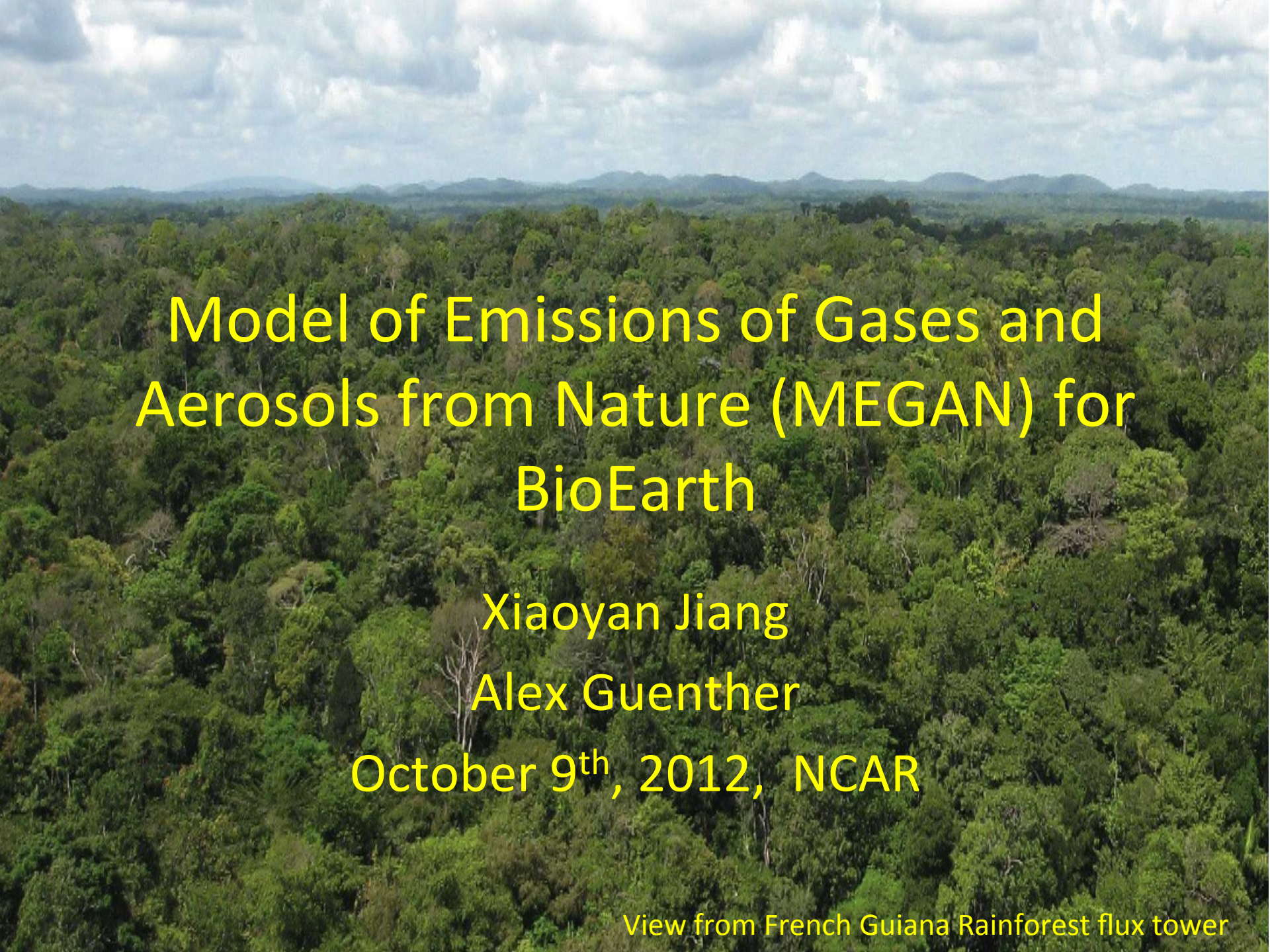


Model of Emissions of Gases and Aerosols from Nature (MEGAN) for BioEarth

Xiaoyan Jiang

Alex Guenther

October 9th, 2012, NCAR

View from French Guiana Rainforest flux tower

Outline

- MEGAN2.1
- Stand-alone MEGAN2.1
- CLM4-MEGAN2.1
- Future work

MEGAN2.1

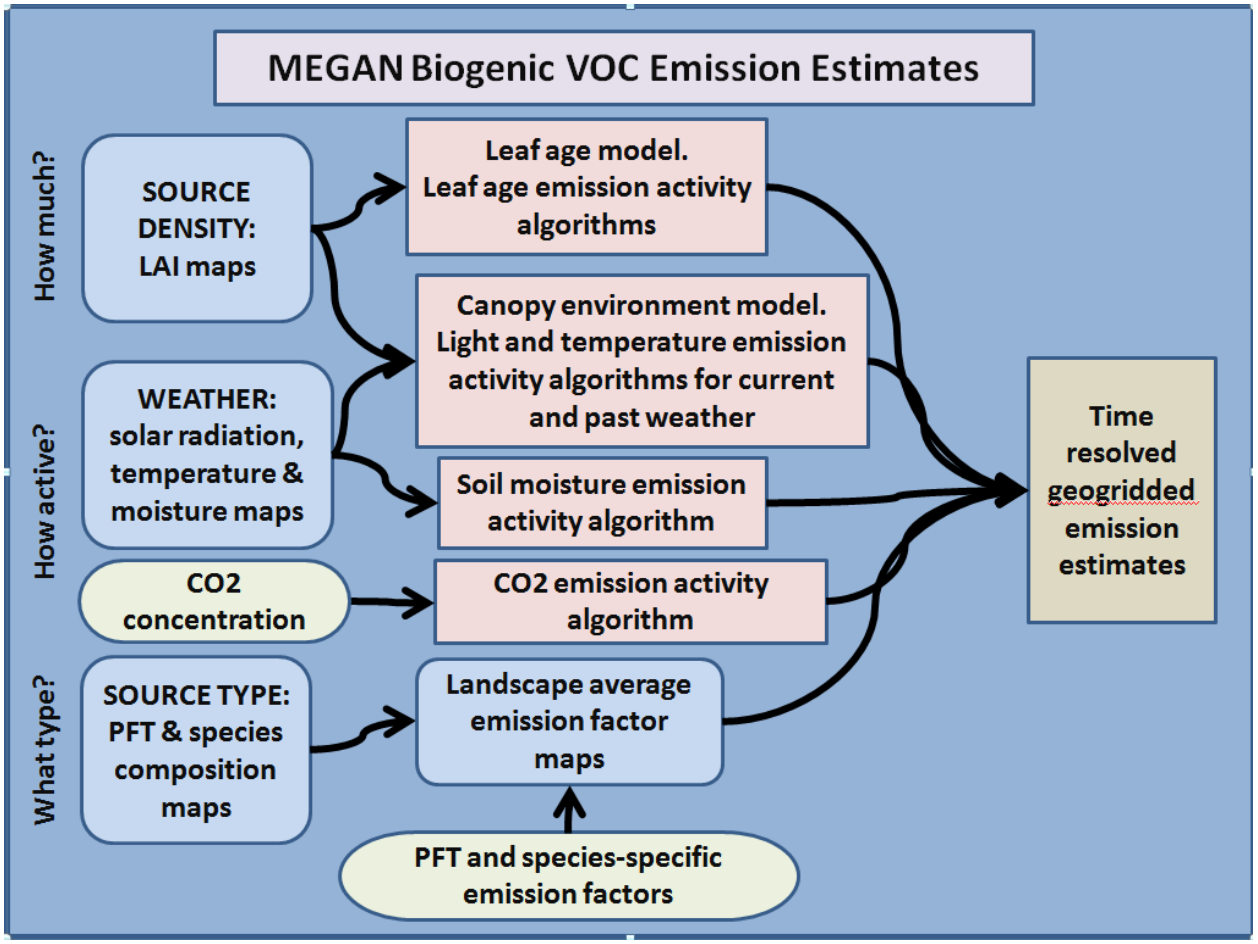
- Available as an offline code and has also been coupled into CLM/ CESM
- Global model with ~ 1 km^2 (or higher) and hourly resolution
- Designed for regional and global modeling
- Explicit (Full) canopy environment model including leaf energy balance
- New emission factors/algorithms
- Isoprene response to CO_2
- Has 147 compounds which are lumped into 19 categories
- Offline source code➔http://bai.acd.ucar.edu/MEGAN
- Oneline code➔http://www.cesm.ucar.edu
- Paper about MEGAN2.1➔http://www.geosci-model-dev-discuss.net/5/1503/2012/gmdd-5-1503-2012.html

19 categories and 147 chemical species in CESM version (stand-alone also includes N2O, NO and NH3) are calculated based on emission factors, PFTs, and environmental controlling factors.

Emission Categories	Compound names
Categories representing individual compounds (14 compounds)	hemiterpenes (isoprene and 232-MBO), monoterpenes (α-pinene, β-pinene, limonene, sabinene, 3-carene, myrcene, *t*-β-ocimene), sesquiterpenes (β-caryophyllene and α-farnesene), methanol, acetone and CO
Other Monoterpenes category (34 compounds)	aromatic monoterpenes (dimethyl styrene, meta-cymenene, p-cymene, and o-cymene), monoterpenes (α-phellandrene, α-thujene, α-terpinene, γ-terpinene, terpinolene, β-phellandrene, camphene, bornene, α-fenchene, allo-ocimene, cis-β-ocimene, verbenene and tricyclene), oxygenated monoterpenes (camphor, fenchone, piperitone, myrtenal, α-thujone, β-thujone, 1,8-cineole, borneol, linalool, 4-terpineol, α-terpineol, cis-linalool oxide, trans-linaool oxide and bornyl acetate) and monoterpenoid-related compounds (β-ionone, ipsenol and estragole).
Other Sesquiterpenes category (30 compounds)	sesquiterpenes (α-bergamotene, β-bisabolene, β-farnesene, α-humulene, acoradiene, aromadendrene, β-bergamotene, α-bisabolene, β-bourbonene, δ-cadinene, δ-cadinene, α-cedrene, α-copaene, α-cubebene, β-cubebene, β-elemene, germacrene B, germacrene D, β-gurjunene, γ-humulene, iso-longifolene, longifolene, longipinene, α-muurolene, γ-muurolene, β-selinene, and δ-selinene), oxygenated sesquiterpenes (cis-nerolidol, trans-nerolidol and cedrol).
Bidirectional exchange category (5 compounds)	ethanol, acetaldehyde, formaldehyde, acetic acid, formic acid
Other compound category (49 compounds)	leaf surface compounds (homosalate, 2-ethylhexyl salicylate, geranyl acetone, oxopentanal, and methyl heptenone), organic halides (methyl bromide, methyl chloride and methyl iodide), sulfur compounds (diallyl disulfide, methyl propenyl disulfide, propenylpropyldisulfide, carbon disulfide, carbonyl sulfide, hydrogen sulfide, methyl mercapten, dimethyl sulfide and dimethyl disulfide), alkanes (methane, ethane, propane, pentane, hexane, heptane), alkenes (butene, propene, 1-dodecene, 1-tetradecene), benzenoids (benzaldehyde, methyl benzoate, 2-phenylacetaldehyde, eugenol, anisole, benzyl acetate, benzyl alcohol, and naphthalene), oxygenated VOC (pentanal, hexanal, heptanal, octanal, nonanal, decanal, octanol, octenol, heptanone, 2-butanone, pyruvic acid, 331-methylbutenol, 321- methylbutenol, neryl acetone, α-terpinyl acetate, phenylacetaldehyde and nonenal)

(Guenther et al., 2012)

$$F_i = \gamma_i \sum \varepsilon_{i,j} \chi_j$$



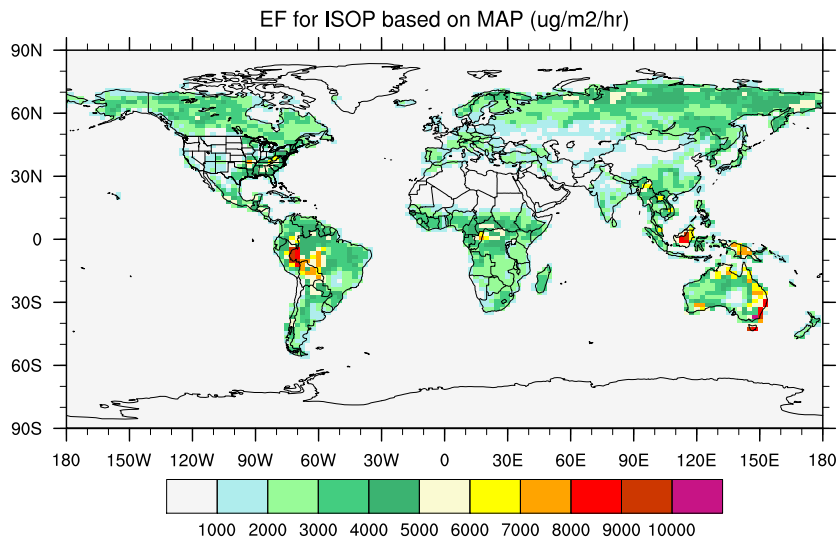
$$F_i = \gamma_i \sum \varepsilon_{i,j} \chi_j$$

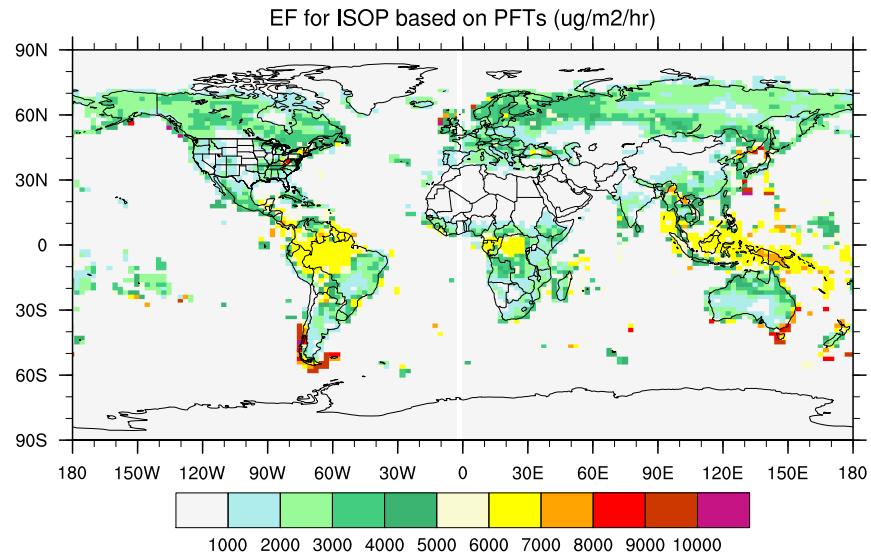
- F_i: emissions of chemical species i
- Υ_i: emission activity factor (environmental and phenological conditions)
- $\varepsilon_{i,j}$: emission factor at standard condition for vegetation type j
- X_j: fractional grid box areal coverage

$\varepsilon_{i,j}$: emission factor

- Options are:
  - Specified from gridded maps based on species composition and species-specific emission factors
  - Calculate from Plant Functional Type (PFT) distributions and the PFT specific emission factors listed in the table (16 PFTs)
- The MEGAN2.1 emission factor represents the net primary emission that escapes into the atmosphere but is not the net flux because it does not include the flux of chemicals from the above canopy atmosphere down into the canopy.

ISOP EFs from MAP and PFT

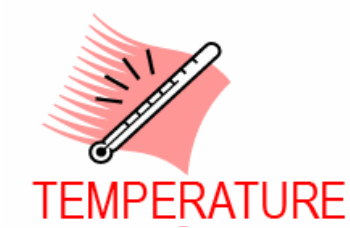




Compound Class	EF_1	EF_2	EF_3	EF_4	EF_5	EF_6	EF_7	EF_8	EF_9	EF_{10}	EF_{11}	EF_{12}	EF_{13}	EF_{14}	EF_{15}
Isoprene	600	3000	1	7000	10 000	7000	10 000	11 000	2000	4000	4000	1600	800	200	1
Myrcene	70	70	60	80	30	80	30	30	30	50	30	0.3	0.3	0.3	0.3
Sabinene	70	70	40	80	50	80	50	50	50	70	50	0.7	0.7	0.7	0.7
Limonene	100	100	130	80	80	80	80	80	60	100	60	0.7	0.7	0.7	0.7
3-Carene	160	160	80	40	30	40	30	30	30	100	30	0.3	0.3	0.3	0.3
t-β-Ocimene	70	70	60	150	120	150	120	120	90	150	90	2	2	2	2
β-Pinene	300	300	200	120	130	120	130	130	100	150	100	1.5	1.5	1.5	1.5
α-Pinene	500	500	510	600	400	600	400	400	200	300	200	2	2	2	2
Other Monoterpenes	180	180	170	150	150	150	150	150	110	200	110	5	5	5	5
α-Farnesene	40	40	40	60	40	60	40	40	40	40	40	3	3	3	4
β-Caryophyllene	80	80	80	60	40	60	40	40	50	50	50	1	1	1	4
Other Sesquiterpenes	200	200	200	200	150	200	150	150	150	150	150	2	2	2	2
232-MBO	200	10	0.01	0.01	0.01	0.01	0.01	2	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Methanol	900	900	900	500	900	500	900	900	900	900	900	500	500	500	900
Acetone	240	240	240	240	240	240	240	240	240	240	240	80	80	80	80
CO	600	600	600	600	600	600	600	600	600	600	600	600	600	600	600
Bidirectional VOC	500	500	500	500	500	500	500	500	500	500	500	80	80	80	80
Stress VOC	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300
Other VOC	140	140	140	140	140	140	140	140	140	140	140	140	140	140	140

Υ_i: emission activity factor

$$\gamma_i = C_{CE}\ LAI\ \gamma_{P,i}\ \gamma_{T,i}\ \gamma_{A,i}\ \gamma_{SM,i}\ \gamma_{C,i}$$



CO_2

Υ_i: emission activity factor

$\gamma_i = C_{CE}\ LAI\ \gamma_{P,i}\ \gamma_{T,i}\ \gamma_{A,i}\ \gamma_{SM,i}\ \gamma_{C,i}$

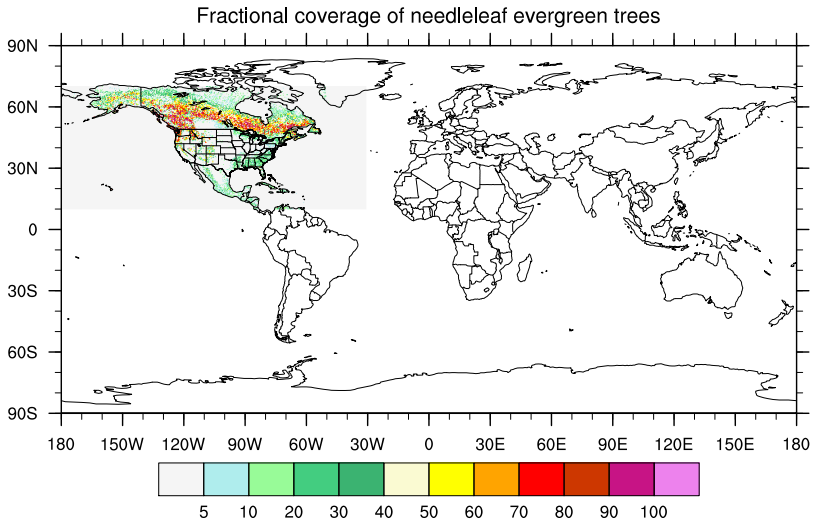
- **Canopy environment coefficient (C_{CE})** : assigned a value that results in γ = 1 for the standard conditions and is dependent on the canopy environment model being used.
- **Light (γ_P)**: $\gamma_{P,i} = (1 - LDF_i) + LDF_i\ \gamma_{P\_LDF}$; where γ_{P_LDF} follows the light-dependent activity factor described for isoprene by Guenther et al. (2006) as $\gamma_{P\_LDF} = C_P\ [(a \cdot PPFD) / ((1 + a^2 \cdot PPFD^2)^{0.5})]$
- **Temperature (γ_T)**: is the weighted average of a light-dependent and light-independent fraction $\gamma_{T,i} = (1 - LDF_i)\ \gamma_{T\_LIF,i} + LDF_i\ \gamma_{T\_LDF,i}$
- **Leaf age (γ_A)**: $\gamma_{A,i} = F_{new} \cdot A_{new,i} + F_{gro} \cdot A_{gro,i} + F_{mat} \cdot A_{mat,i} + F_{sen} \cdot A_{sen,I}$; where $A_{new,i}$, $A_{gro,i}$, $A_{mat,i}$, and $A_{sen,i}$ are empirical coefficients
- **Soil moisture (γ_{SM})**: $\gamma_{SM,isoprene} = 1$ $\quad \theta > \theta_1$
  $\gamma_{SM,\ isoprene} = (\theta - \theta_w) / \Delta\theta_1$ $\quad \theta_w < \theta < \theta_1$
  $\gamma_{SM,\ isoprene} = 0$ $\quad \theta < \theta_w$
- **Leaf area index (LAI)**
- **CO_2 for isoprene (γ_C)**: $\gamma_{CO2,isoprene} = I_{Smax} - [(I_{Smax}\ (C_i)^h) / ((C^*)^h + (C_i)h\ )]$

PFT data

- **High resolution (60m) PFT data for North America :**

Available at: http://bai.acd.ucar.edu/MEGAN

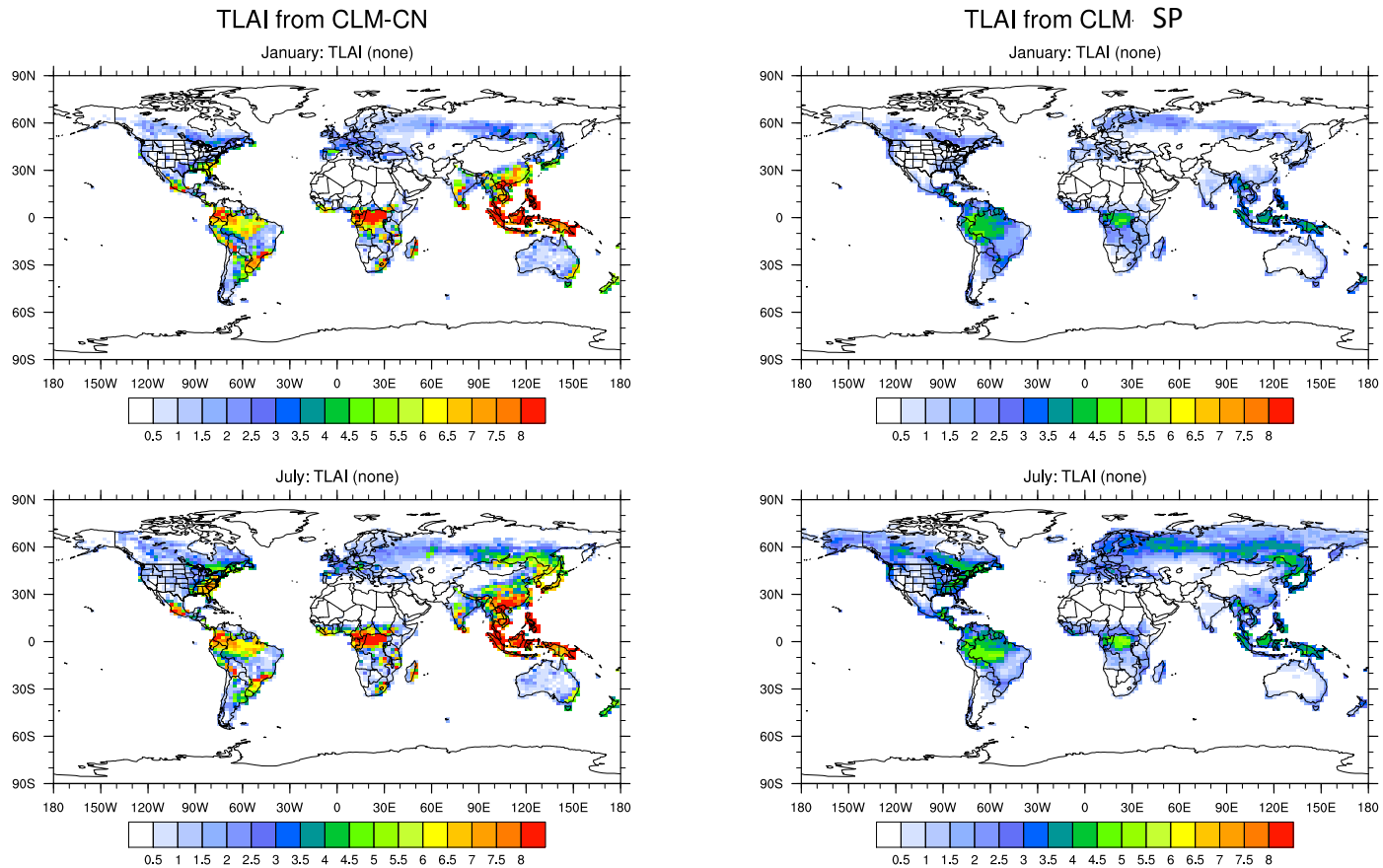
Created by combining the National Land Cover Dataset (NLCD, Homer et al. 2004) and the Cropland Data Layer (see http://nassgeodata.gmu.edu/CropScape/), which are based on 30-m LANDSAT-TM satellite data, with vegetation species composition data from the Forest Inventory and Analysis (see www.fia.fs.fed.us) and the soil database of the Natural Resources Conservation Services (see http://sdmdataaccess.nrcs.usda.gov/).



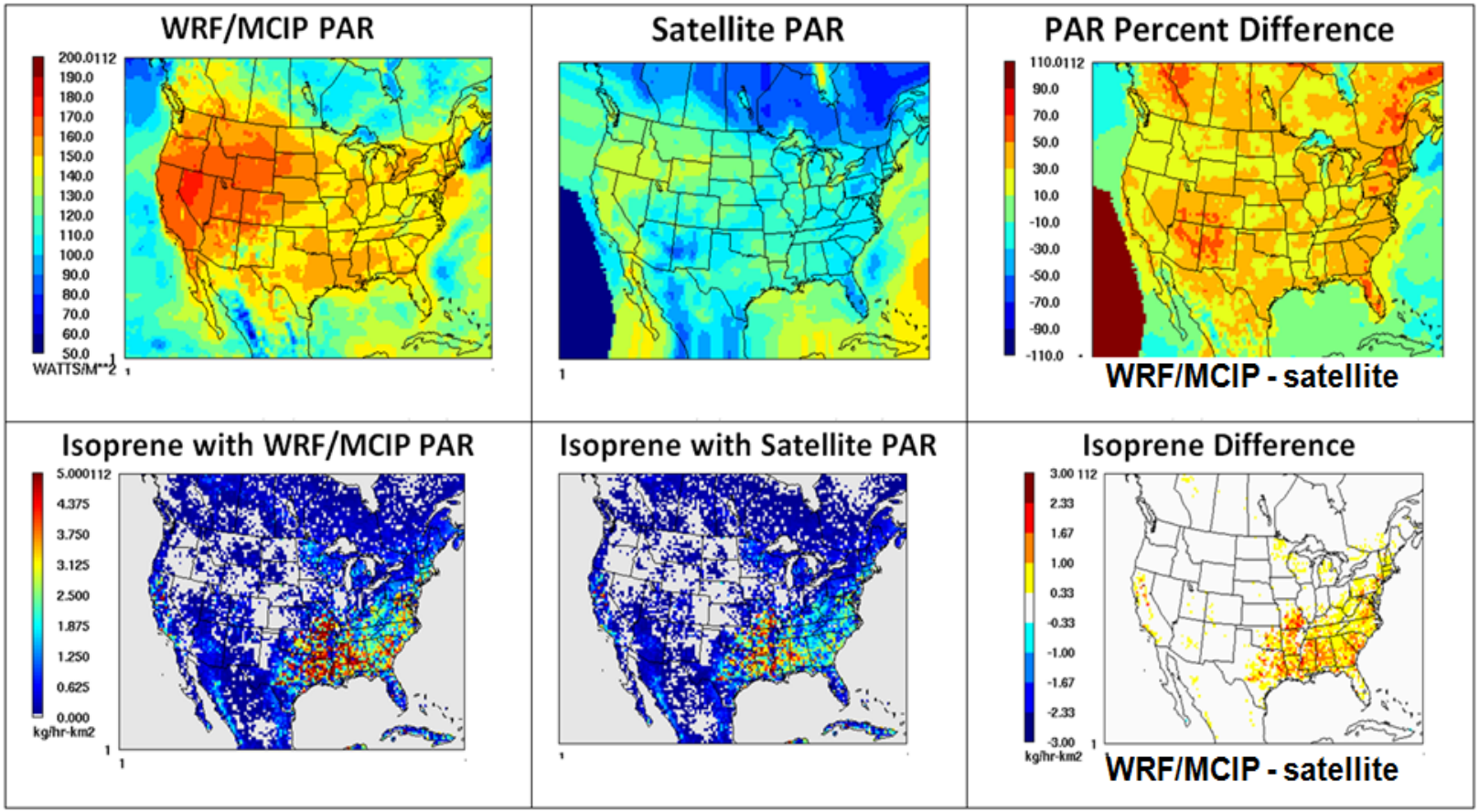
- **0.3 min global PFT data from CLM website**

Leaf Area Index data

- MEGAN uses LAI to quantify the amount of foliage at a given location and uses changes in LAI to estimate the age of the foliage. LAI data for driving MEGAN can be obtained from dynamic vegetation models or from satellite datasets.
- Offline MEGAN2.1 uses 8-day LAI

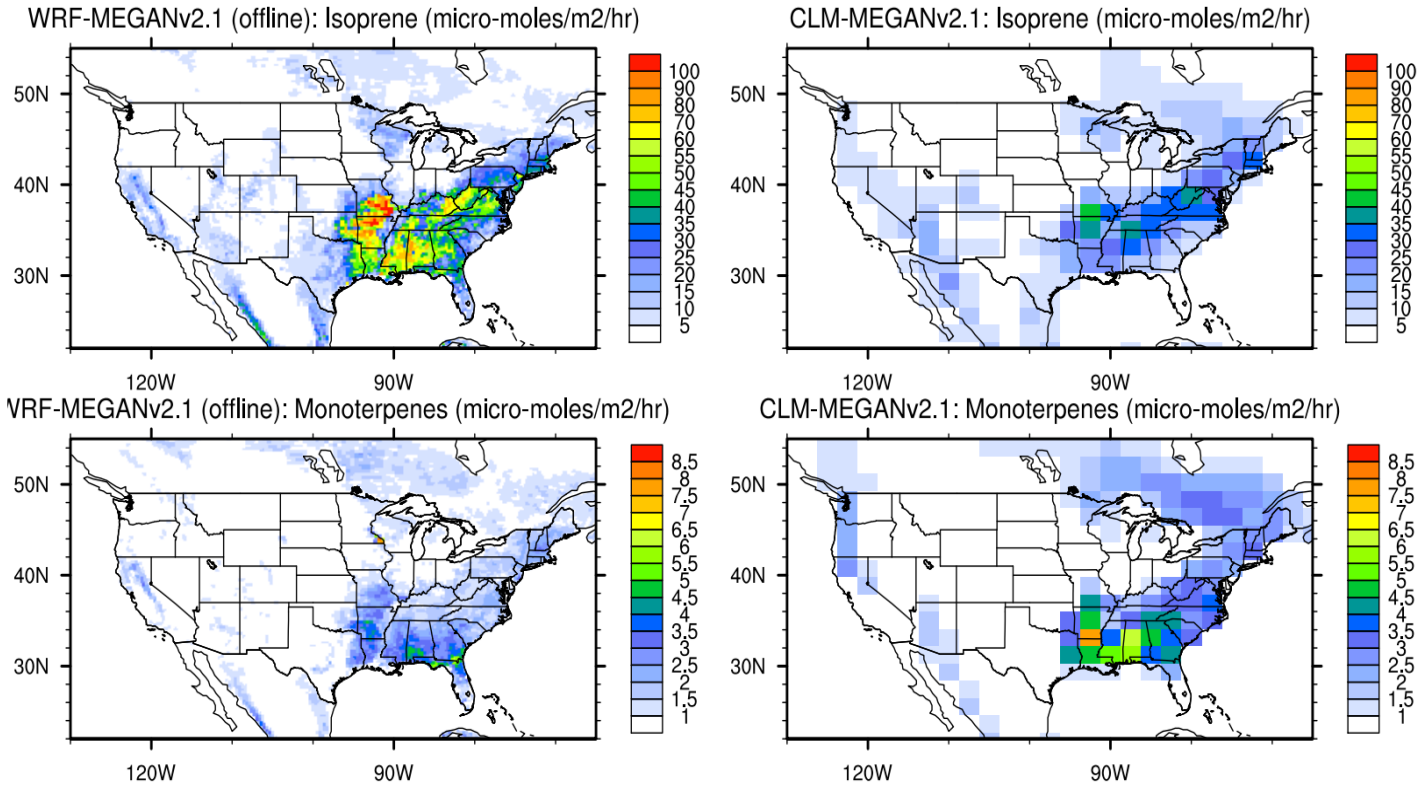


Radiation impact on isoprene emissions



- 3-18 July, 2008, period average estimates of PAR (W m^{-2}) from WRF/MCIP (top left) and satellite (top middle) and percent difference for WRF/MCIP – Satellite (top right) and associated isoprene emissions (kg h^{-1} km^{-2}) using MEGAN2.1 in WRF-AQ driven by WRF/MCIP PAR (bottom left) and satellite PAR (bottom middle) and difference (bottom right).

MEGAN2.1 Estimates with WRF/CLM



Offline MEGAN2.1 with WRF forcing Online MEGAN2.1 within CLM

Stand-alone MEGAN2.1 USER'S GUIDE

MEGAN version 2.10 User's Guide

Xiaoyan Jiang, Alex Guenther, and Tiffany Duhl
Atmospheric Chemistry Division
NCAR Earth System Laboratory
PO Box 3000 Boulder CO USA
contact: xjiang@ucar.edu

Tan Sakulyanontvittaya
Jeremiah Johnson
ENVIRON
Novato, CA, USA

Xuemei Wang
Sun-Yat Sen University
Guangzhou, China

http://bai.acd.ucar.edu/MEGAN

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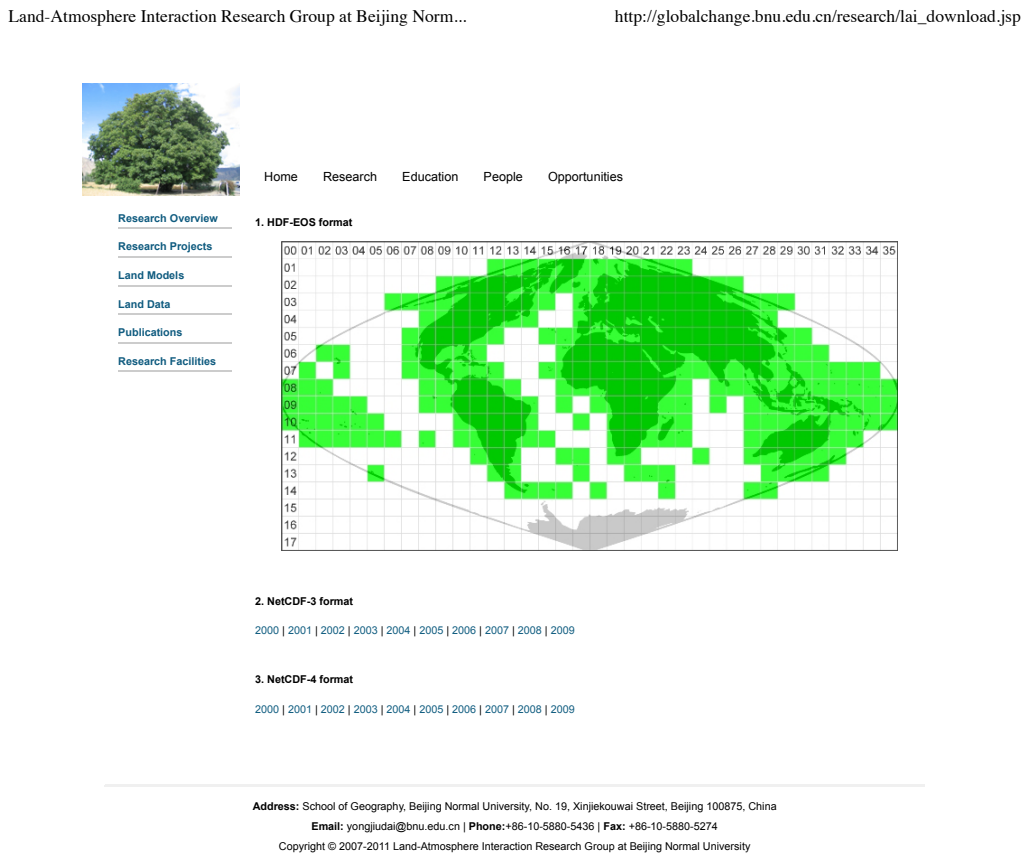
New global 30s MODIS LAI data

- http://globalchange.bnu.edu.cn/research/lai_download.jsp



MEGAN2.1 with CLM4 in CESM

- Climate change impacts➔

  Land use/cover change impacts➔
- On changes in biogenic emissions

  On changes in atmospheric chemistry
- Feedbacks

$F_i = \gamma_i \sum \varepsilon_{i,j} \chi_j$

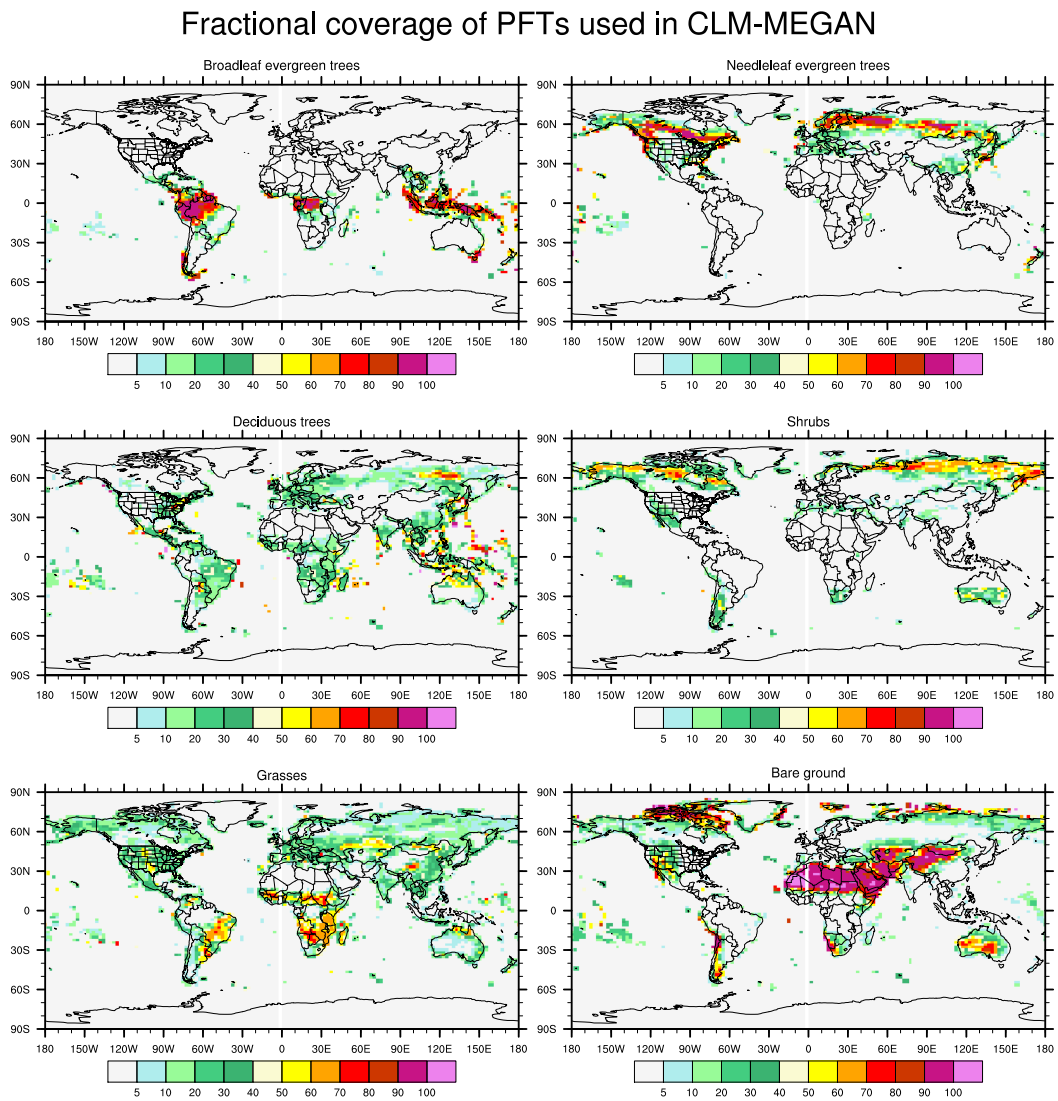
- The calculated emissions of chemical species (F_i) are passed to CAM-Chem through the namelist option:

```
&megan_emis_nl
megan_factors_file = '/work/CESM_NCAR/new_emiss_factors/new_factor.nc'
 megan_specifier = 'ISOP = isoprene',
                   'C10H16=myrcene+sabinene'
```

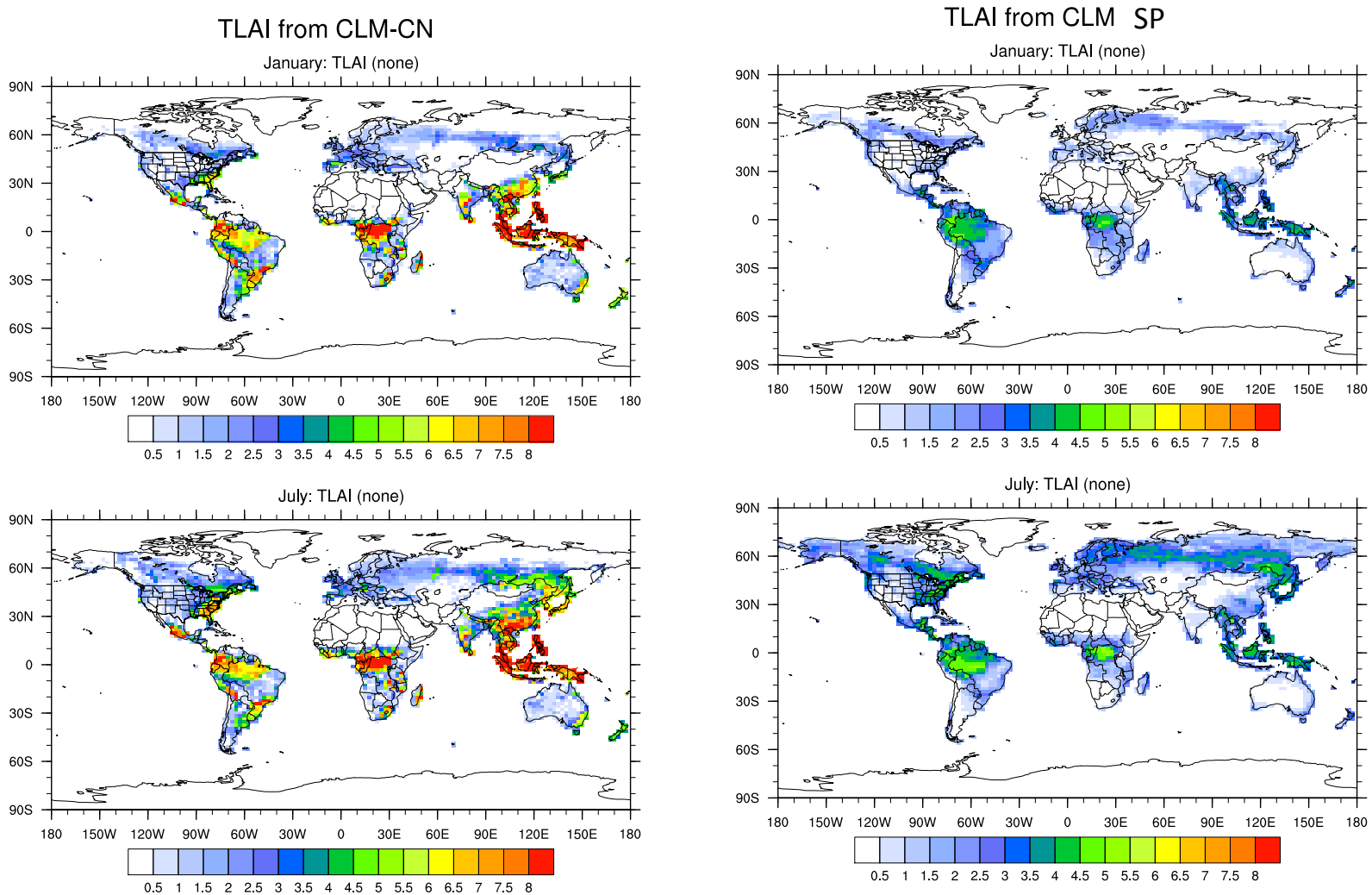
Υ_i: emission activity factor (environmental and phenological conditions)

- **Dependent on PFT, temperature, radiation, LAI, leaf age and soil moisture. For isoprene, CO_2 effect is also included.**
- PFT: vegetation fractional coverage, and emission factors
- Temperature (vegetation): biogeophys/CanopyFluxesMod.F90
- Radiation (direct and diffuse radiation): biogeophys/ SurfaceRadiationMod.F90
- LAI, leaf age (sunlit fraction of canopy, one-sided leaf area index): biogeochem/CLM/CN or CLM/SP
- Soil moisture: from CLM hydrology under biogeophys/
- CO_2: from biogeophys/CanopyFluxesMod.F90: leaf stomatal resistance and leaf photosynthesis. This is also linked with the current CN module in CLM.

CLM4 surface data and initial conditions

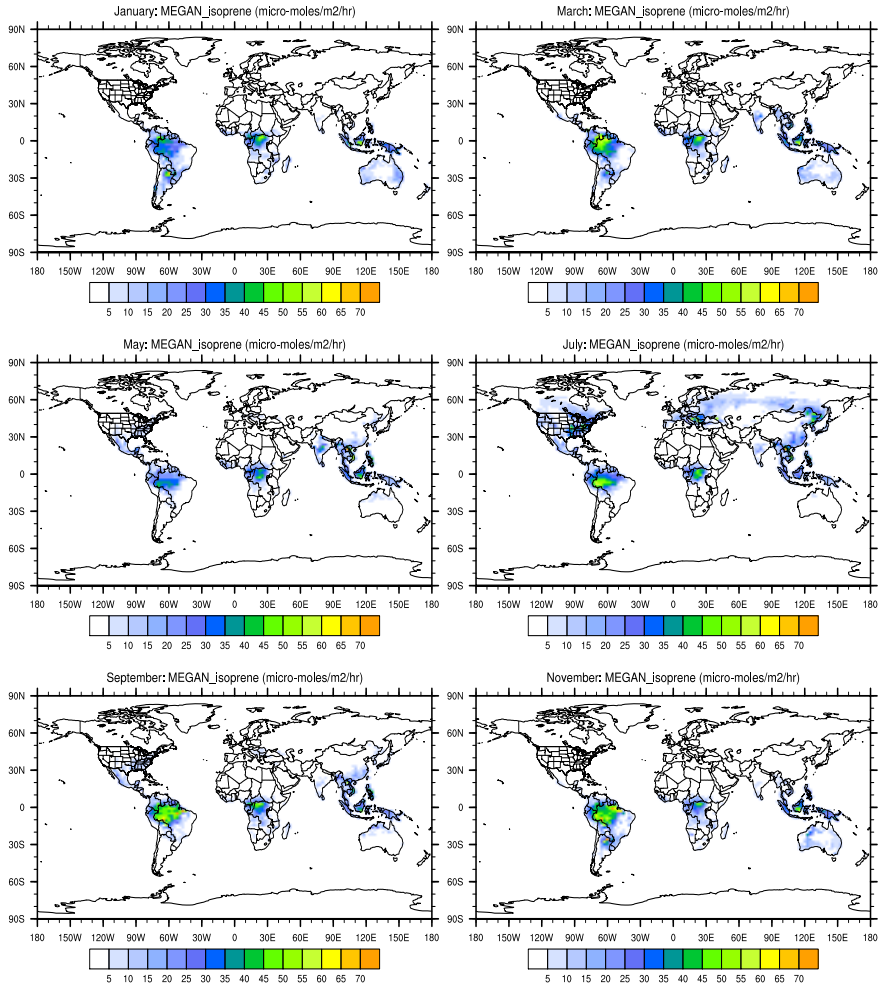


LAI from CLM-CN vs. CLMSP

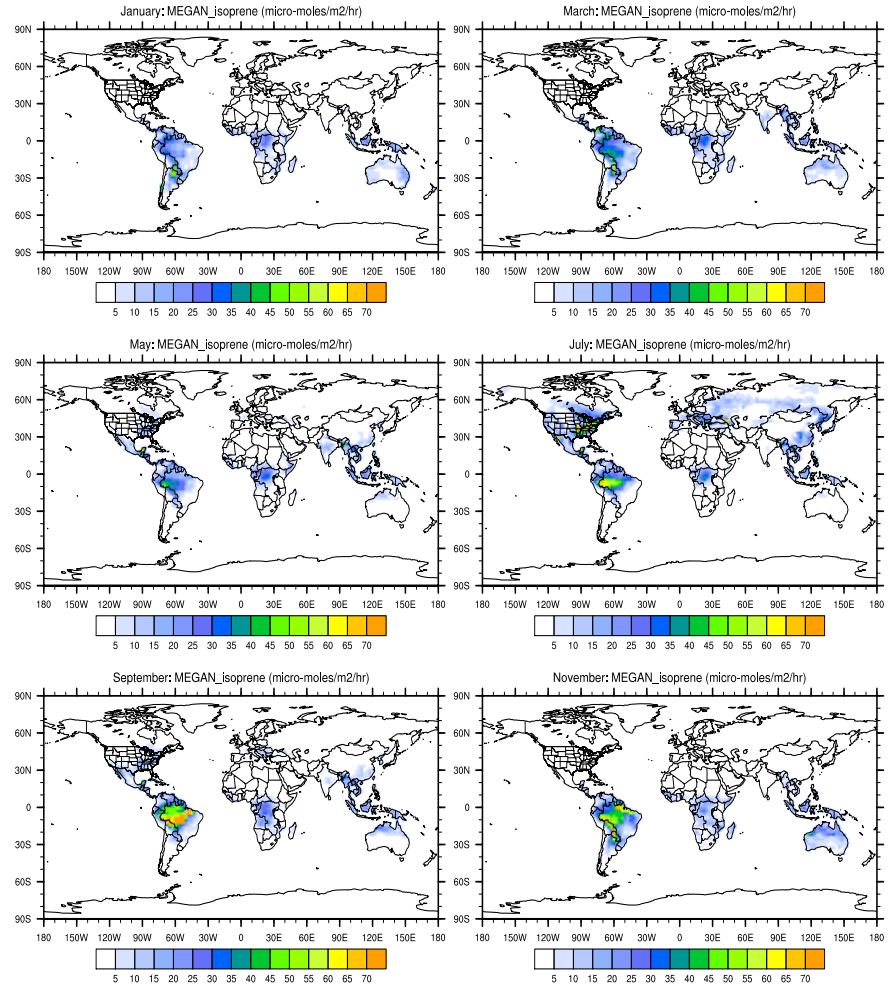


Impacts on isoprene emissions

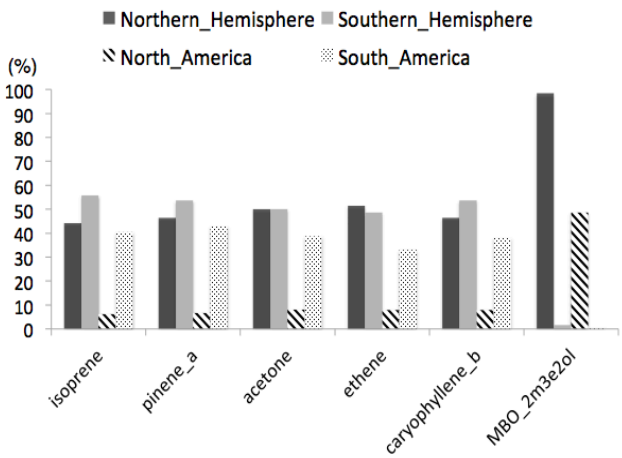
MEGAN isoprene from CLMCN-MEGAN

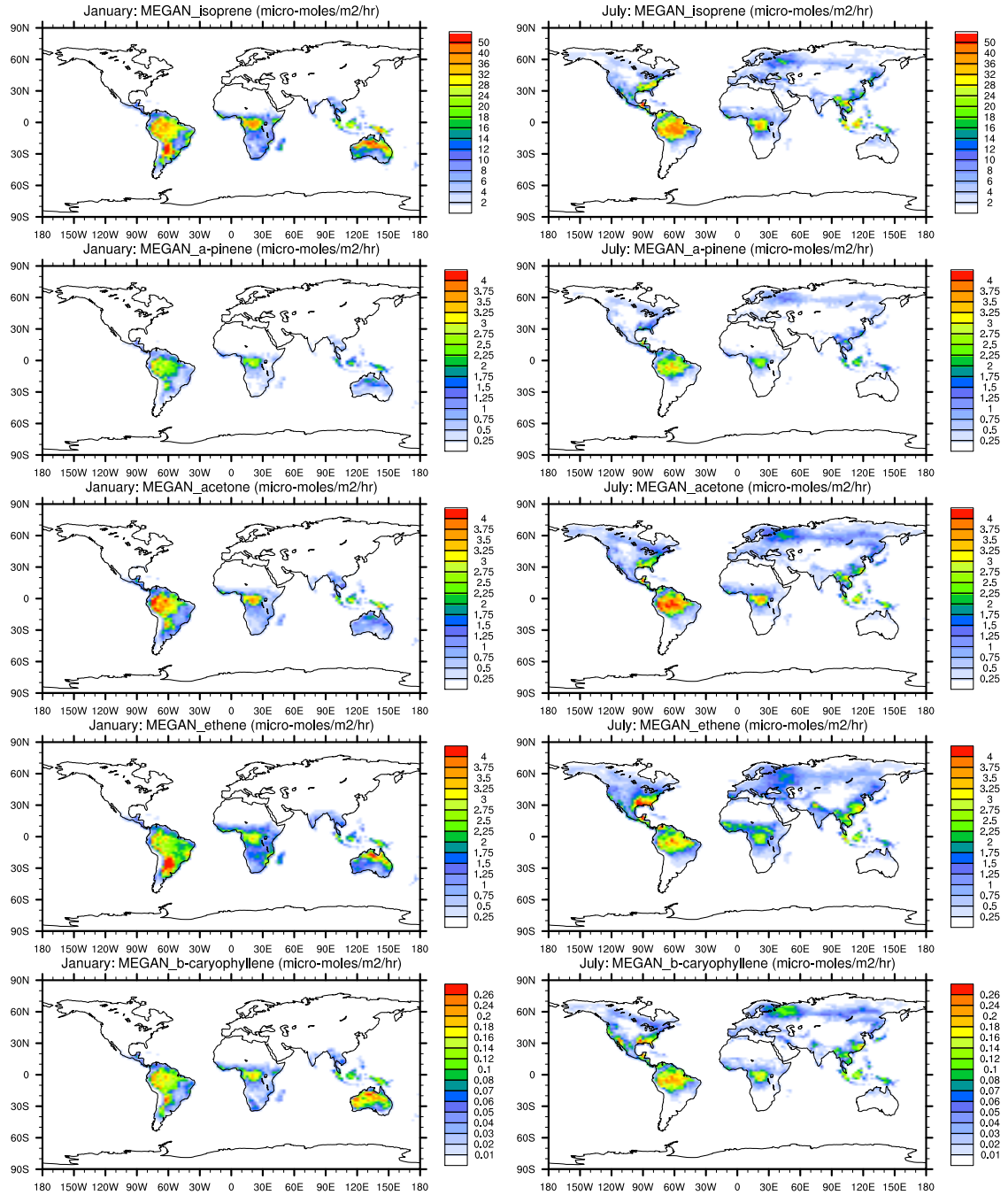


MEGAN isoprene from CLMSP-MEGAN



Global simulation of different compounds





Global totals

Table 3. CLM4 global land area (10^{12} km^2) and isoprene, monoterpene (MT) and other (VOC and CO) emissions for individual Plant Functional Types estimated using MEGAN2.1 algorithms in CLM4 for year 2000.

CLM PFT Number	Description	Land Area	Isoprene Tg yr^{-1}	MT Tg yr^{-1}	Other Tg yr^{-1}
	Bare	40.7			
1	Needleleaf Evergreen Temperate Tree	5.46	1.61	7.38	11.6
2	Needleleaf Evergreen Boreal Tree	10.6	5.9	6.63	9.42
3	Needleleaf Deciduous Boreal Tree	1.46	0.0002	0.52	0.89
4	Broadleaf Evergreen Tropical Tree	15.6	244	82.9	127
5	Broadleaf Evergreen Temperate Tree	2.64	21.9	4.0	8.71
6	Broadleaf Deciduous Tropical Tree	12.9	178	45.0	74.3
7	Broadleaf Deciduous Temperate Tree	5.33	35.4	5.86	13.1
8	Broadleaf Deciduous Boreal Tree	2.14	4.79	0.99	2.02
9	Broadleaf Evergreen Temperate Shrub	0.18	0.23	0.08	0.33
10	Broadleaf Deciduous Temperate Shrub	4.15	21.8	6.77	16.4
11	Broadleaf Deciduous Boreal Shrub	9.33	2.93	1.07	3.3
12	Arctic C3 Grass	4.94	0.97	0.02	1.45
13	Cool C3 Grass	14.3	11.2	0.25	26.1
14	Warm C4 Grass	13.2	5.93	0.49	51.3
15	Crop1	16.3	0.02	0.36	44.5
	Total (all PFTs)	159	535	162	390

Compound Class	Compounds	Emissions (Tg yr^{-1})
Isoprene	Isoprene	535
α-Pinene	α-Pinene	66.1
t-β-Ocimene	t-β-Ocimene	19.4
β-Pinene	β-Pinene	18.9
Limonene	Limonene	11.4
Sabinene	Sabinene	9.0
Myrcene	Myrcene	8.7
3-Carene	3-Carene	7.1
Other Monoterpenes	Camphene	4.0
	β-phellandrene	1.5
	Terpinolene	1.3
Sum of the other 31 compounds in this category		14.9
α-Farnesene	α-Farnesene	7.1
β-Caryophyllene	β-Caryophyllene	7.4
Other Sesquiterpenes	β-Farnescene	4.0
	α-Humulene	2.1
	α-Bergamotene	1.3
Sum of the other 27 compounds in this category		7.1
232-MBO	232-MBO	2.2
Methanol	Methanol	99.6
Acetone	Acetone	43.7
Bidirectional VOC	Ethanol	20.7
	Acetaldehyde	20.7
	Formaldehyde	5.0
	Acetic acid	3.7
	Formic acid	3.7
Stress VOC	Ethene	26.9
	C3-hexenal	4.9
	DMNT	4.9
	C3-hexenol	2.9
Sum of the other 11 compounds in this category		7.8
Other VOC	Propene	15.8
	Butene	8.0
	Homosalate	2.0
	Geranyl acetone	0.8
Sum of the other 45 compounds in this category		5.5
Total VOC	Sum of 146 VOC	1006
CO	CO	81.6
Total	VOC and CO	1088

(Guenther et al., 2012)

Future work

- Add biological particles: pollen scheme completed, fungal spores and other particles in development
- Improved soil nitrogen emissions
- Extend CLM PFT scheme to approach that can adequately describe BVOC emissions (~50 PFTs)
- Improved canopy environment model
- Evaluate and improve using aircraft and tower based flux and measurements
- Incorporate measurements into a community biogenic emission model testbed

Thank you!