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

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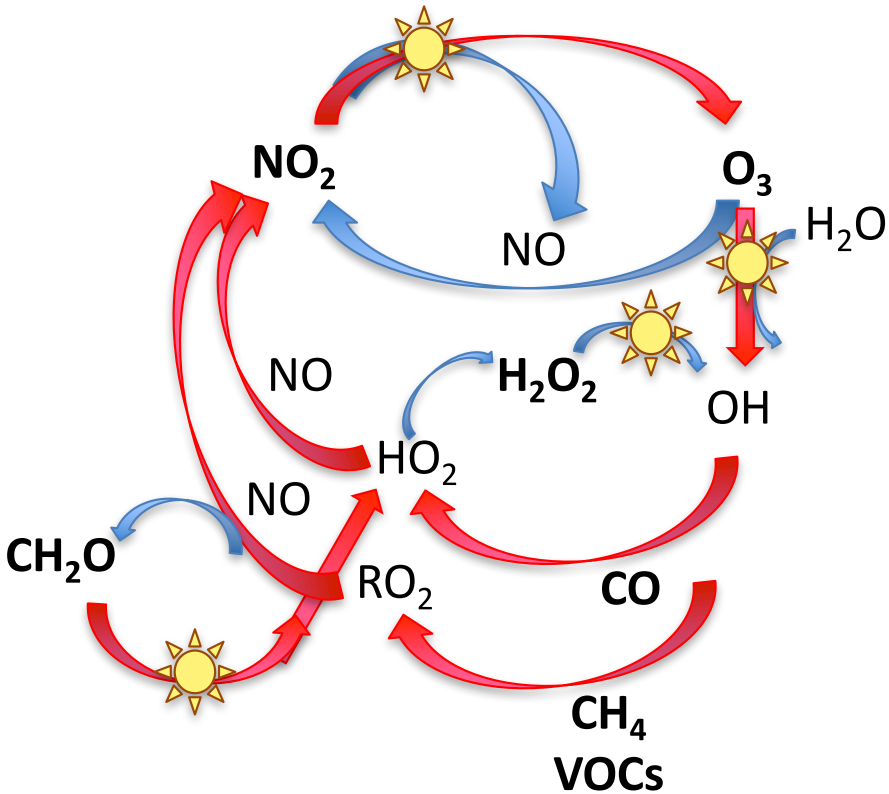
Chemical Production of Ozone

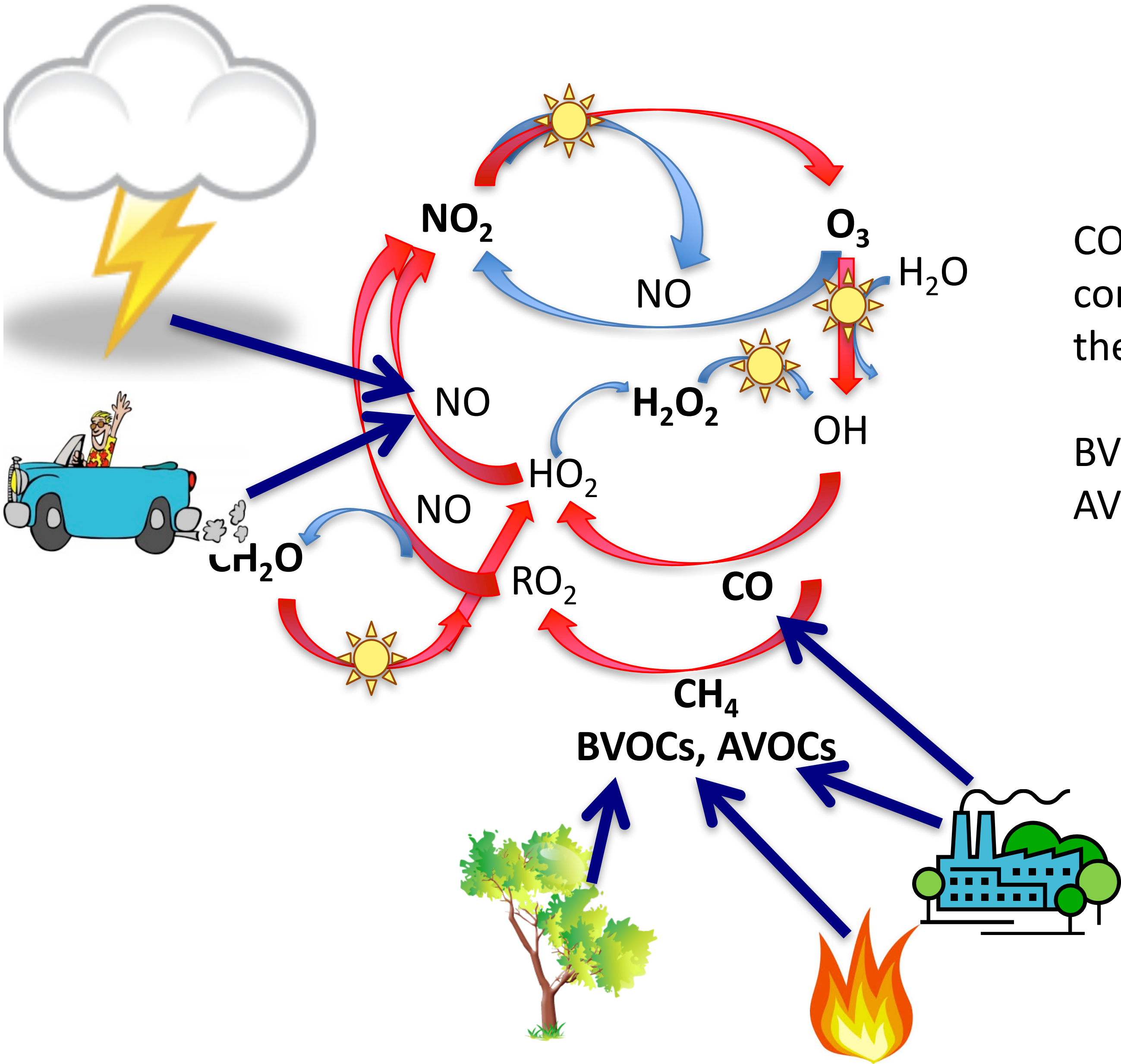
(Atmospheric Chemistry 101)



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

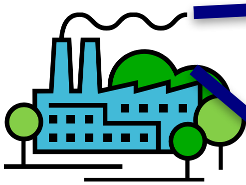


CO, CH_4, and volatile organic compounds (VOCs) are the fuel for the chemistry

BVOC = biogenic VOC
AVOC = anthropogenic VOC

Emissions and Aerosols

Oceans → DMS → SO_2 → $\mathbf{SO_4}$

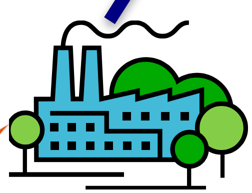


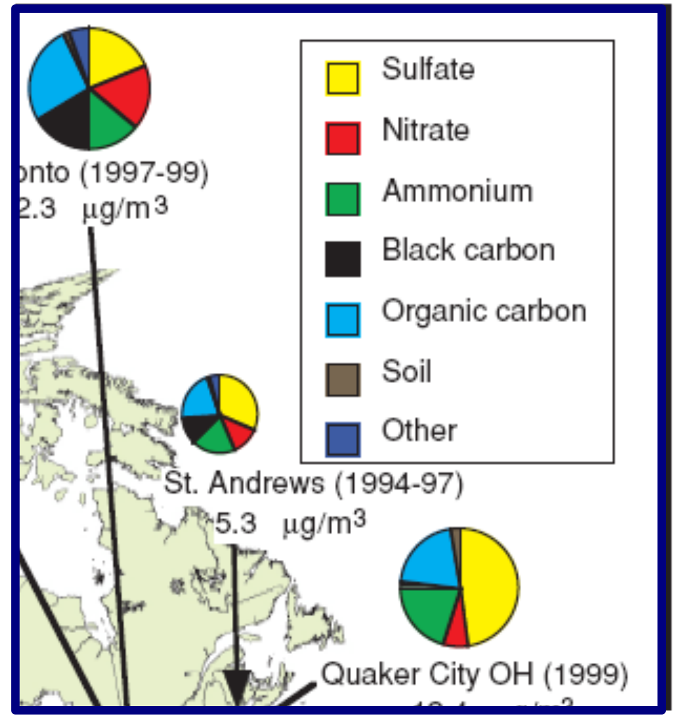
$HNO_3 - NH_3 - SO_4$ equilibrium → $\mathbf{(NH_4)_2SO_4}$, $\mathbf{NH_4HSO_4}$, $\mathbf{NH_4NO_3}$ aerosols

NO

$VOC + O_3$ → SVOC

$SVOC + O_3$ → **SOA**





(NARSTO, 2004)

Dust, Sea salt

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

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)

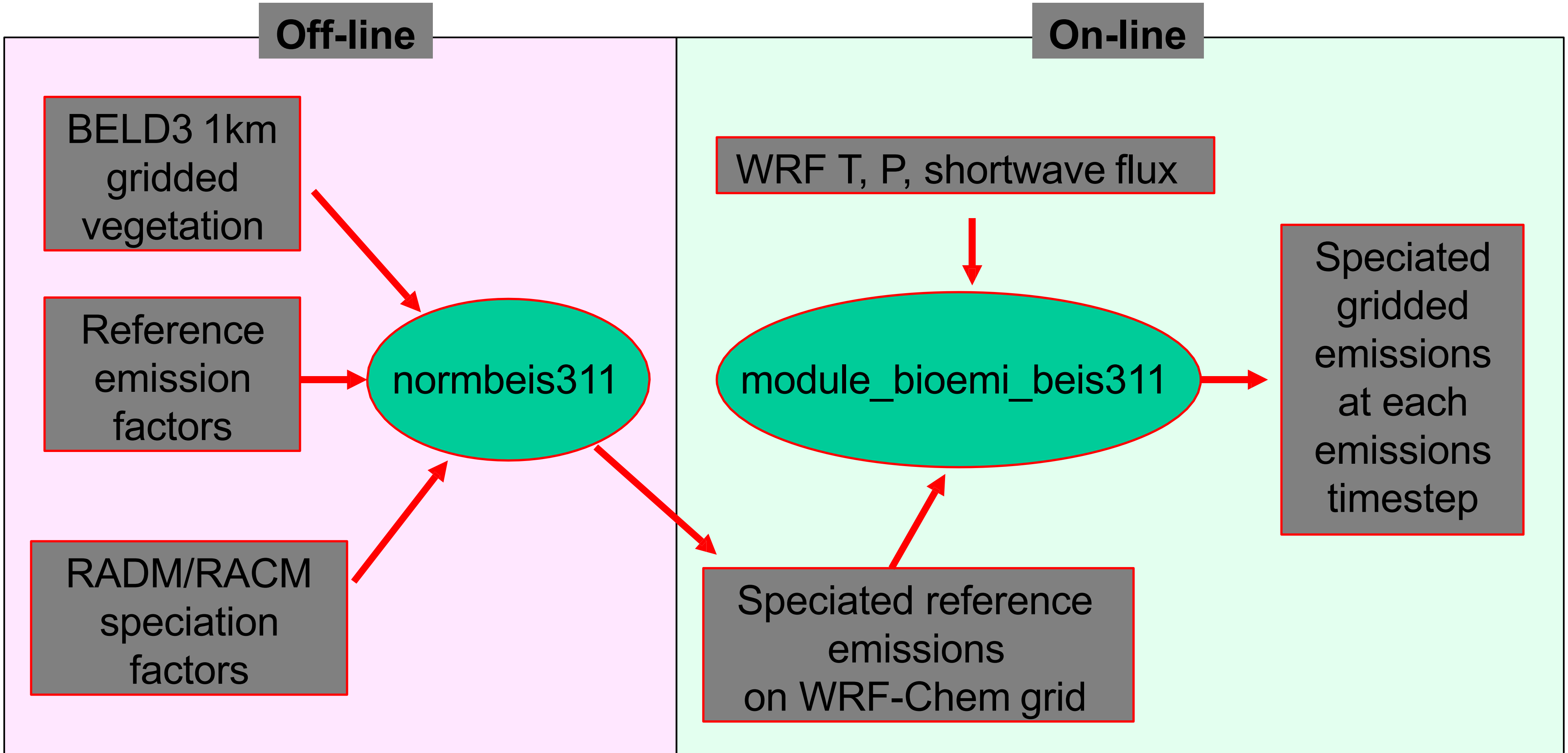
- **Simple Guenther approach** (bio_emiss_opt = 1):
  - Landuse based emissions following Guenther et al (1993, 1994), Simpson et al. (1995). Emissions depends on both temperature and photosynthetic active radiation.
  - No additional input data files.

- **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 2.04 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

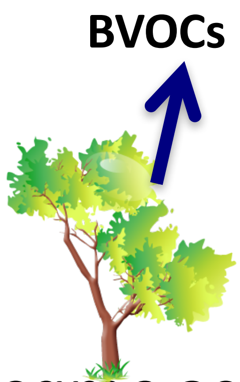
Based on EPA BEIS3 v14 for SMOKE processor



RACM species emitted by BEIS3:
ISO, API, LIM, XYL, ETH, HC3, ETE, OLT, OLI, HCHO, ALD, KET, ORA2, CO, NO

Biogenic Emissions Modeling: MEGAN

- **<u>MEGAN</u>:**
  Model of Emissions of Gases and Aerosols from Nature
  - Guenther et. al., *Atmospheric Chemistry and Physics*, 2006
    - Version 2.1 coupled to CLM will be in WRF-Chem 4.0
  - 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

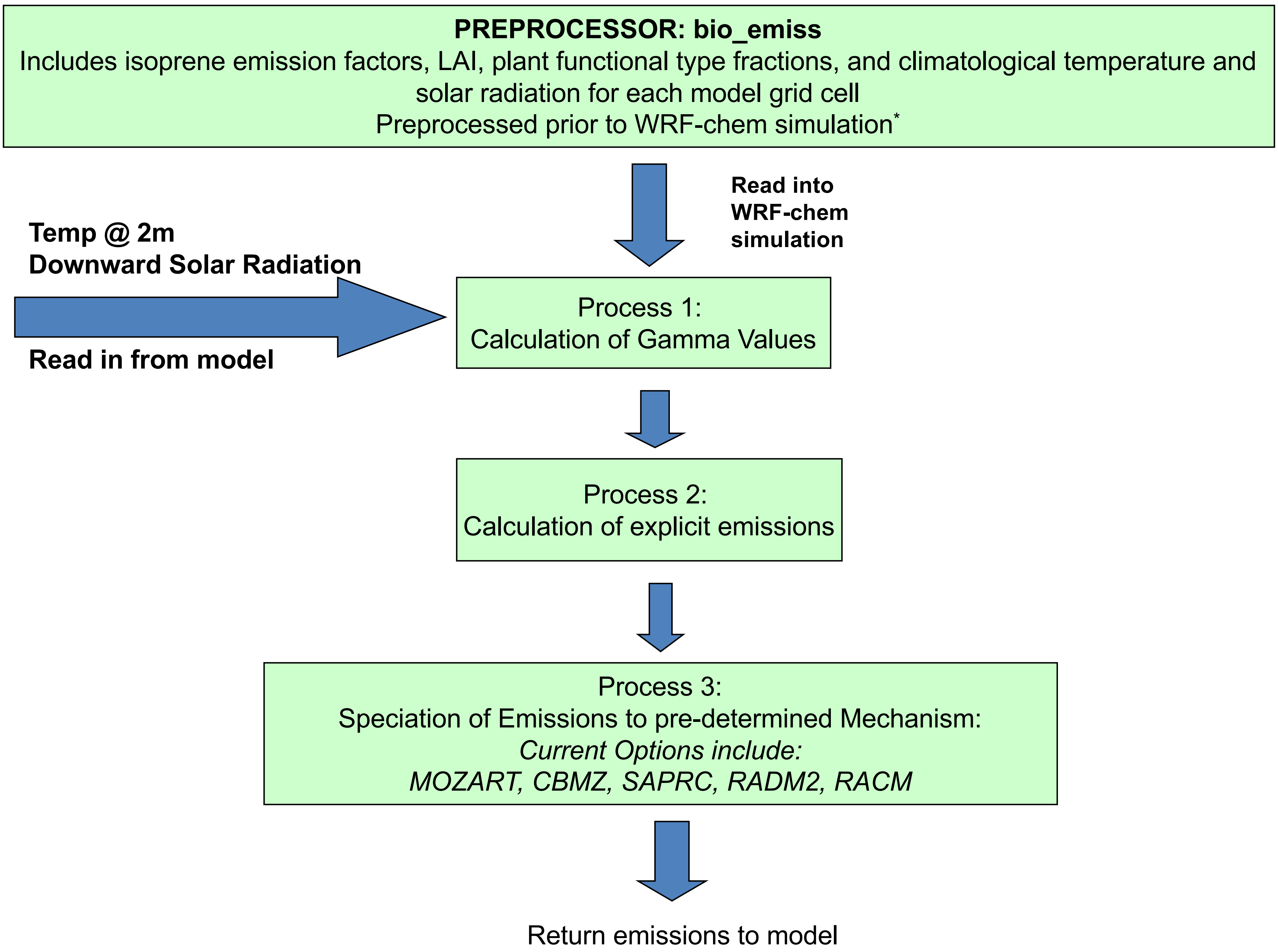
MEGAN Framework: Calculation of emissions

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

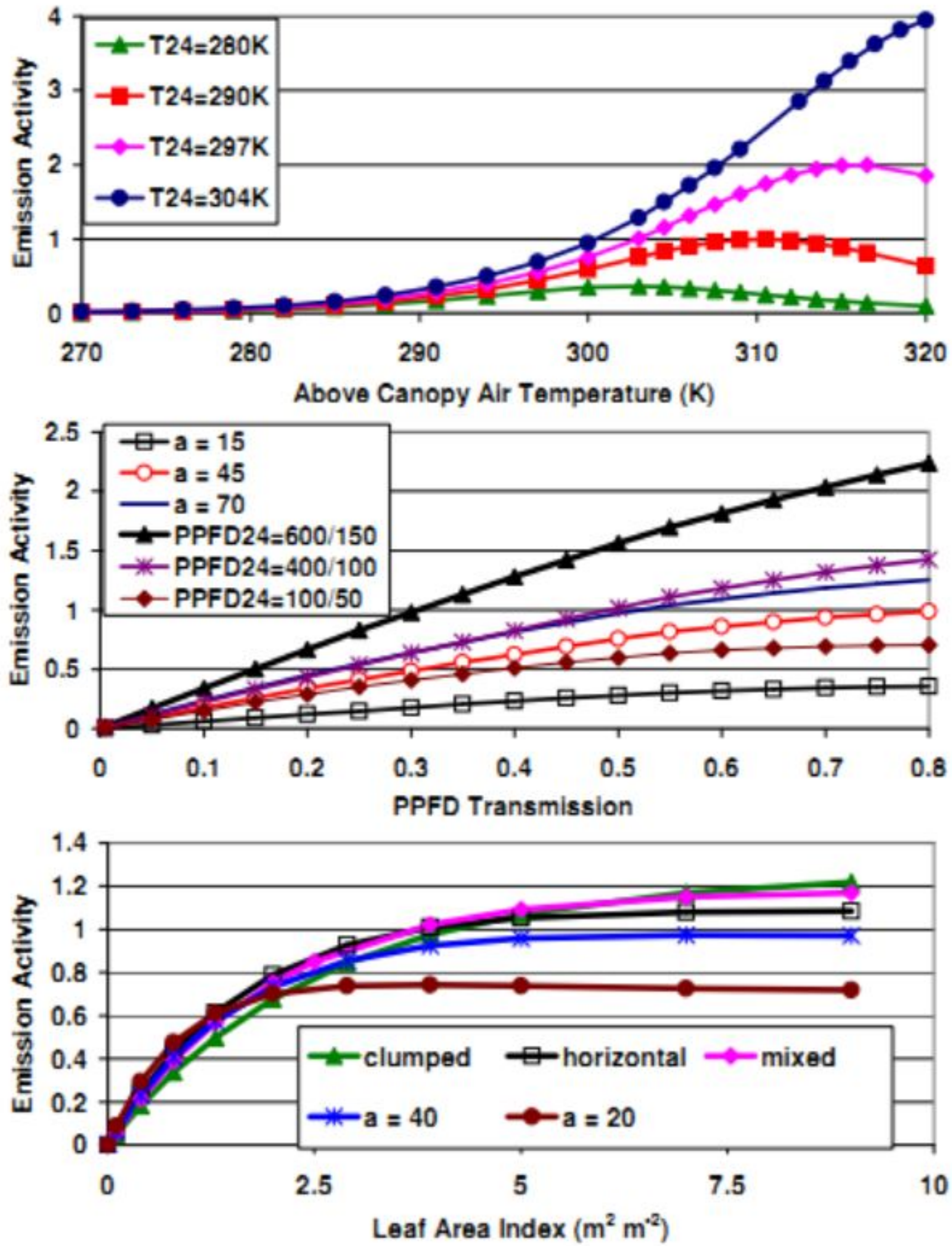
$$\gamma_{CE} = \gamma_{LAI} \bullet \gamma_{P} \bullet \gamma_{T}$$

EM: Emission ($\mu g\ m^{-2}\ hr^{-1}$)
ε: Emission Factor ($\mu g\ m^{-2}\ hr^{-1}$)
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*
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



Guenther et al., 2006, *ACP*

Emissions increase as

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

Emission Factors for Isoprene

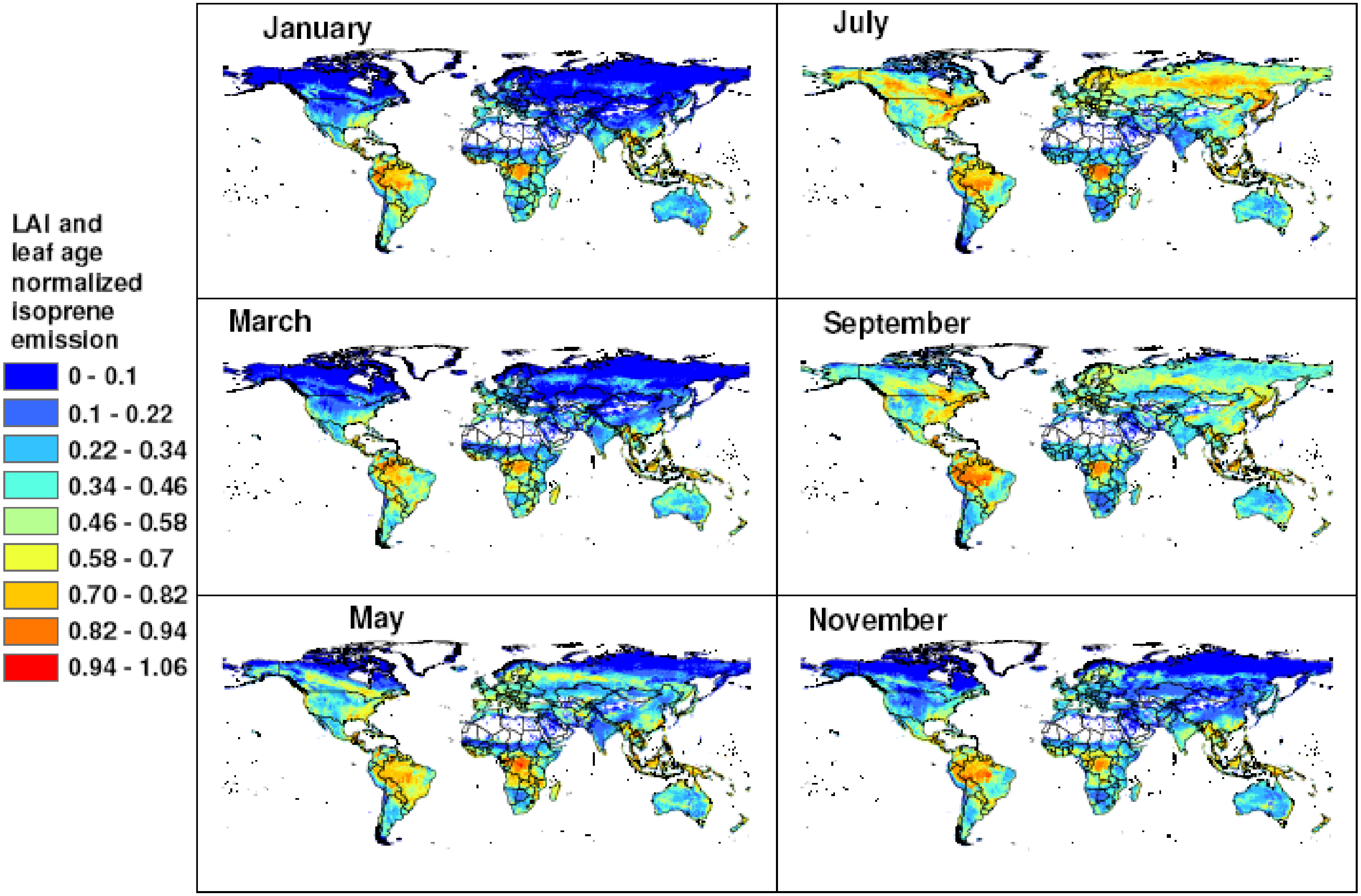


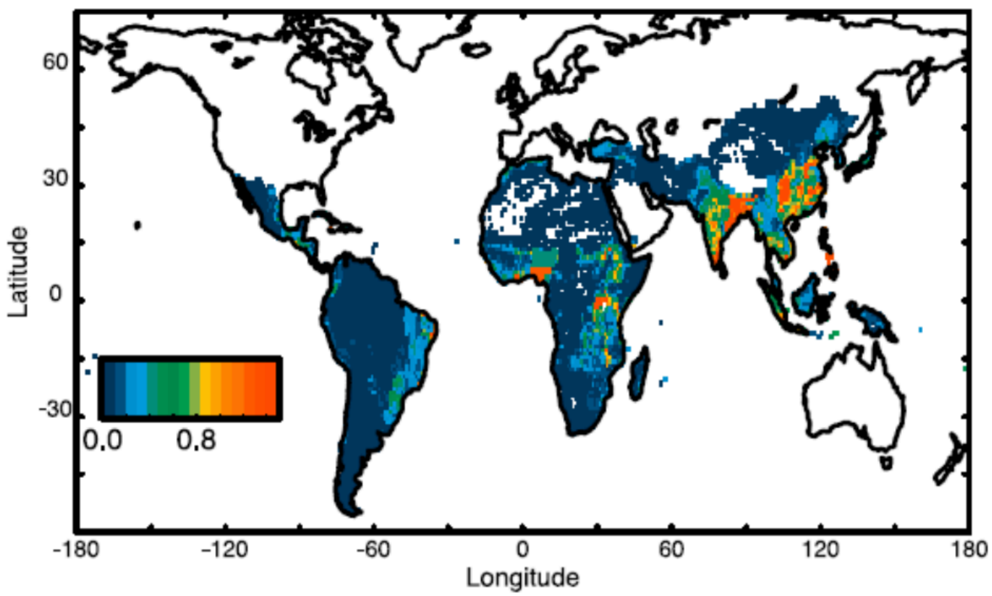
Fig. 5. Monthly normalized isoprene emission rates estimated with MEGAN for 2003. Rates are normalized by the emission estimated for standard LAI ($=5\,m^2\,m^{-2}$) and leaf age (80% mature leaves). These normalized rates illustrate the variations associated with changes in only LAI and leaf age; i.e.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

Biofuel burning in the developing world

Emissions_Yevich_Logan

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

Woodfuel (fuelwood and charcoal) use



PREP-CHEM-SRC

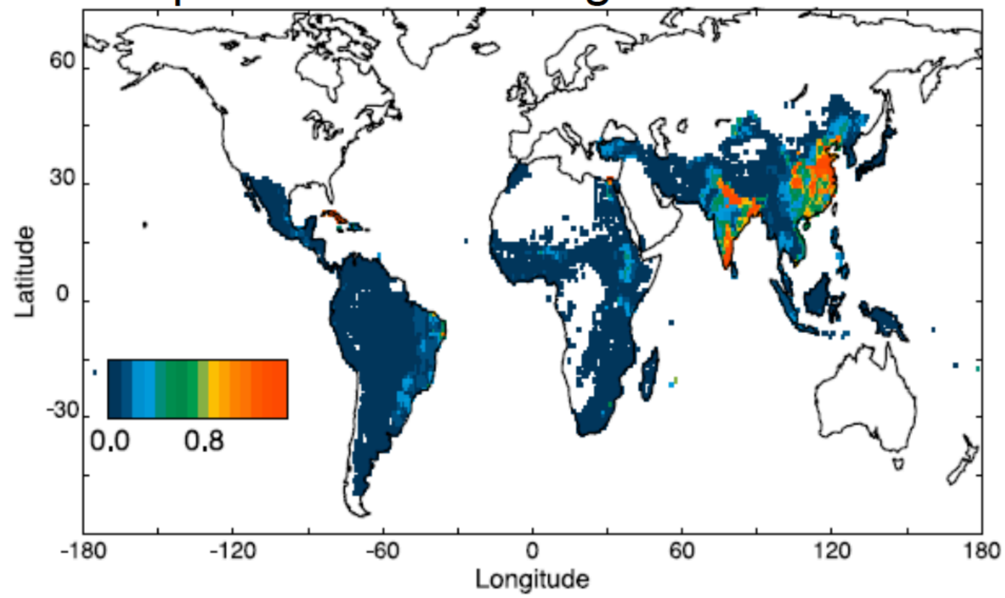
use_fwbawb =1

OR use HTAP:

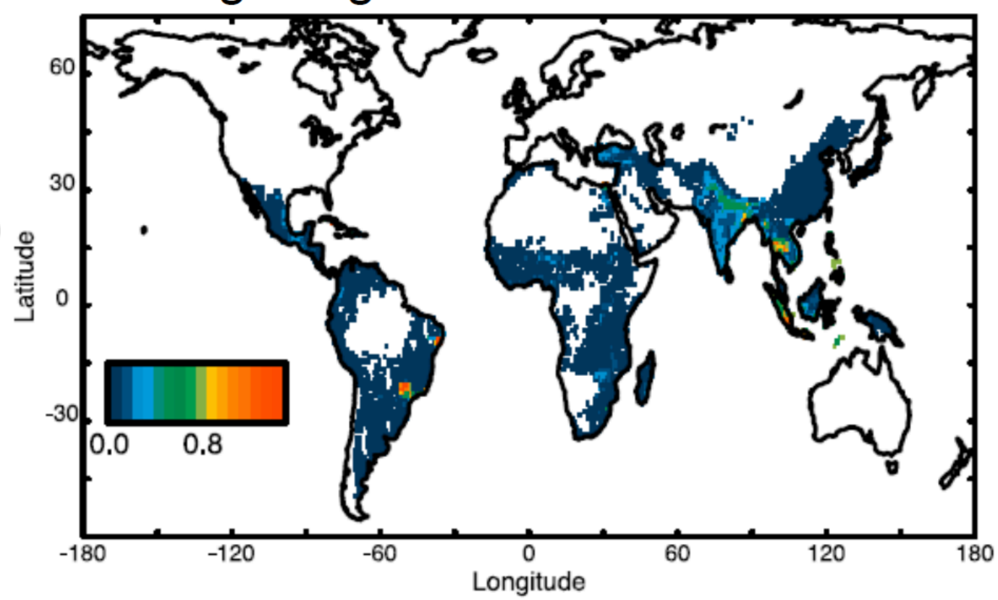
use_edgar = 3

use_fwbawb = 0

Crop residue and dung use



Burning of agricultural residue in the fields

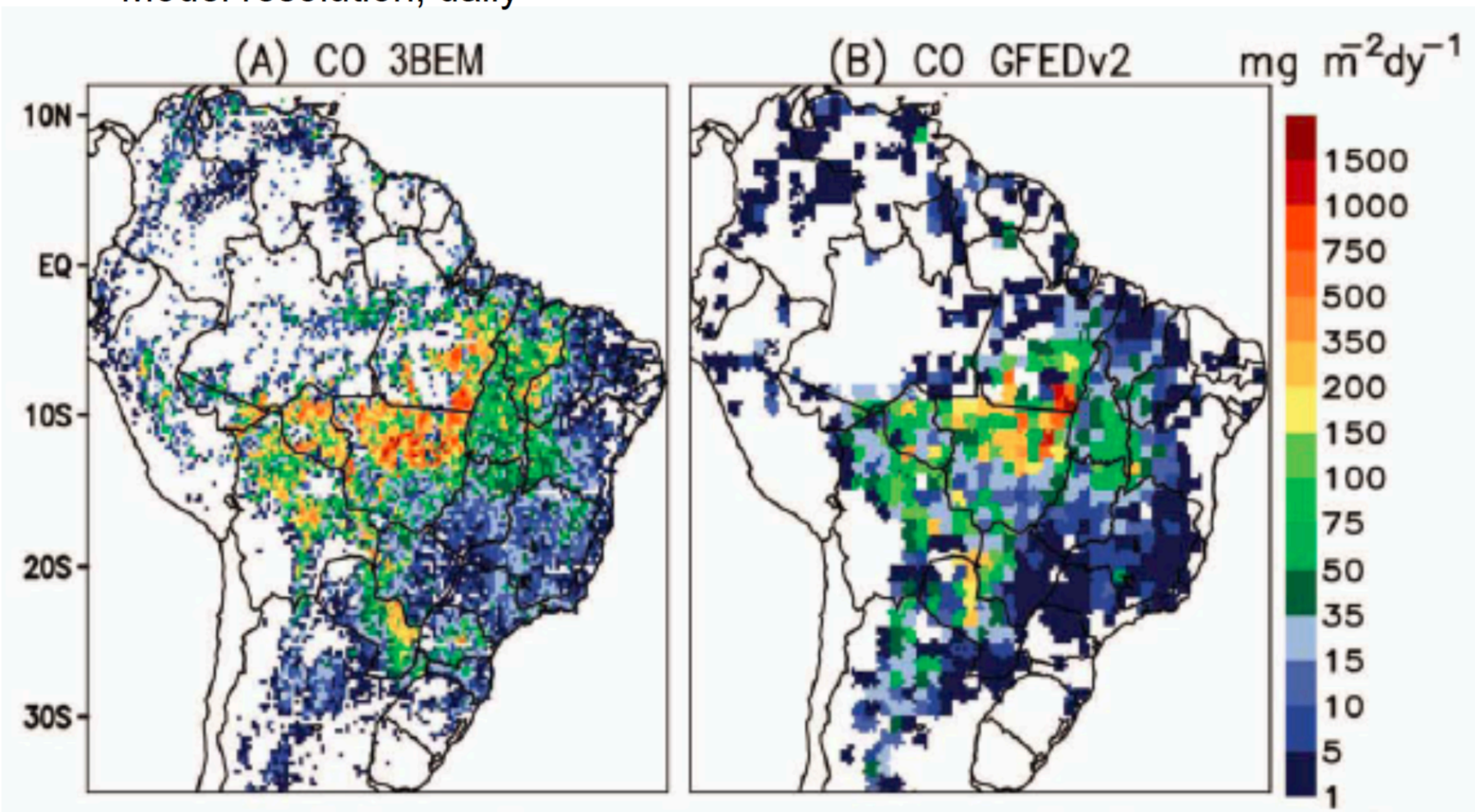


Yevich and Logan, 2003

Biomass burning emissions

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

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



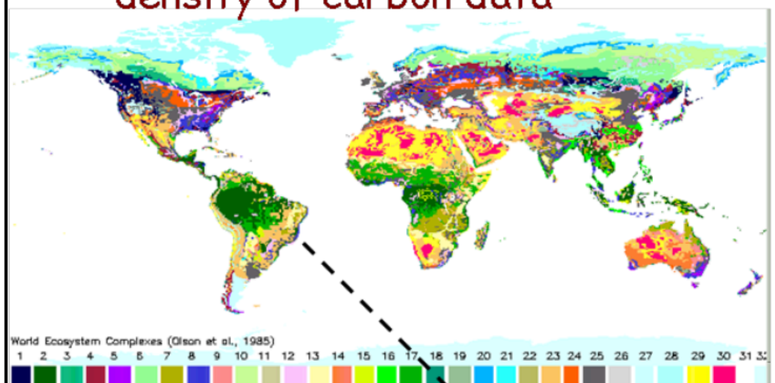
Average daily CO emissions, Aug.-Oct. 2002, 35 km

Freitas et al. (2011)

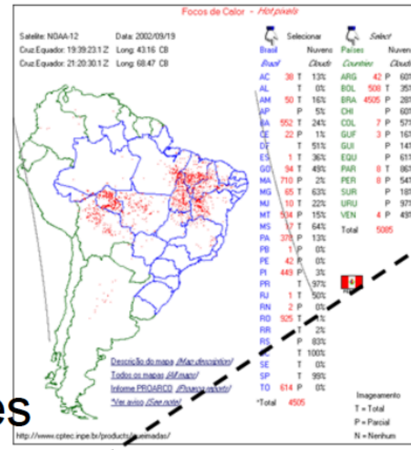
3BEM

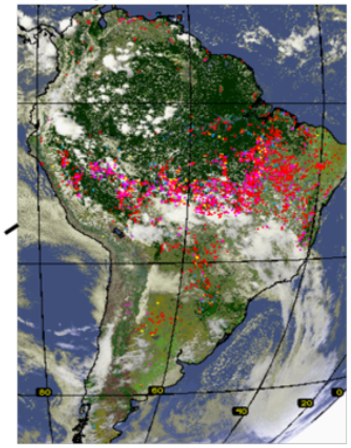
Biomass burning emissions inventory
Regional scale – daily basis

density of carbon data



near real time fire product

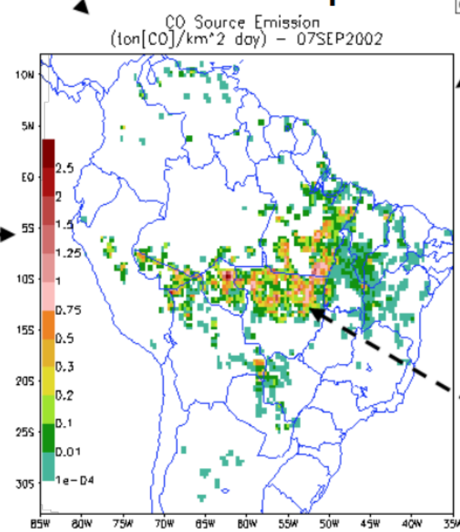




6 types of biomes

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

$$M_{[\eta]} = \alpha_{veg} . \beta_{veg} . \mathrm{E}f_{veg}^{[\eta]} . a_{fire},$$

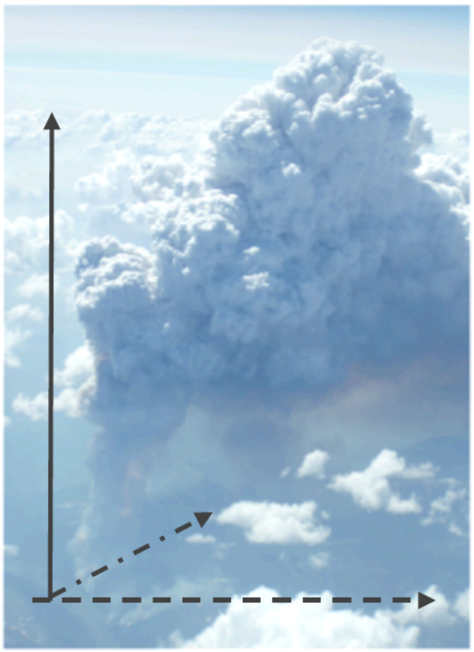
CO source emission (kg m^{-2}day^{-1})

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.

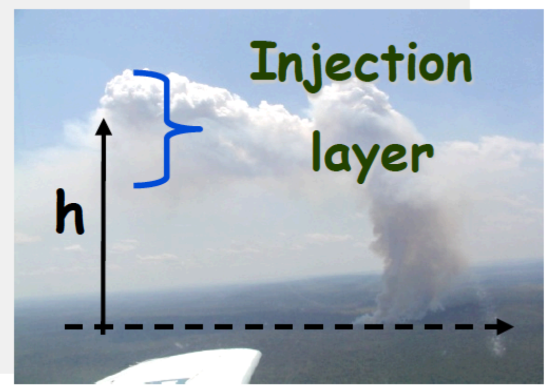


Plume rise model

total emission flux: F_η being λ the smoldering fraction

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

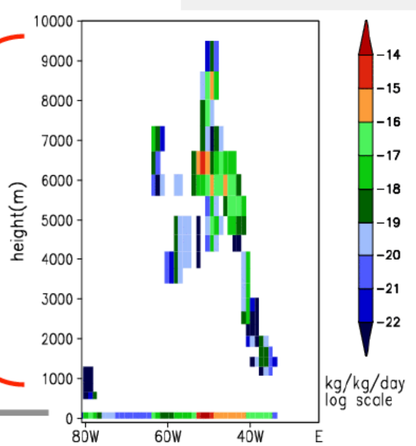
flaming term : $$E_\eta = \frac{(1-\lambda) F_\eta}{\rho_{air}\Delta z_{\text{injection layer}}}$$



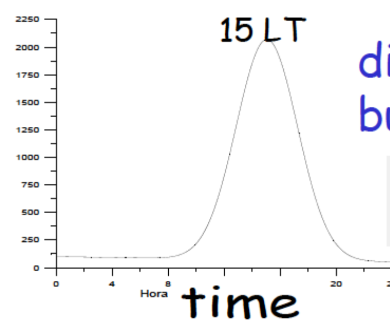
Example in the model:

flaming emission

smoldering emission



$r(t)$



diurnal cycle of the burning for S. America:

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

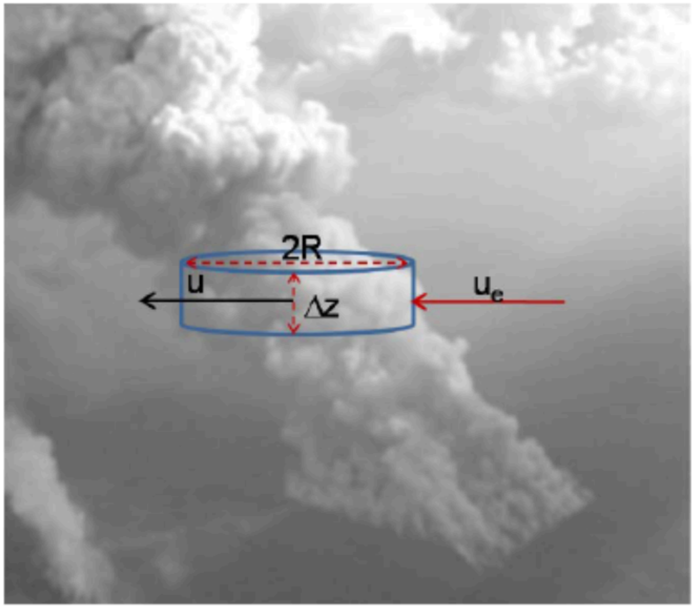
Freitas et al. (2011)

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

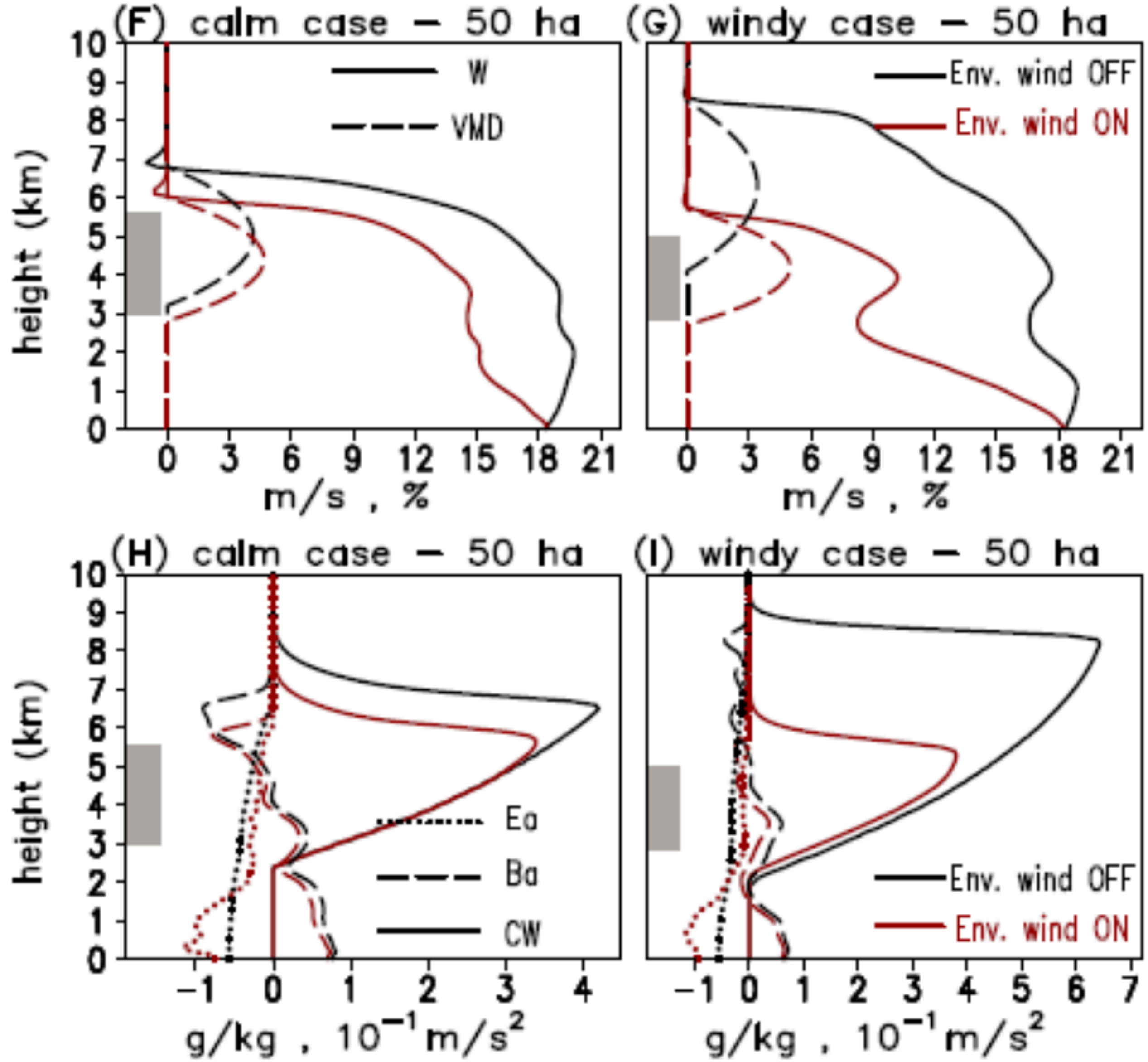


$$\lambda_{\text{entr}} = \frac{2\alpha}{R}|w|$$

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

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)

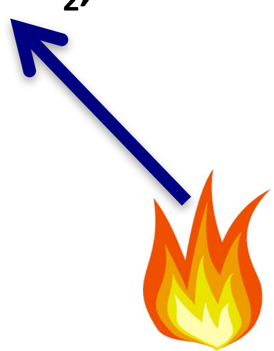
Fire Emissions: Fire INventory from NCAR (FINN)

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
- Daily global FINN emissions (v1.6, updated November 2017) and a global waste burning emissions inventory available for hindsight and forecast model applications at http://bai.acom.ucar.edu/Data/fire/
- Daily current global emissions (FINN version1) are available for forecast applications at: https://www.acom.ucar.edu/acresp/forecast/fire-emissions.shtml and http://www.acom.ucar.edu/acresp/MODELING/finn_emis_txt/
- Utilities to include FINN emissions are also at: http://bai.acom.ucar.edu/Data/fire/

CO, NO_x,
VOCs, SO_2, PM



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.

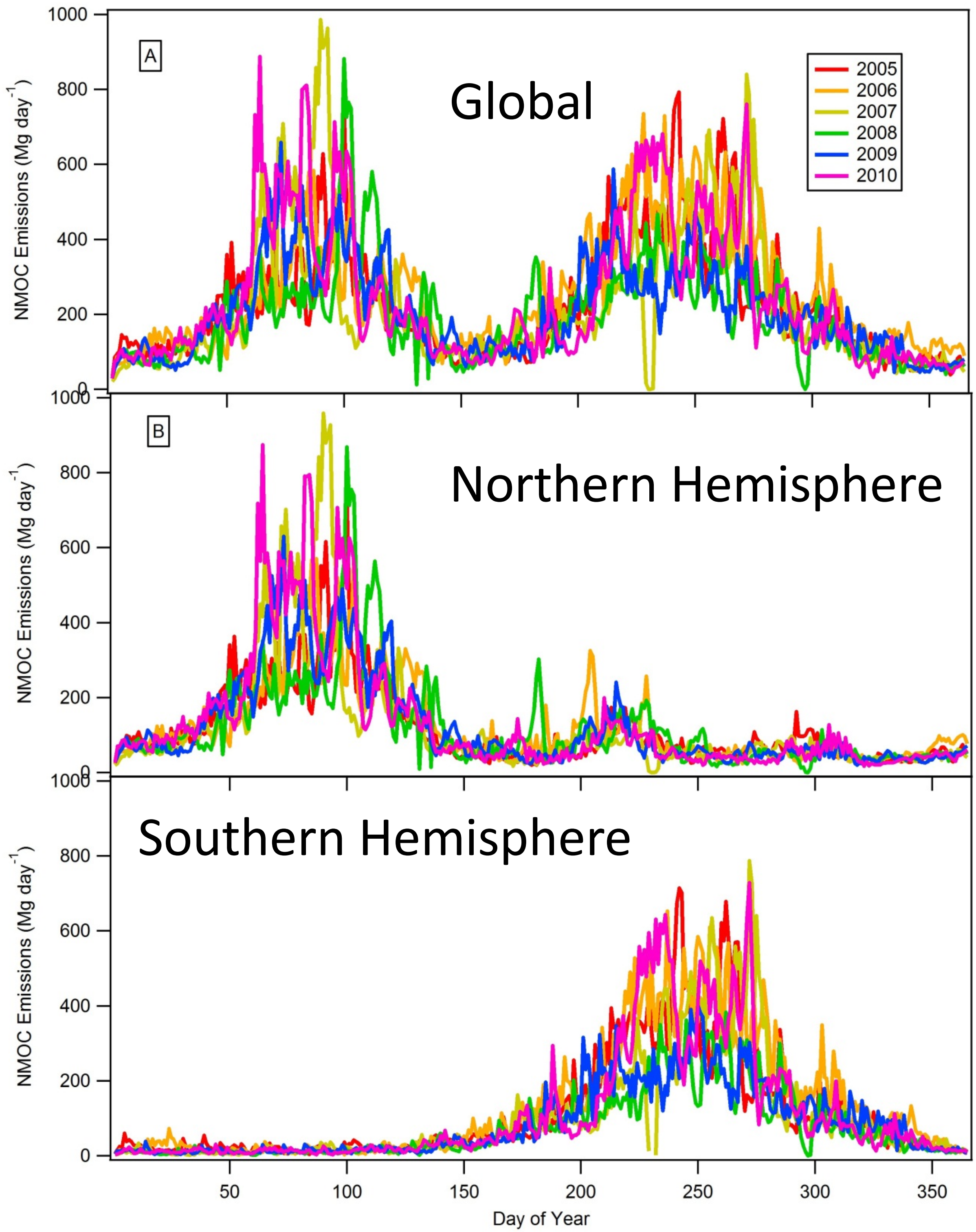
Speciation of VOCs provided for MOZART-4, SAPRC99, GEOS-Chem

Plume rise option available- *but requires additional inputs*

Global Daily Emissions

Emissions highly variable

- Daily
- Season
- Spatial

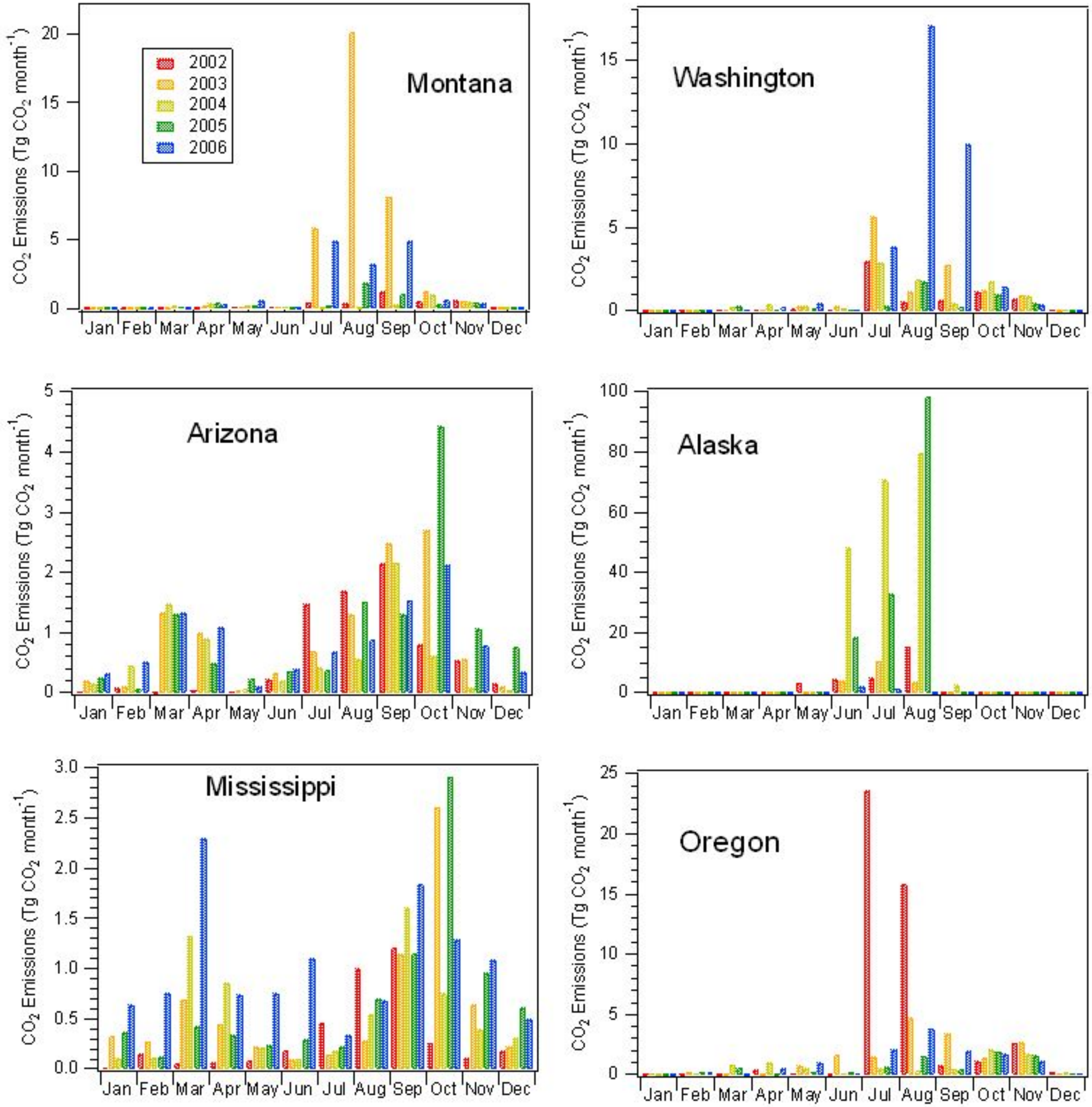


Wiedinmyer et al., *GMD*, 2011

Fire Emissions Variability:

-Spatial

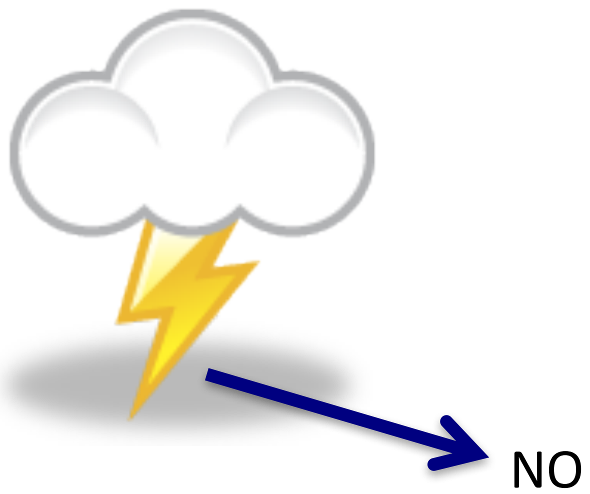
-Temporal



Wiedinmyer and Neff,
Carbon Balance and Management,
2007

Lightning-NO_x Emissions

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



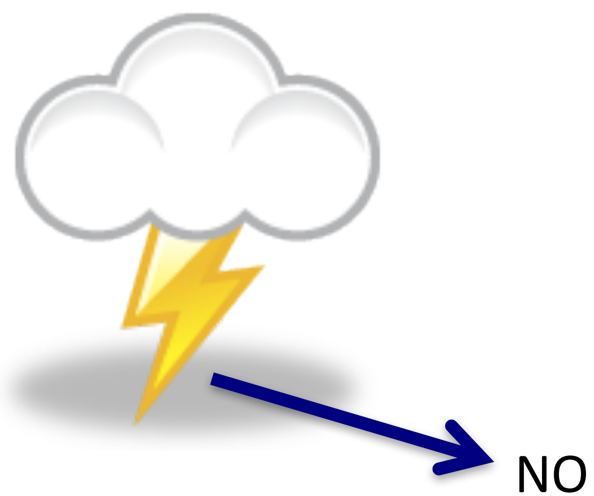
When lightning is triggered,
- Temperature increases to 1000s degrees
- This splits many molecules including N_2 and O_2

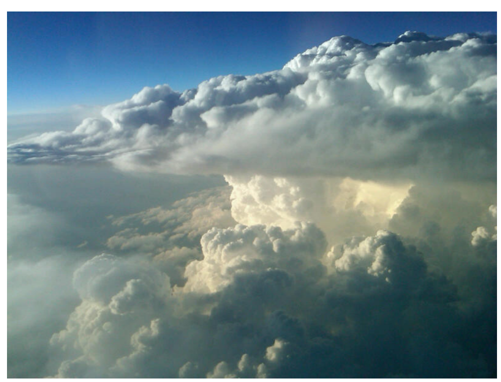
When temperature drops to normal,
- Some of the N and O atoms recombine with each other

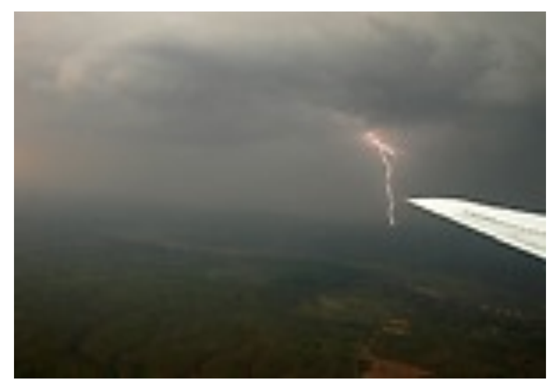
→ NO (nitric oxide)

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

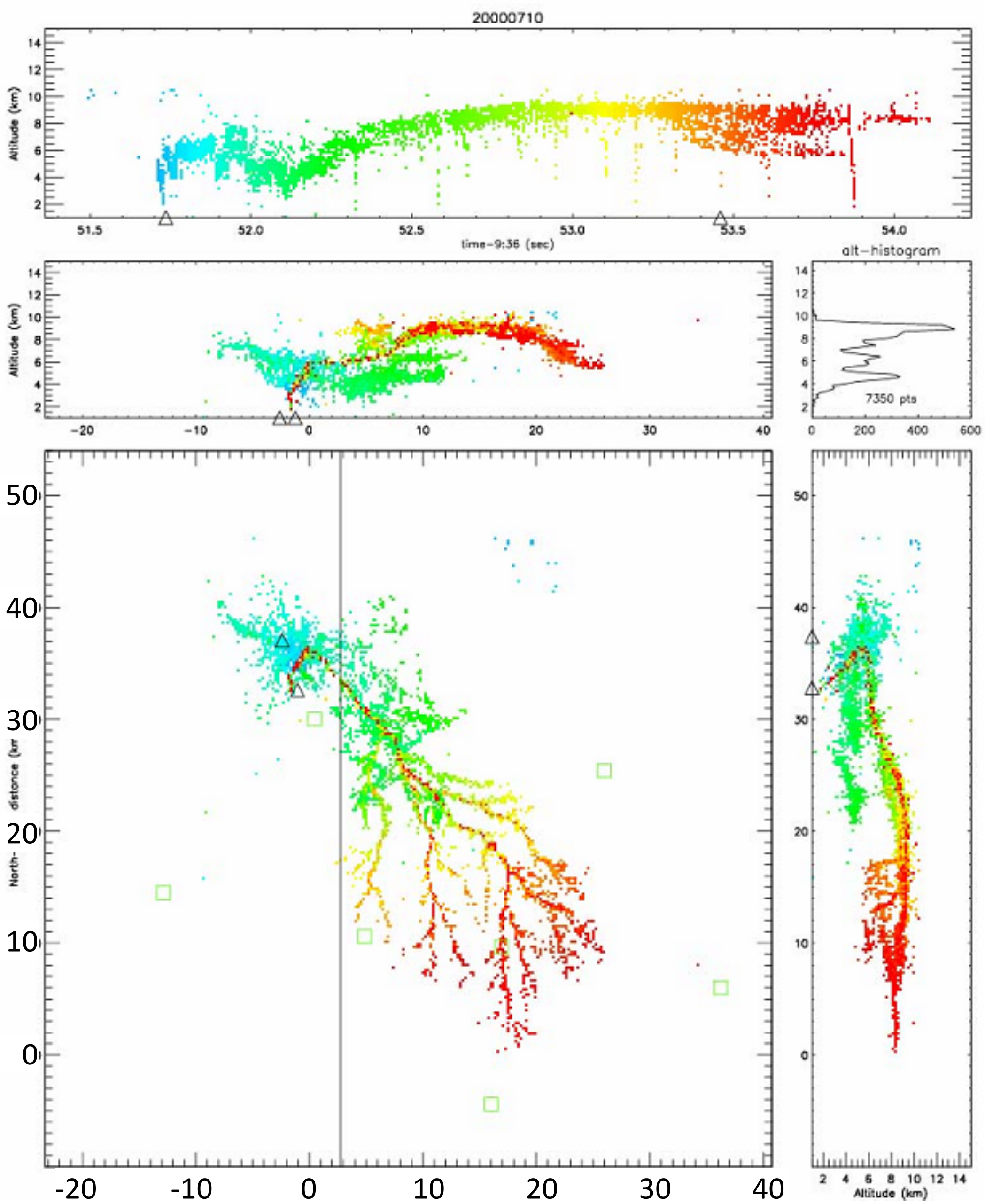






Example Lightning Flash

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)	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

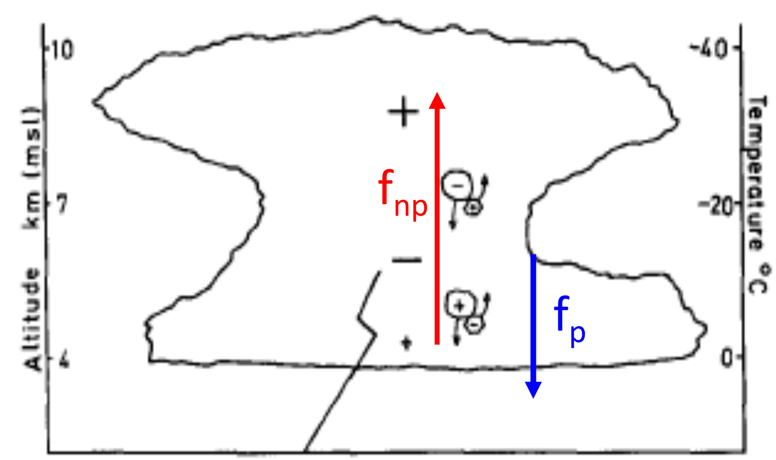


FIG. 2. A schematic of graupel–ice-crystal charge transfer above and below the reversal temperature level in a thunderstorm.

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)

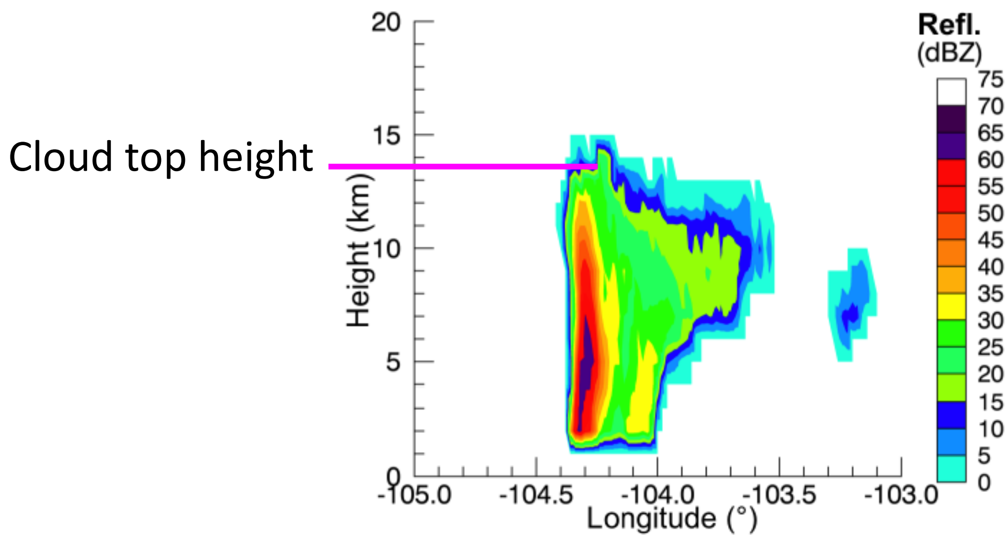
  H = cloud top height of the 20 dBZ contour

- 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



<u>Note:</u>
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

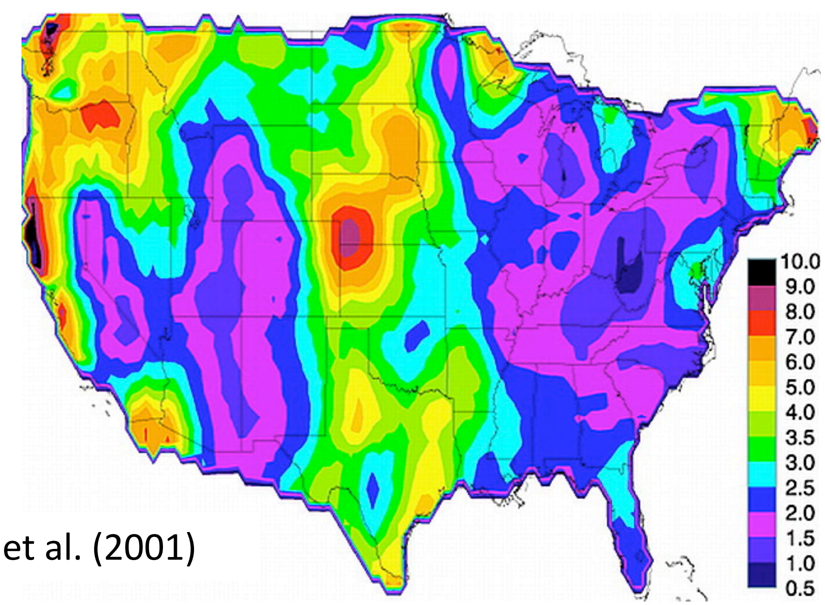
- Prescribed Values
  1) Set to a specified value everywhere
  2) Set to a very coarsely prescribed climatology (Boccippio et al., 2001)
  3) Gridded input – need to provide input

- 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., GMD,

  Placed throughout the grid cell

3) Determine where to put the NO emissions

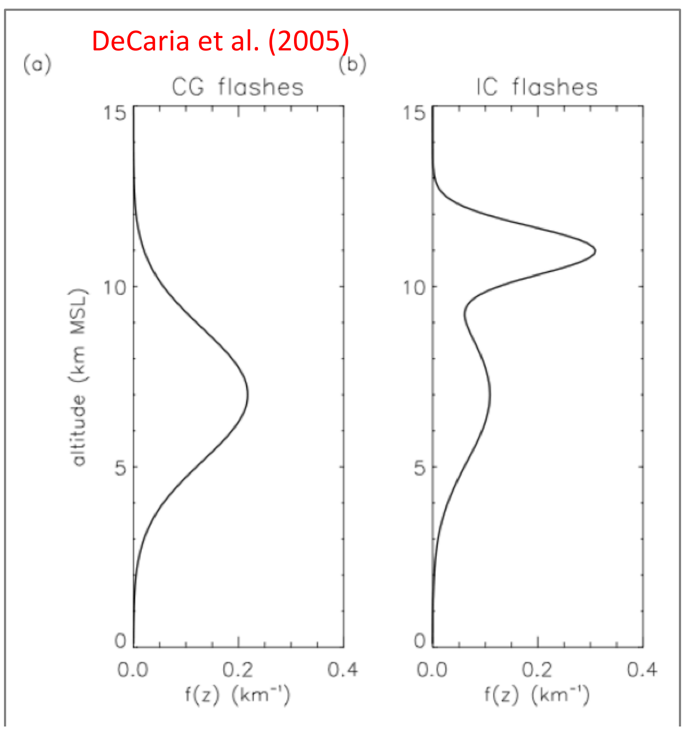
<u>Vertical Placement</u>

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

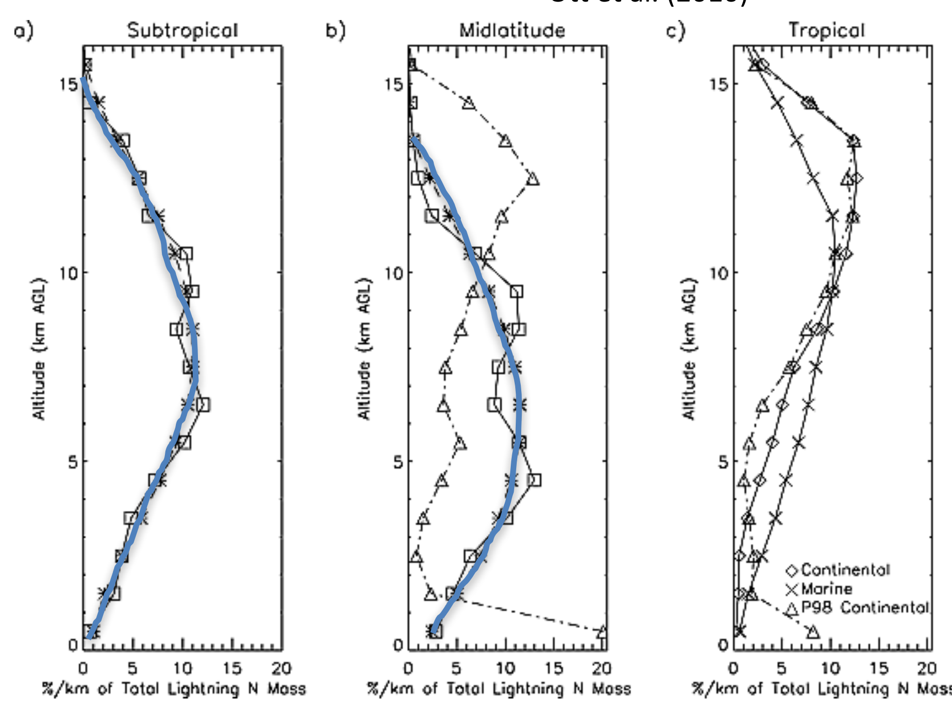
  Uses DeCaria et al. (2005) curves

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

  Uses Ott et al. (2010) curves



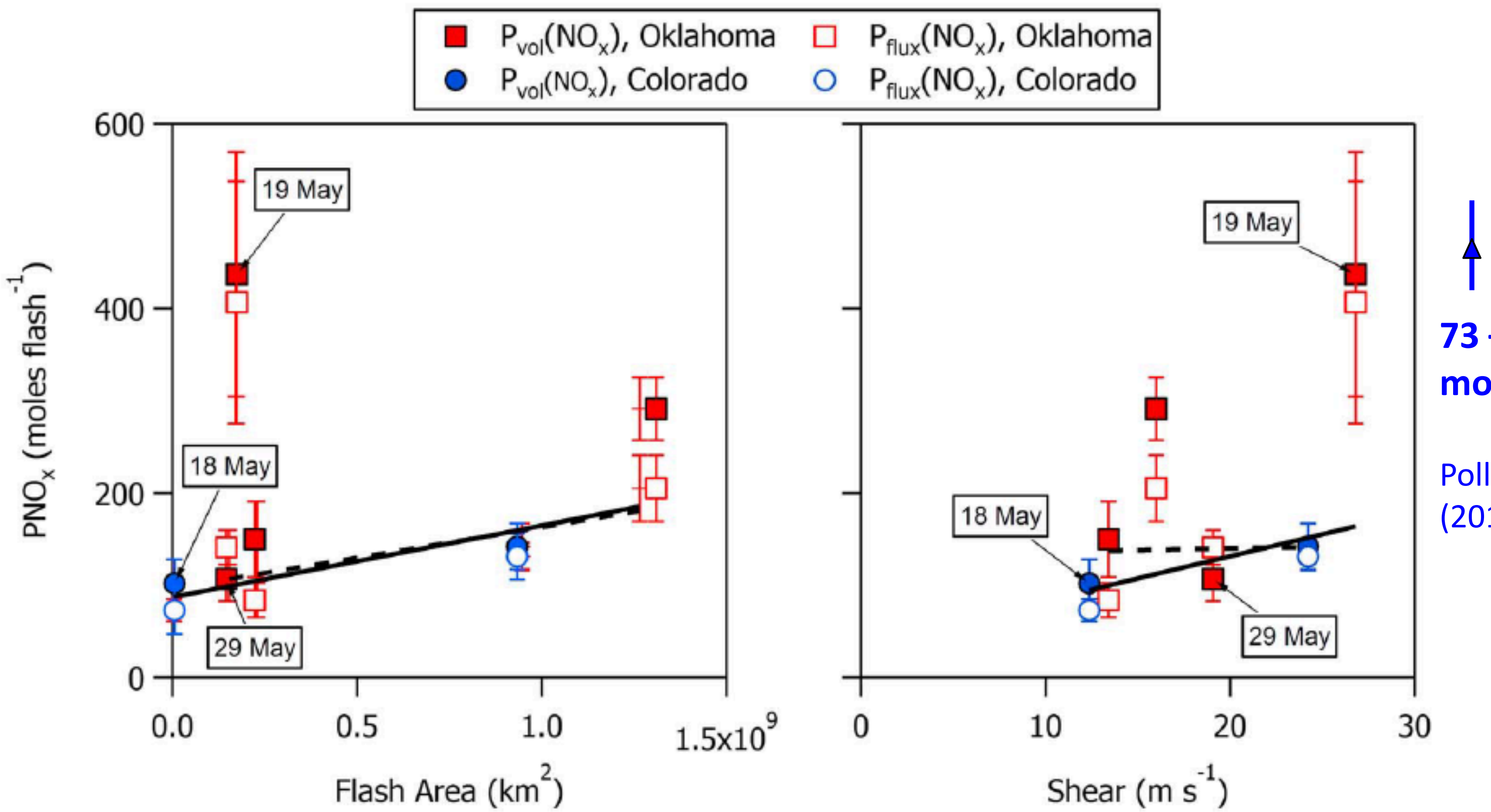
Ott et al. (2010)



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

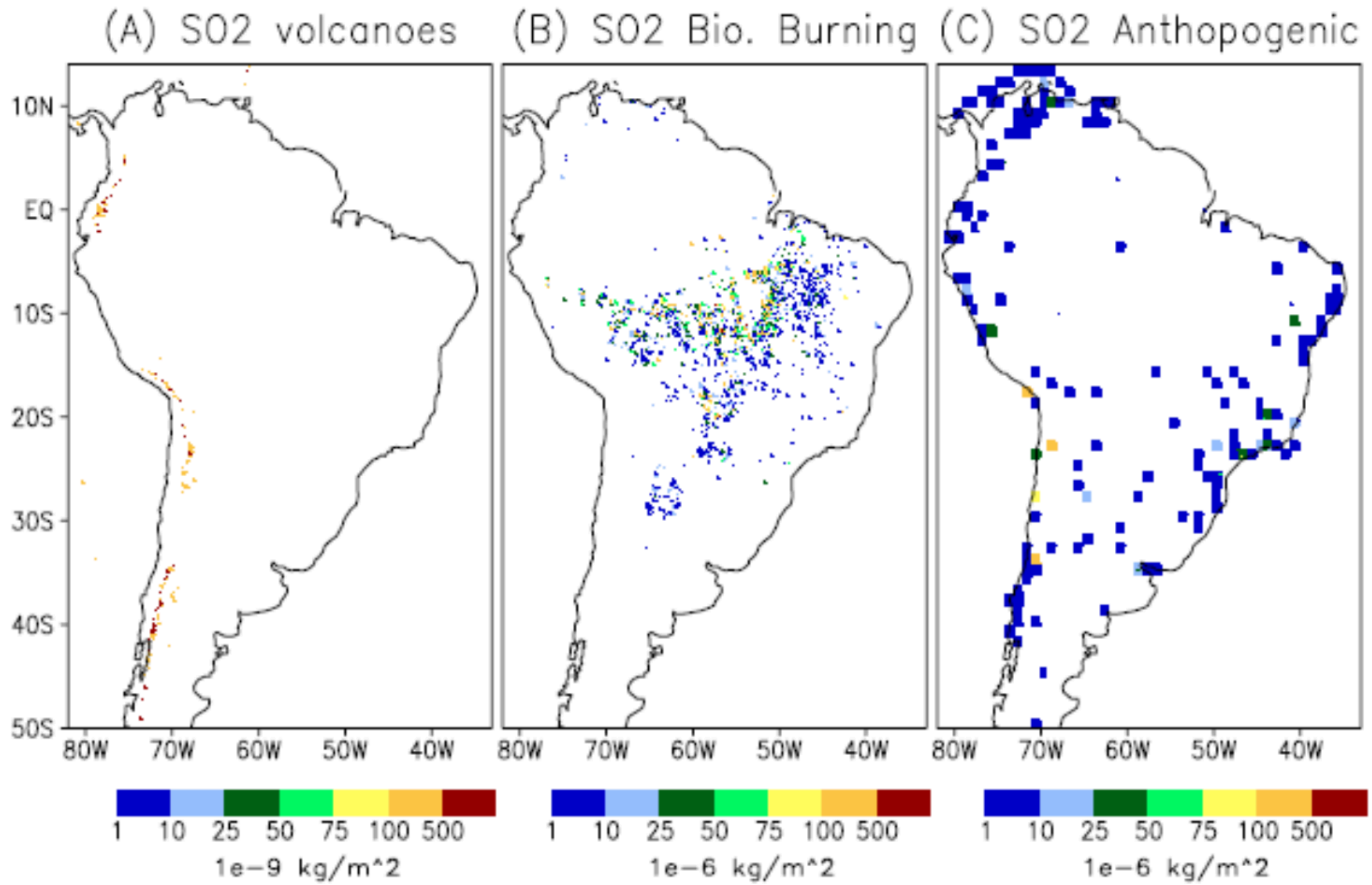


73 – 407 moles/flash

Pollack et al. (2016)

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)

Contact the following people with your questions

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