Winners of Atmospheric Environment's

2016 Haagen-Smit Prize

Grell, GA; Peckham, SE; Schmitz, R; McKeen, SA; Frost, G; Skamarock, WC; Eder, B., Fully coupled "online" chemistry within the WRF model. Atmospheric Environment, 39, 6957-6975, 2005.

Sillman, S., The relation between ozone, NOx and hydrocarbons in urban and polluted rural environments. Atmospheric Environment, 33(12), 1821-1845, 1999.

Emission Inventory Options within WRF/Chem

Stu McKeen, Ravan Ahmadov, Megan Bela, Greg Frost

(CIRES/University of Colorado, NOAA/ESRL)

- WRF/Chem design considerations
- Putting anthropogenic emissions in the model
- How good are the North American inventories?
- Global inventories

WRF/Chem design considerations

(current configuration)

Basic emissions are specified "outside" of WPS or WRF system

- 4-dimensional arrays (I,J,K,time) for each emitted species
- Emission variables specified in the Registry (e_co, e_so2…etc.)
- Time dependent handled in share/mediation_integrate (e.g., anthro)
- Time-independent em. data added to wrfinput_<d0x> files (e.g., biogenic)

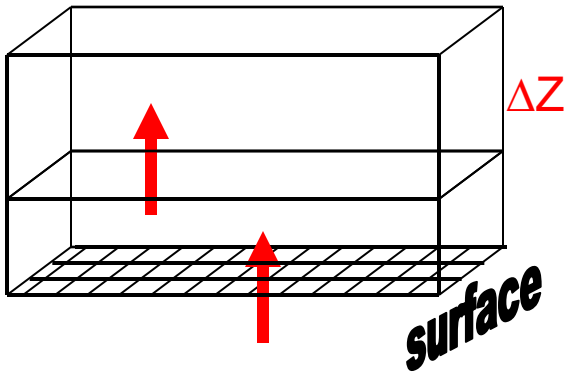
Practical Constraints:

- WRF domain (horizontal and vertical) must be pre-defined - real.exe
- Up to User to link:
  - Emissions inventory - Chemical Mechanism
  - Spatial Allocation - Temporal Variations
- No internal coupling with WRF for anthropogenic plume rise calculations
  (But biomass burning options do incorporate plume rise!)

Chemistry mechanisms in WRF-Chem3.6

Chemical mechanisms	*Fixed versions*	*KPP*	*Coupled to the aerosol schemes*
RADM2	**Yes**	**Yes**	**MADE/SORGAM, GOCART**
RACM	**None**	**Yes**	**MADE/SORGAM, GOCART**
RACM-MIM	**None**	**Yes**	**None**
RACM-ESRL	**None**	**Yes**	**MADE/SORGAM, MADE/SOA_VBS**
CB4	**None**	**Yes**	**None**
CBMZ	**Yes**	**Yes**	**MOSAIC**
MOZART	**None**	**Yes**	**GOCART**
SAPRC99	**None**	**Yes**	**MOSAIC**
NMHC9	**None**	**Yes**	**None**
CRIMECH	**None**	**Yes**	**MOSAIC**

How are emissions added within WRF/Chem?



adopted convention:

Emission units: moles/km^2/hr - gas phase
μg/km^2/hr - aerosol

For both surface and elevated sources

WRF/Chem gas/aerosol units

Gas-phase: ppmv (parts per million by volume)

Aerosol: μg/kg$_{(dry\ air)}$

dyn_em/solve_em.F → share/solve_interface.F → chem/chem_driver.F → chem/module_emissions_anthropogenic.F

chem/module_emissions_anthropogenic.F → add_anthropogenics subroutine
chem/module_emissions_anthropogenic.F → add_biogenics subroutine

$$\chi_{(new)} = \chi_{(old)} + \Delta t \bullet [Emission]/\Delta Z/\rho_{AIR}$$

[ΔZ, and ρ_{AIR} are not constant]

Where are the emissions data and processing routines?

ftp://aftp.fsl.noaa.gov/divisions/taq

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emissions_data_2011/

(NEI-2011 inventory – 4km res., North America)

Name

- em11v1_file1.tar
- em11v1_file2.tar

Use emiss_v04.F included in em11v1_file1.tar to process

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global_emissions/

(EDGAR/HTAP inventory – 2010 base year, 0.1 degree res., Global)

GoCART aerosol options

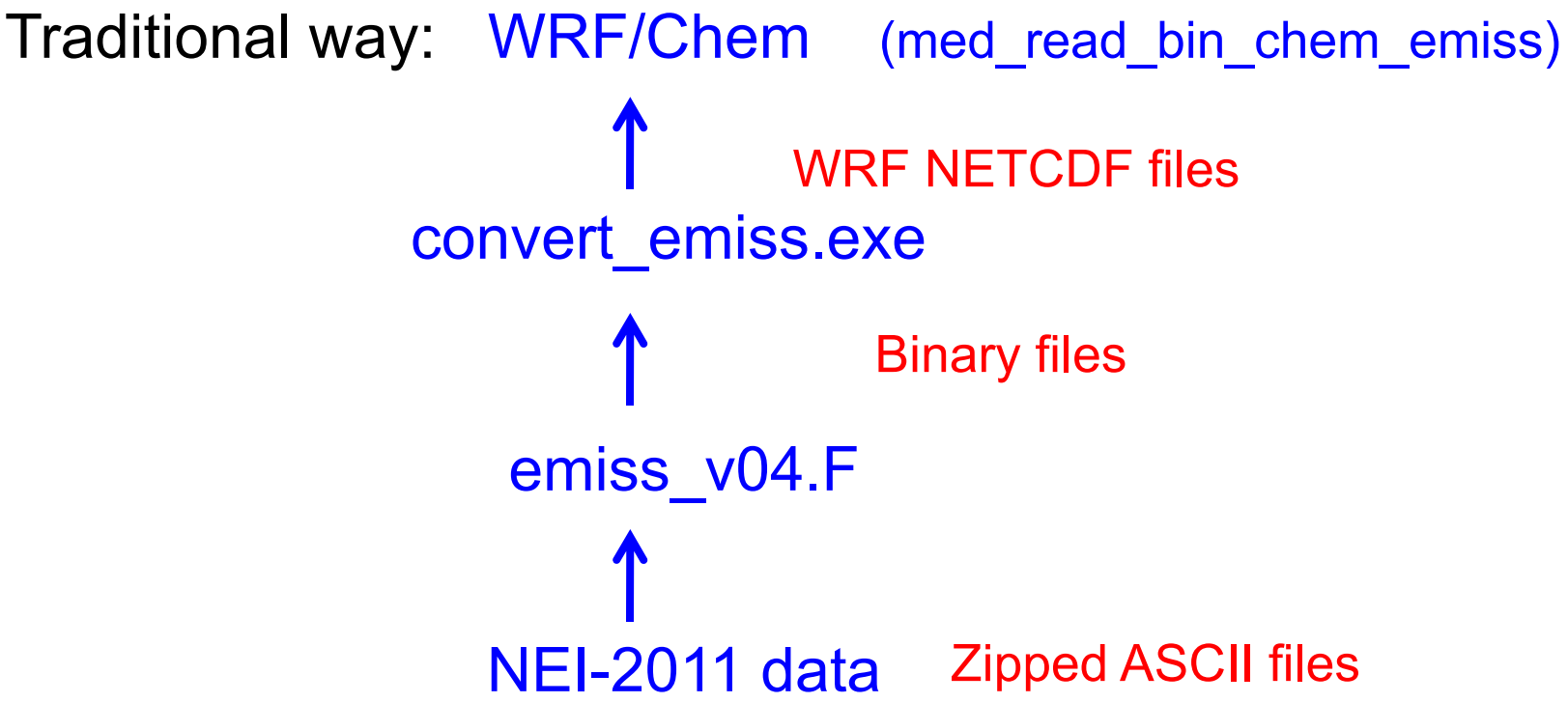
Domains outside of North America

Name

- global_emissions_v3_02aug2012.tar.gz
- global_emissions_v3_24aug2015.tar.gz
- prep_chem_sources_v1.4_08aug2013.tar.gz
- prep_chem_sources_v1.5_24aug2015.tar.gz

Use prep_chem_sources_v1.5 to process

Incorporating the NEI-2011 emissions within WRF/Chem



- Auxiliary input files can be used for emissions (also with parallel option)
- Emission variables defined in Registry
- Specify filenames, timing, …etc. in namelist.input file

The netcdf anthropogenic emission files

(read in convert_emiss.F)

- Hourly emissions for the 3-D grid (K=1,kemit)
- Emission variables must match photochemical mechanism (emiss_opt, chem_opt) and variable assignments in the Registry (i.e. e_co, e_so2 … etc.)

Naming Convention:

io_style_emissions=1

wrfchemi_<hour>_d<domain_id> (wrfchemi_00to11z_d01 and wrfchemi_12to23z_d01)
Average emissions (typical summer day) : used for each day of the simulation

io_style_emissions=2

wrfchemi_d<domain_id>_<date/time> (wrfchemi_d01_2006-04-06_00:00:00)
Day specific emissions: time and date in netcdf header must match simulation date

Anthropogenic emission options (within the namelist file)

emiss_opt = 2 (use RADM2 anthropogenic emissions)
emiss_opt = 3 (use RADM2/MADE/SORGAM anthropogenic emissions)
emiss_opt = 4 (use CBMZ/MOSAIC anthropogenic emissions)
emiss_opt = 5 (biomass burn with RACM/GoCart PM2.5)
emiss_opt = 6 (biomass burn with simple GoCart PM2.5)
emiss_opt = 7 (MOZART emissions)
emiss_opt = 8 (MOZART + GoCart PM2.5 emissions)

How are the netcdf anthropogenic emission files generated?

Three step process:

1. Generate “Binary Intermediates” with variables and format defined in: convert_emiss.F
2. Run real.exe to generate netcdf header and domain information (wrfinput_d01 file)
3. Compile and run convert_emiss.F

Considerations when using convert_emiss.F

Convert_emiss is broken for WRF/Chem version 3.7 and later
- there are work arounds (compile/run convert_emiss from version 3.6)

Must be run twice (00 to 12Z emissions, 12Z to 24Z emissions) for io_style_emissions=1

Namelist for real.exe run must have proper variable specification (emission update interval, kemit, date/time for io_style_emissions=2, domain definitions)

Binary intermediate filename(s) are specified in the namelist.

The “binary intermediate” emissions files can be generated by: emiss_v04.F

- Use emiss_v04.F as a template for your particular chemical mechanism and emission option.

- Number of emitted species, specie names, 3-D emission fields from 00Z to 01Z, 3-D fields from 01Z to 02Z,….etc.

- Species number and order must match what’s in convert_emiss.F.

- Emission variable names must match chemical mechanism (emiss_opt, chem_opt) and variable assignments in the Registry (i.e. e_co, e_so2 … etc.)

- Two “binary intermediate” files are expected in convert_emiss.F (e.g. wrfem12k_00to12z and wrfem12k_12to24z)

emiss_v04.F

- For North America only
- U.S. EPA NEI-2011 emission inventories (4km resolution)
- Includes U.S. and Canadian point emissions from CEMS measurements of 2006
- VOC speciation according to SAPRC-11 and RACM2 photochemical mechanisms

- Uses “raw” emissions files (zipped ASCII, hourly, NEI-2011 emissions)

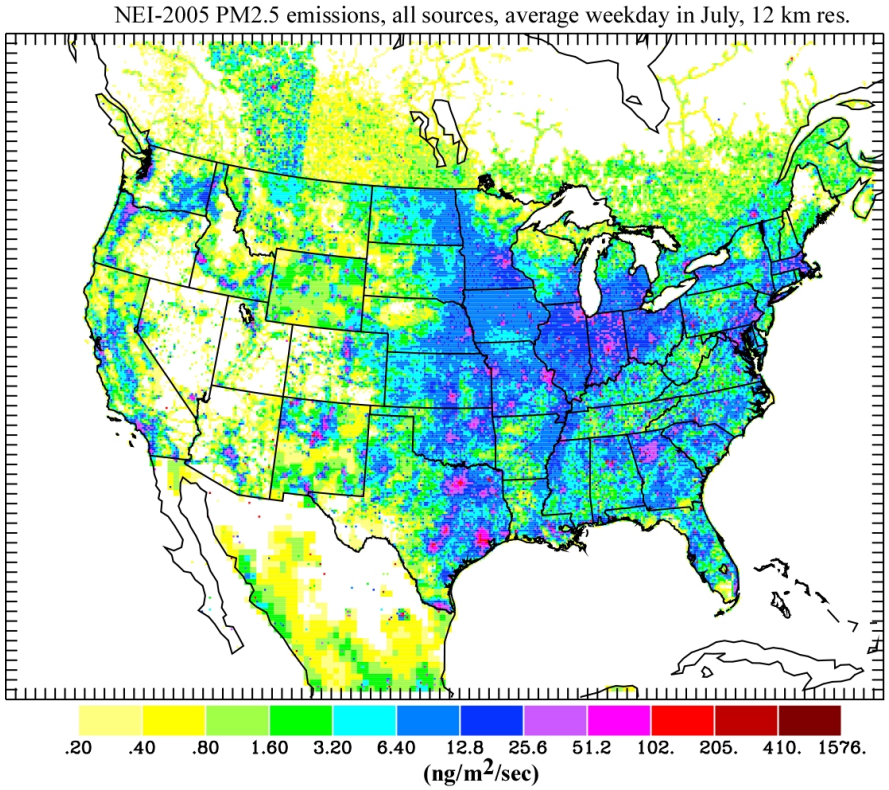
- Domain, including vertical height levels, must be defined (nesting options)
  (Lambert Conformal, Polar Stereographic currently supported)

- Simple grid dumping from 4km domain into user domain

- Any plume-rise from point sources must be specified here -
  (momentum lift only in current configuration)

- Requires VOC conversion table from SAPRC-11/RACM2 VOC
  to user photochemical mechanism (table for RACM in standard release)

Gridded domain defined by U.S. EPA 4-km spatial surrogate file



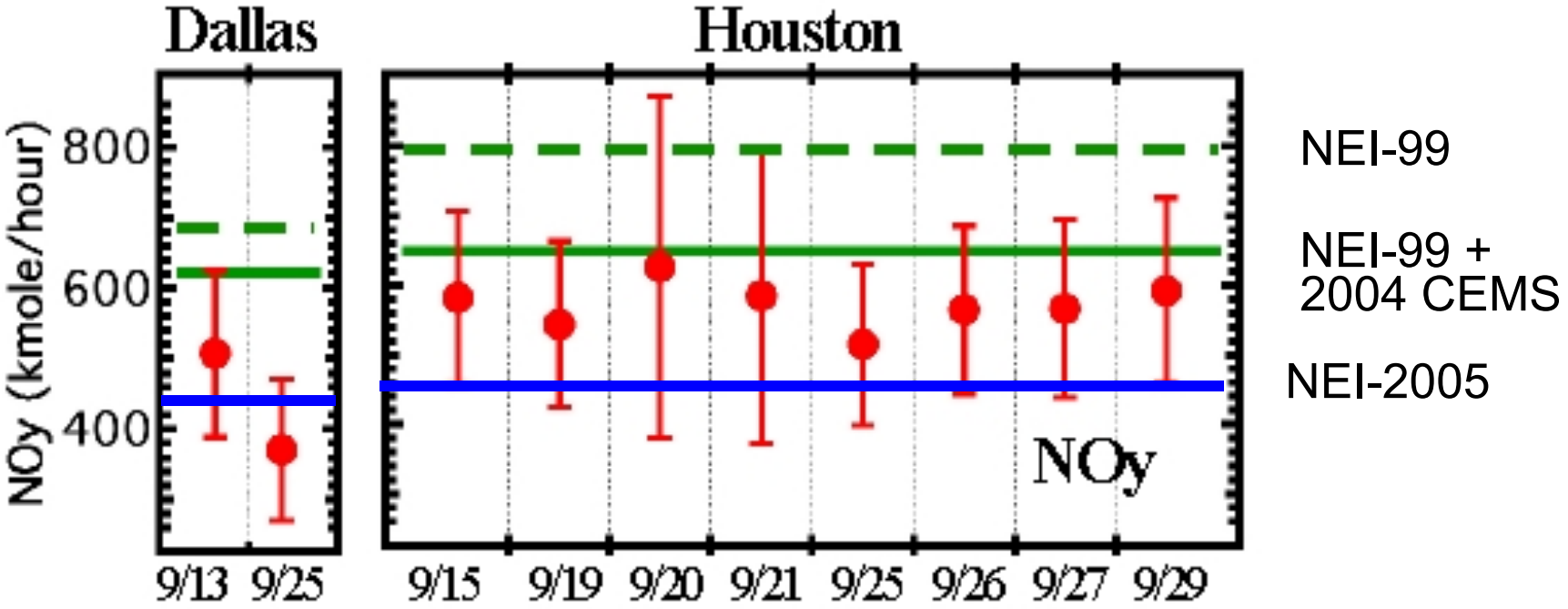
Canada:
Area sources: U.S. EPA, base year 2000
Point sources: EC's NPRI, August 2006
16707 total, 79 CEMS

U.S.:
Area sources from U.S. EPA:
NEI-2011 onroad/nonroad from MOBILE
NEI-2011 for other area sources
Point sources: 2011 CEMS, NEI-2011
151040 total, 4455 CEMS

Mexico (from WRAP program):
Area sources from U.S. EPA, base year 1999
36 km resolution only
Point sources (1999): 769 total

Some Devils in the Details:
66 spatial surrogates for U.S., 63 for Canada, 2 for Mexico
No biomass burning from non-agricultural fires (wild or prescribed)
Ship emissions outside of ports spread over large areas (no ship tracks)
Canadian point emissions rely on SIC to U.S. EPA SCC translation table
etc……

NOy emissions determined from mass-balance method by NOAA/ESRL/CSD.
11:00 am LT emissions from Houston and Dallas during TexAQS-2006.
Derived from upwind/downwind transects within the PBL,
observed winds, PBL heights and NOy measurements



Uncertainty limits in observations include PBL and background uncertainties

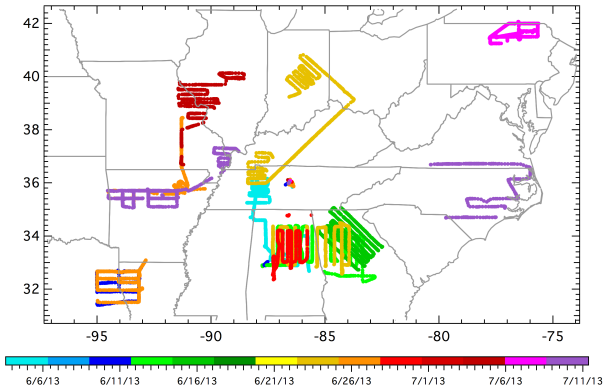
Emission inventory from 11:00am to noon, LT (representative of daylight average)

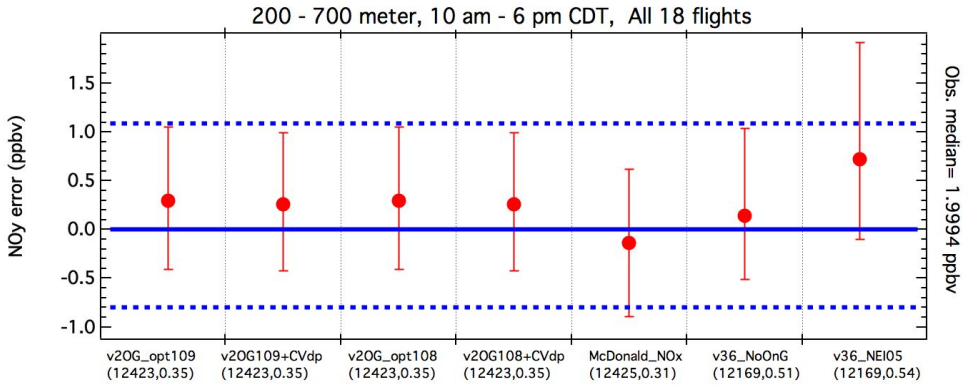
over pre-determined ~100 X 100 km^2 domains

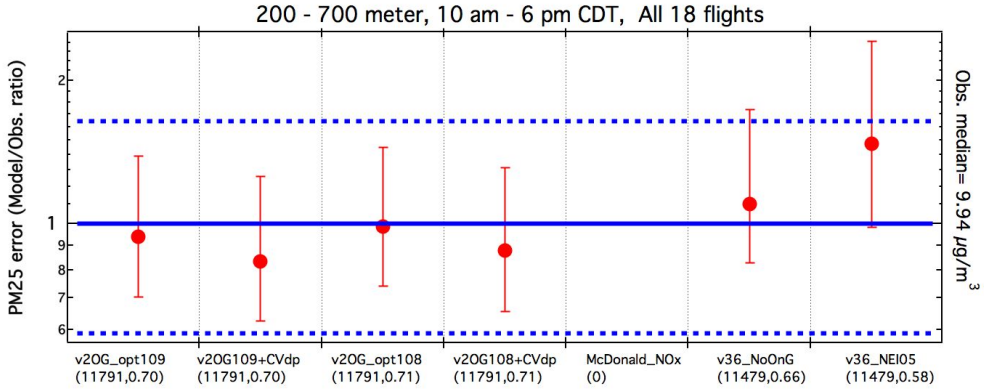
Anderson et al. (2014):
NEI-2011 NOy emissions high by a factor of 2 in the eastern U.S

Travis et a. (2016):
NEI-2011 NOy emissions high by a factor of 30 to 60% U.S

SENEX-2013 NOAA/ESRL/CSD field campaign



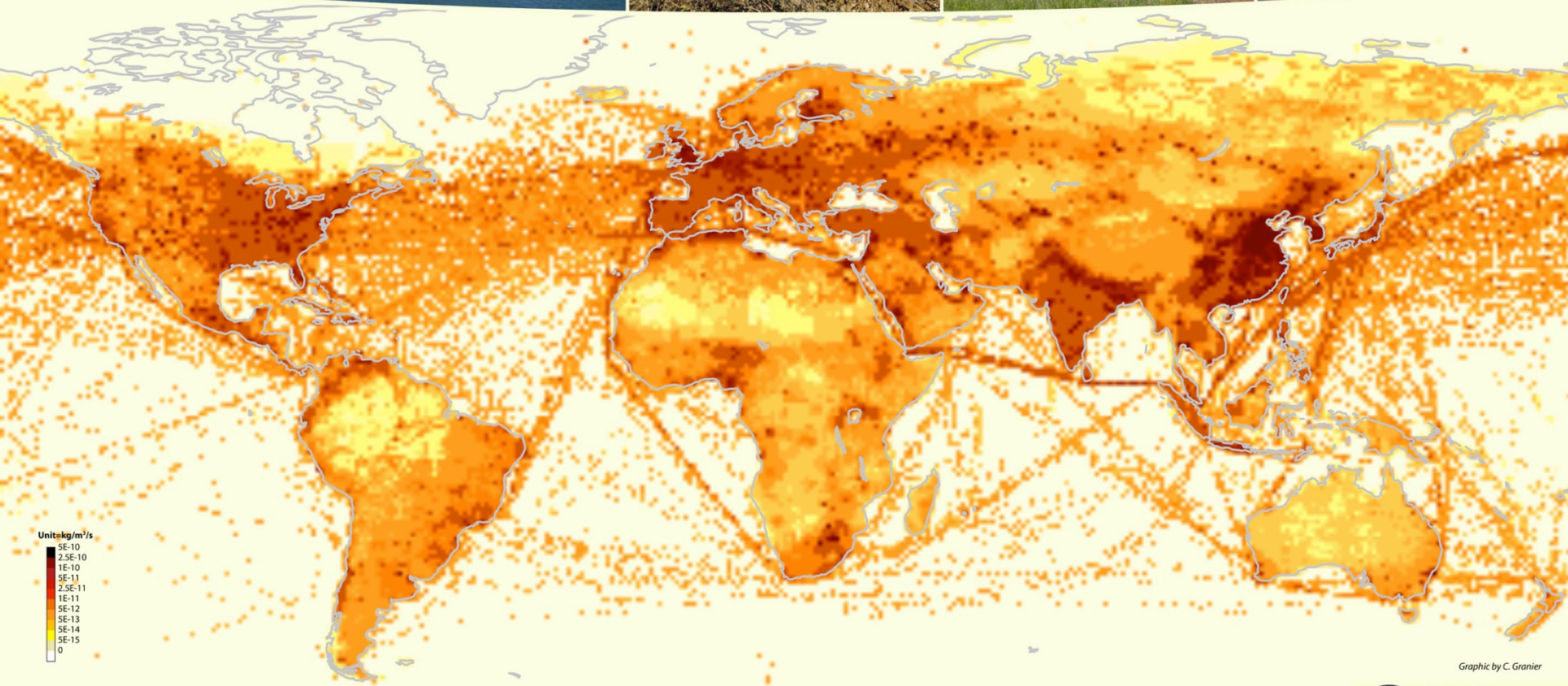




NOy – median 15% high (was 30%)
PM2.5 – 5% low (was 45% high)







Graphic by C. Granier

Emissions of Nitrogen Oxides from all Anthropogenic Activities in 2010

Data provided by Claire Granier and Gregory Frost.

The MACCity inventory quantifies trace gases and aerosols emitted by a variety of human activities, including energy production, industry, transportation and agriculture.

GEIA
Global Emissions InitiAtive





A list of recent global inventories

Author	Acronym	Reference or Website	Years	Resolution
Lamarque et al.	ACCMIP	eccad.sedoo.fr	1900-2000	0.5x0.5
Riahi et al.	RCPs	eccad.sedoo.fr	2000-2100	0.5x0.5
Granier et al.	MACCity	eccad.sedoo.fr	2000-2015	0.5x0.5
Maenhout et al.	EDGAR4.2	edgar.jrc.ec.europa.eu	1970-2008	0.1x0.1
Crippa et al.	EDGAR4.3	edgar.jrc.ec.europa.eu	1970, 2010	0.1x0.1
Maenhout et al.	HTAPv2	edgar.jrc.ec.europa.eu	2008, 2010	0.1x0.1
Klimont et al.	ECLIPSE v4, v5	iiasa.ac.at	1990-2030	0.5x0.5
Schultz et al.	RETRO	juelich ftp	1960-2000	0.5x0.5
Bond et al.	Bond	Hiwater.org	1850-2000	country
Junker&Liousse	J&L	eccad.sedoo.fr	1860-2003	1x1
Huang Y. et al.	PKU	inventory.pku.edu.cn	1960-2009	0.1x0.1
Smith et al.	PNNL	sedac.ciesin.columbia.edu	1850-2005	1x1

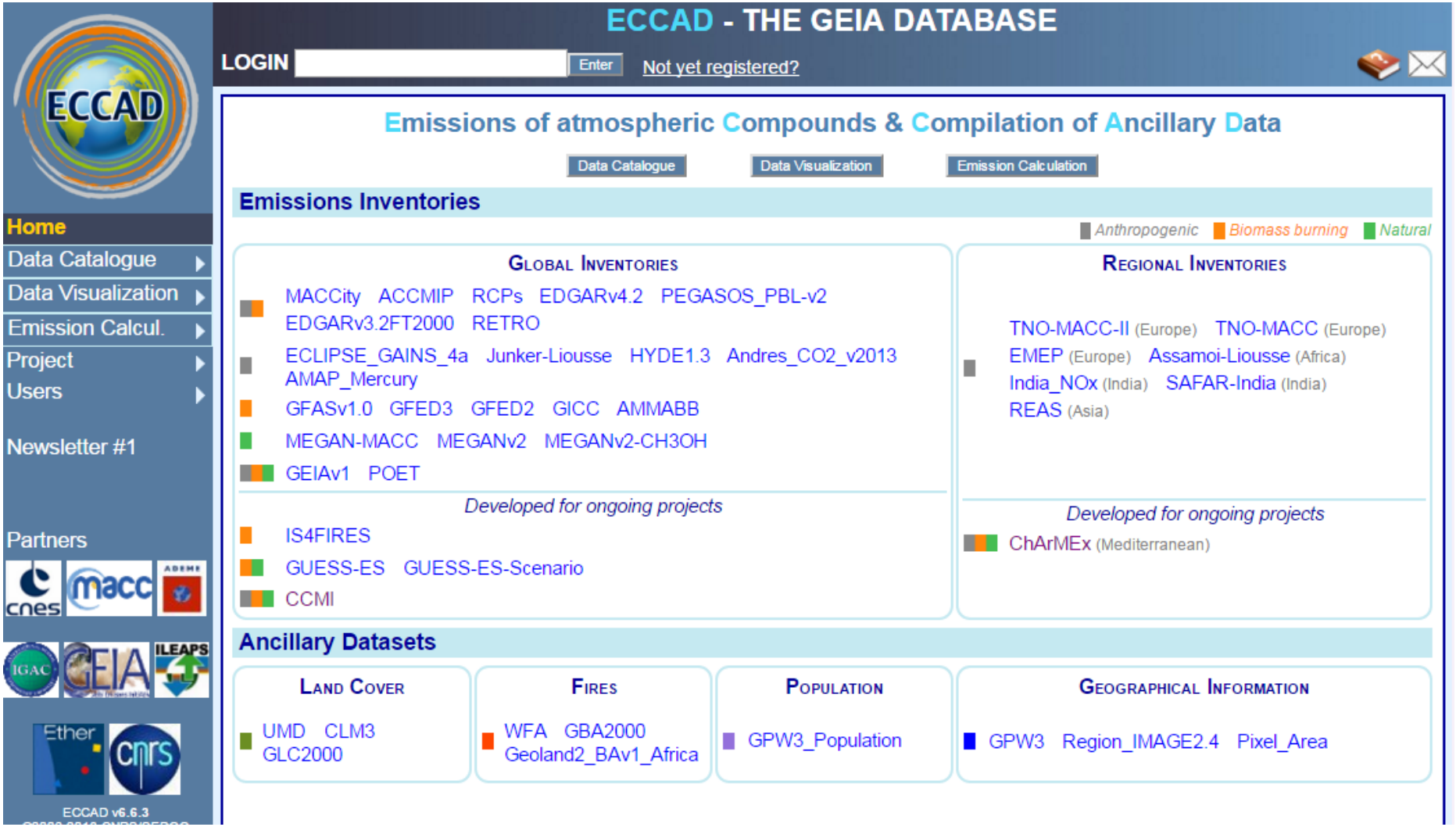
Blue: inventories providing just a few species

All the data are publicly available. Most available at: eccad.sedoo.fr, the database of the **Global Emissions InitiAtive (GEIA)**

Where can you get most of these emissions ?

=> ECCAD : Atmospheric Compounds and Compilation of Ancillary Data

http://pole-ether.fr/eccad



Global Anthropogenic Emission Inventories Available in WRF/Chem

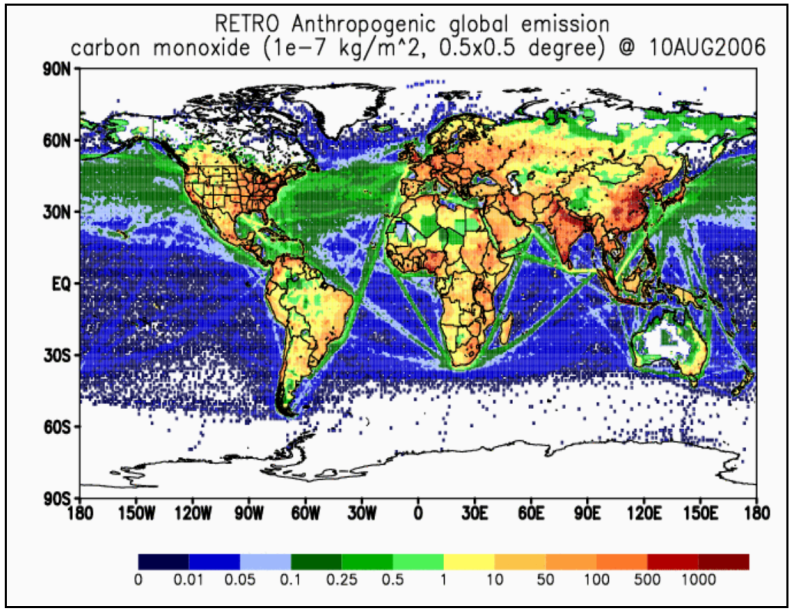
(use prep_chem_sources package to generate binary files)

HTAP v2.2 (0.1º x 0.1º, monthly, 2010)
CH_4, CO, SO_2, NOx, NMVOC, NH_3, PM10, PM2.5, BC and OC

RETRO (0.5^0 x 0.5^0, monthly, 1960-2000)
CO, SO_2, NOx, NMVOC, NH_3, PM10, PM2.5, BC and OC

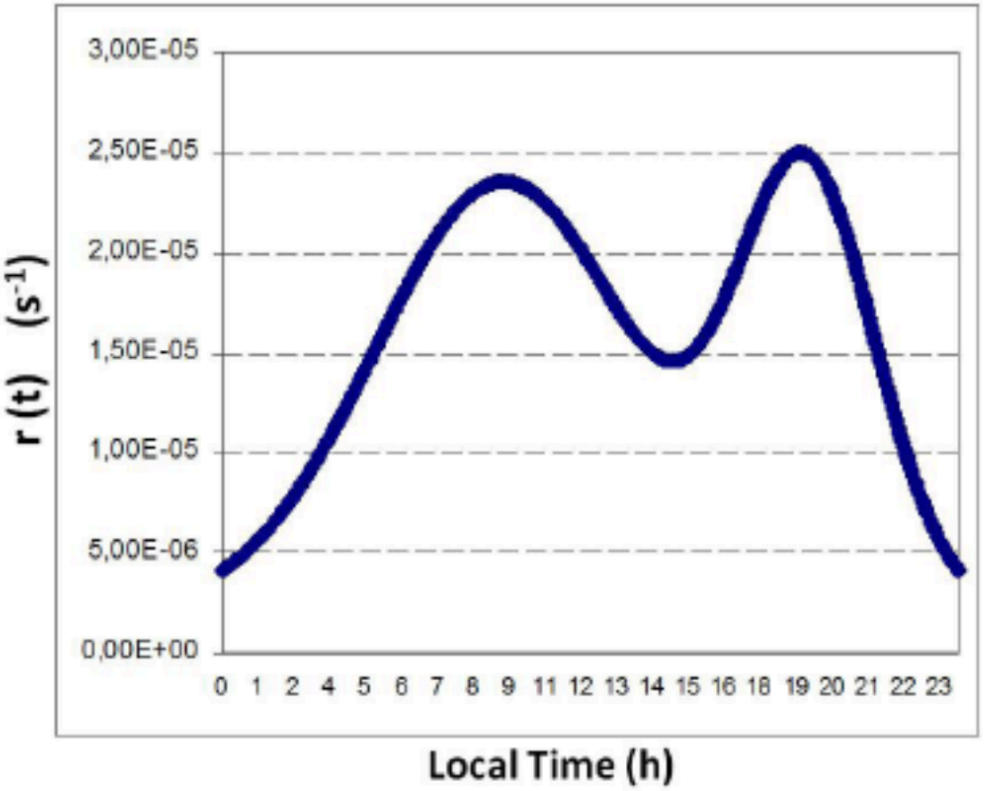
GOCART
OC, BC and SO_2 (1^0 x 1^0, annual, 2006)
DMS (1^0 x 1.25^0, monthly)
NO_3, H_2O_2 and OH (3D, 1^0 x 1.25^0 monthly, 2006)

EDGAR v4.2 (0.1º x 0.1º, annual, 1970-2008)
RETRO plus CO_2, CH_4, N_2O, HFCs, PFCs, SF_6



Anthropogenic emissions

Diurnal cycle is applied inside WRF



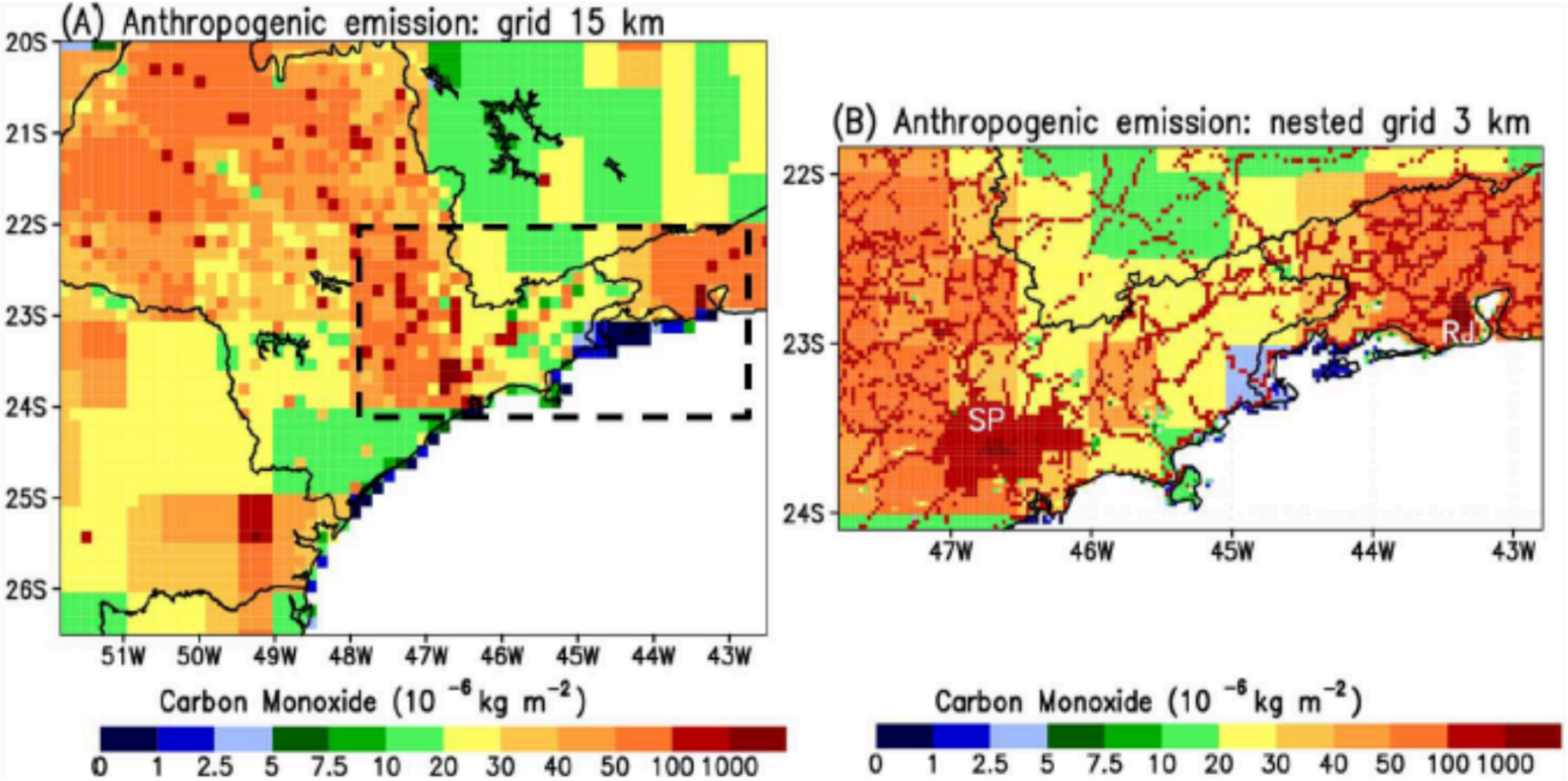
$$\int_0^{86400} r(t)dt = 1,$$

$$\bar{E}_\eta(k,t) = \begin{cases} \dfrac{F_\eta}{\bar{\rho}(k_1)\ \Delta z_1} r(t),\ k=1 \text{ (surface)} \\ 0,\ k>1 \text{ (above)} \end{cases},$$

Alonso et al. (2010)

Anthropogenic emissions

AREA DELIMITER algorithm distributes emissions on high resolution grids



Alonso et al. (2010)

Thank you

Any Questions?