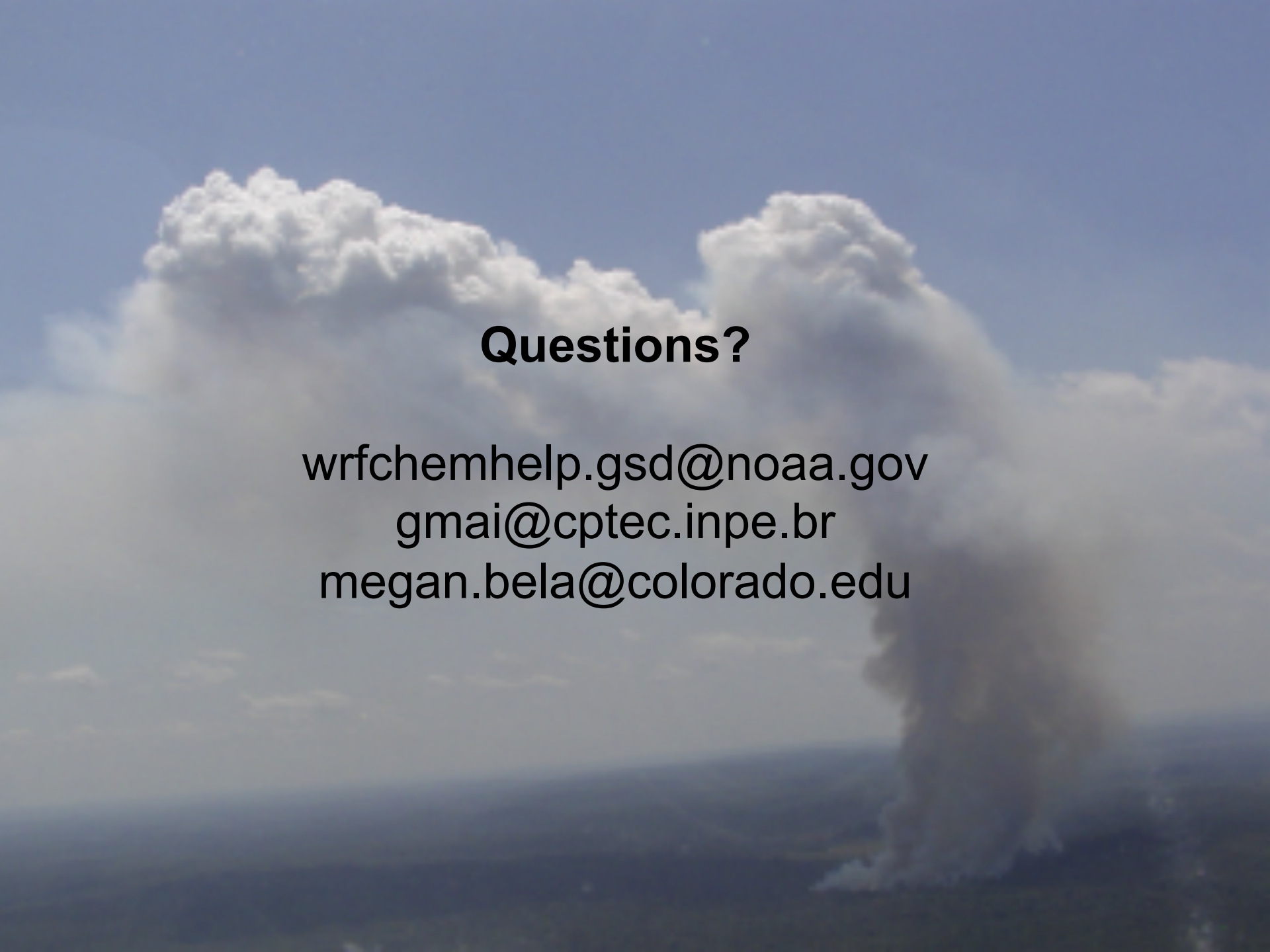
Freitas, S. R., K. M. Longo, R. Chatfield, D. Latham, M. A. F. Silva Dias, M. O. Andreae, E. Prins, J. C. Santos, R. Gielow and J. A. Carvalho Jr.: Including the sub-grid scale plume rise of vegetation fires in low resolution atmospheric transport models. Atmospheric Chemistry and Physics, v. 7, p. 3385-3398, 2007.

Freitas, S. R.; Longo, K. M.; M. Andreae. The impact of including the plume rise of vegetation fires in numerical simulations of associated atmospheric pollutants. Geophys. Res. Lett., 33, L17808, doi:10.1029/2006GL026608, 2006.

Yevich, R. and J.A. Logan, An assessment of biofuel use and burning of agricultural waste in the developing world, Global Biogeochemical Cycles, 2003



Questions?

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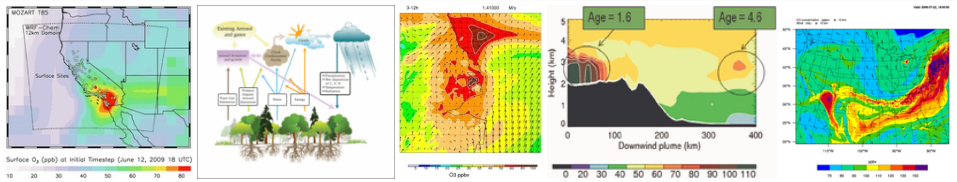
gmai@cptec.inpe.br
megan.bela@colorado.edu

Using MEGAN with WRF-Chem

Gabriele Pfister, Stacy Walters, Christine Wiedinmyer, Alex Guenther, Mary Barth, Louisa Emmons, Tiffany Duhl

Preprocessors available from: *www.acd.ucar.edu*



WRF-Chem

WRF-Chem is the Weather Research and Forecasting (WRF) model coupled with Chemistry. The model simulates the emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the meteorology. The model is used for investigation of regional-scale air quality, field program analysis, and cloud-scale interactions between clouds and chemistry.

The development of WRF-Chem is a collaborative effort among the community. NOAA/ESRL scientists are the leaders and caretakers of the code. The Official WRF-Chem web page is located at the NOAA web site. Our model development is closely linked with both NOAA/ESRL and DOE/PNNL efforts. Description of PNNL WRF-Chem model development is located at the PNNL web site as well as the PNNL Aerosol Modeling Testbed .

Use the MOZART Download page to retrieve MOZART-4 model results.

Information on running WRF-Chem with the MOZART chemical mechanism can be found in the MOZCART User's Guide.

Processors Available to the Community:

NEW (November 2011): Preprocessors have been updated to work for lat/lon projections in addition to Lambert, Mercator and Polar. The mozbc tool has been updated to enable time interpolation.

mozbc

NCAR/ACD has developed a program to create time-varying chemical 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). To obtain mozbc, see the **Download** section below.

bio_emiss

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

preprocessor tools

Pre-processor tools for running WRF-Chem / MOZCART. See the **Download** section below.

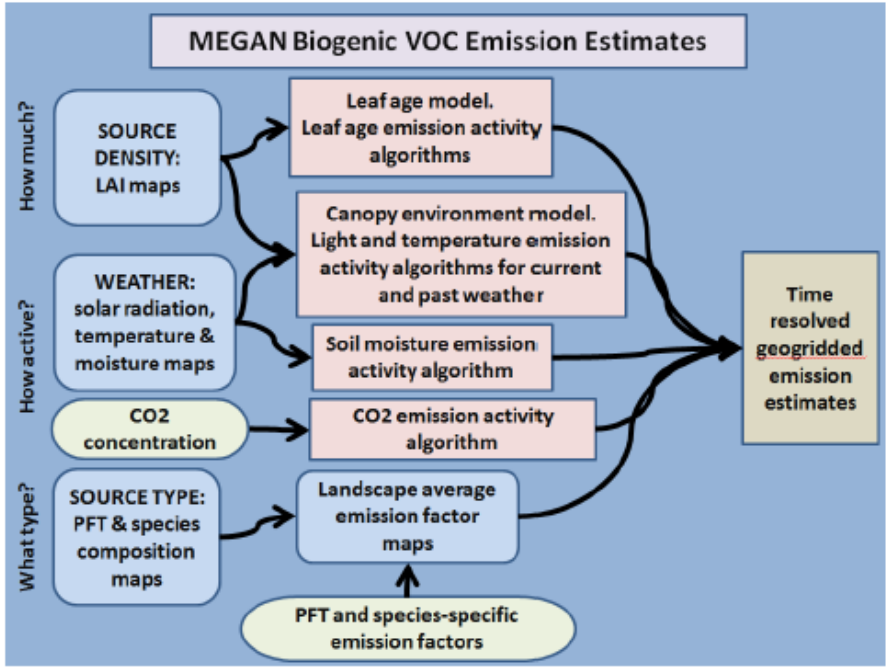
Download

- Preprocessors are in FORTRAN
- README details compilation and execution
- Require netcdf libraries; work on Portland Group or IBM fortran 90 compilers
- Domain information derived from wrfinput_d<domain>

MEGAN online biogenic emissions

Model of Emissions of Gases and Aerosols from Nature

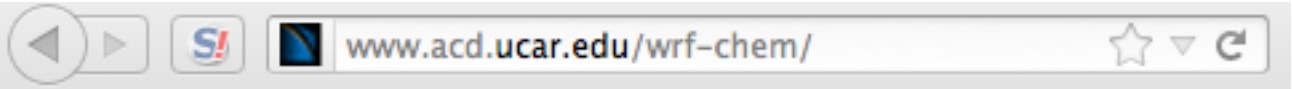
- Estimate emissions of VOCs, NOx and CO from vegetation
- Driving variables include landcover, LAI, weather, and atmospheric chemical composition
- Reference: *Guenther et al.*, GMD 2012 (for MEGAN v2.1)
- Note: as of current land cover used in MEGAN differs from that used within WRF-Chem
- Planned:
  - Update to latest MEGAN
    current version in WRF-Chem: 2.04
  - link to WRF-Chem land cover/CLM



from Guenther et al., 2012

MEGAN preprocessor

- Static input fields needed to run with online MEGAN biogenic emissions: *Isoprene Emissions Factors, past/current conditions (monthly LAI, solar radiation & temperature), Fractional coverage of broadleaf and needelleaf 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



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_emiss - 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)
/
```

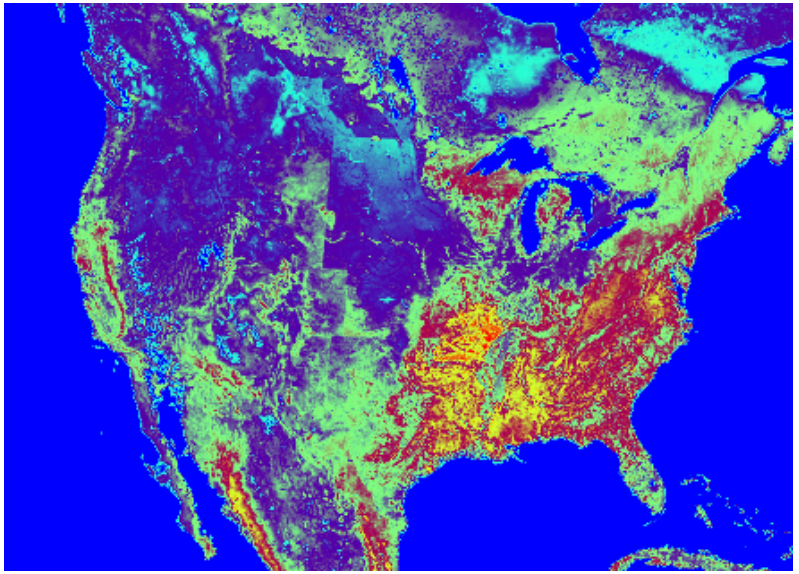
- To run : *megan_bio_emiss < megan_bio_emiss.inp > megan_bio_emiss.out*

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)
   ne_area = # chemical species
```



EBIO_ISO, 20 July 2008 21 UTC

For Questions:

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