Anthropogenic and Biogenic emissions processing within WRF/Chem

Stu McKeen, Steven Peckham
(CIRES/University of Colorado, NOAA/ESRL)

- WRF/Chem design considerations
- Putting anthropogenic emissions in the model
- Biogenic emission options
- How good are the inventories?
- Future plans

WRF/Chem design considerations

(current configuration)

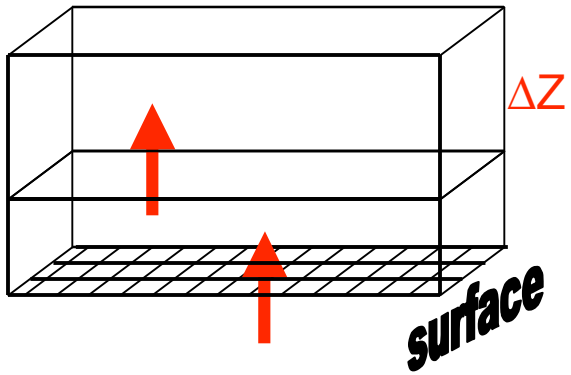
Basic emissions are specified "outside" of WPS or WRF system

- 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 new biomass burning options do incorporate plume rise!)

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, add_biogenics subroutine

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

[ΔZ, and ρ_{AIR} are not constant]

The netcdf anthropogenic emission files

(read in module_input_chem_data.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)

How are the netcdf anthropogenic emission files generated?

Three step process:

1. Generate “Binary Intermediates” with variables and format defined in: module_input_chem_data.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 (get a script from someone)

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: med_read_bin_chem_emiss subroutine of module_input_chem_data.F

The “binary intermediate” emissions files

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

- 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)

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

emiss_v03.F

- For North America only
- U.S. EPA NEI-99 emissions inventory (4km resolution)
- Updated U.S. point emissions from CEMS measurements to 2004
- VOC speciation according to SAPRC-99 photochemical mechanism

emiss_v03.F

- Uses “raw” emissions files (zipped ASCII, hourly, NEI-99/SAPRC-99 emissions)

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

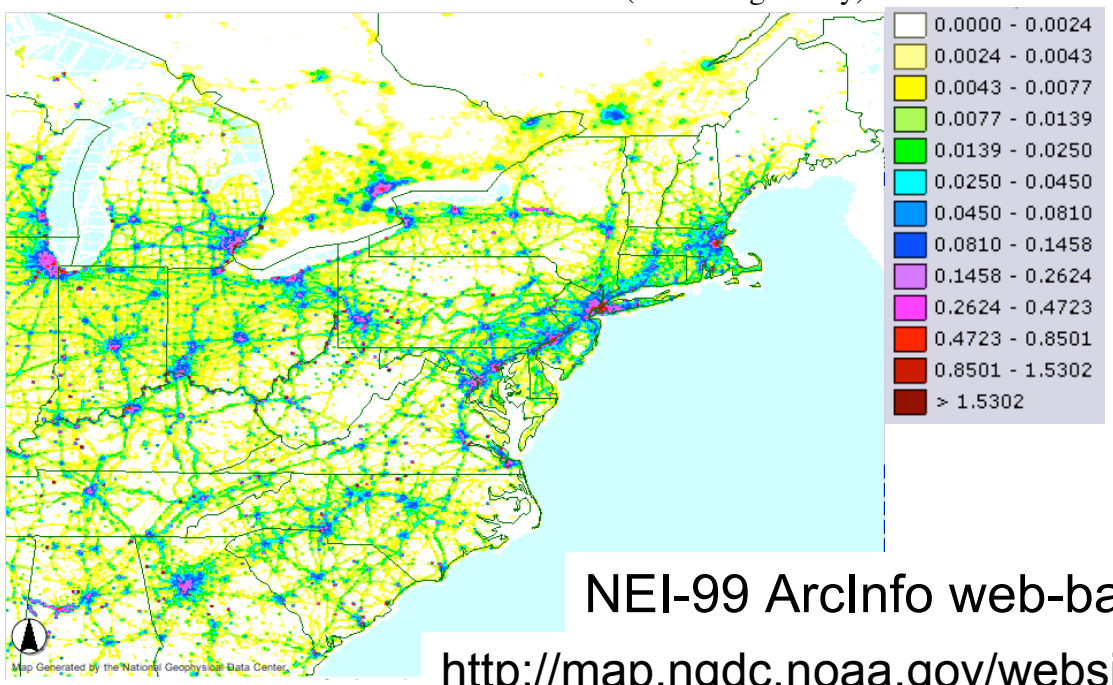
- Simple grid dumping from 4km domain into user domain

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

- Requires VOC conversion table from SAPRC-99 to user photochemical mechanism

How “good” are the NEI-99 emissions?

NEI-99 NOx emission rate(ton/4km grid/day)

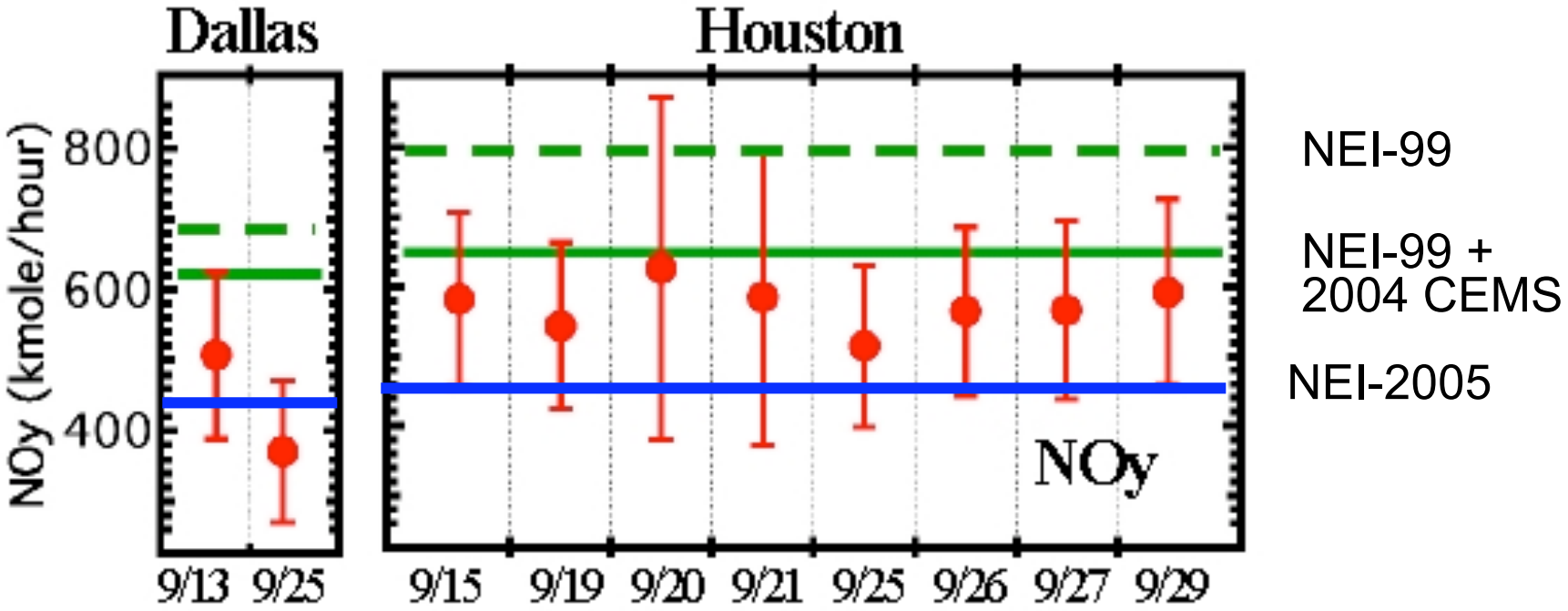


NEI-99 ArcInfo web-based emissions viewer:

http://map.ngdc.noaa.gov/website/al/emissions/viewer.htm

Kim, S.-W., et al., Eastern U.S., NO2 satellite columns, GRL, 2006
Warneke, et al., Houston, New England, Los Angeles, VOC, JGR 2007
Kim, S.-W., et al., Western U.S., NO2 satellite columns, submitted to JGR 2008
Warneke, et al., Tennessee, New England, Texas, Bio-VOC, submitted to JGR 2008
McKeen et al., Houston/Dallas, NOy, CO, VOC, PM2.5, to be submitted to JGR 2008

Observed NOy 11:00 am LT emissions from Houston and Dallas
Derived from upwind/downwind transects within the PBL,
observed winds, PBL heights and NOy measurements

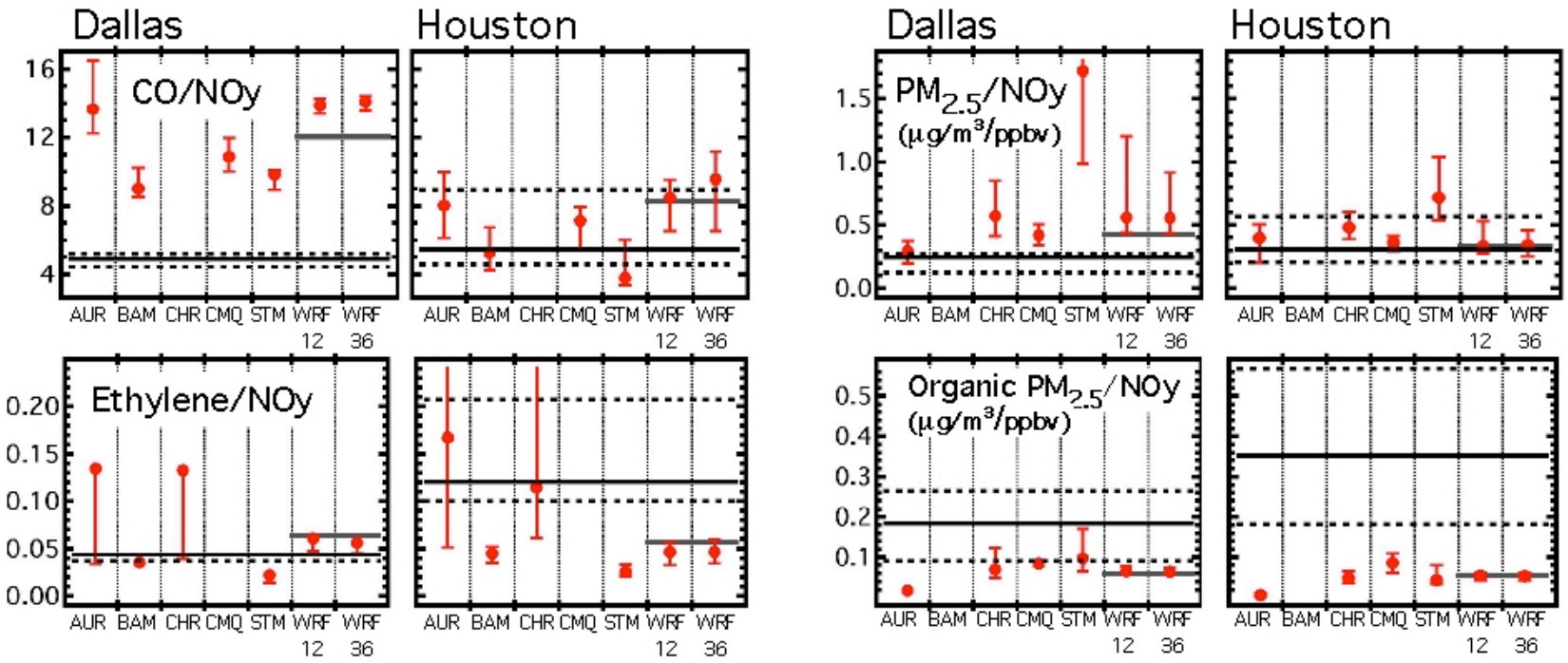


Uncertainty limits in observations include PBL and background uncertainties

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

over pre-determined ~1000 km^2 domains

Model and Observed concentration difference ratios (and NEI-99 emission ratios) downwind (< 50 km) of Houston and Dallas



Red circles: Model median ratios (whiskers - central 2/3 of sorted distributions)

Black lines: Observed medians (dashed lines - central 2/3 of sorted distributions)

Gray lines over WRF/Chem models - From NEI-99 (used in WRF/Chem runs)

Future Plans

2005 NEI inventory available (since Nov. 2007) from U.S. EPA
- Gridded data ready for WRF/Chem - shooting for October 2008
- Additional species: CO2, CH4, several toxics
- More speciated VOC - matches SAPRC07 (toxics) mechanism
- Updated Emissions from Canada and Mexico (2002 NEI)

BEIS3.13 - Automate to minimize User intervention
- Reference files put on same 4km anthro inventory grid
- Create pre-processor (similar to emiss_v03.F)

Plume-rise calculations within WRF-Chem
- Two options: standard Briggs, and new Freitas