Biogenic, Fire, Lightning Emissions and Chemical Boundary Conditions

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Emissions for Chemical Transport Models

- Anthropogenic
  - Point, Area, Mobile
- Biogenic
- Biomass Burning
- Lightning
- Volcanoes
Chemical Production of Ozone
(Atmospheric Chemistry 101)

To make ozone, need sunlight
NO\textsubscript{x} = NO + NO\textsubscript{2}
HO\textsubscript{x} = OH + HO\textsubscript{2}

HO\textsubscript{x} precursors are CO, CH\textsubscript{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

$\text{DMS} \rightarrow \text{SO}_2 \rightarrow \text{SO}_4$

$\text{HNO}_3 - \text{NH}_3 - \text{SO}_4$ equilibrium $\rightarrow (\text{NH}_4)_2\text{SO}_4, \text{NH}_4\text{HSO}_4, \text{NH}_4\text{NO}_3$ aerosols

$\text{VOC} + \text{O}_3 \rightarrow \text{SVOC}$

$\text{SVOC} + \text{O}_3 \rightarrow \text{SOA}$

Dust, Sea salt

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

(NARSTO, 2004)
Mass conserving anthropogenic emissions preprocessor

**anthro_emis**: creates WRF-Chem gridded anthropogenic emission files from latitude-longitude gridded input anthropogenic emission files

- Both diurnal (wrfchemi_00z_d<nn>) and serial (wrfchemi_d<nn>_<date>) files can be created
- Capable of handling both regional and global input datasets
- Tested with MACCity, EDGAR-HTAP and SEAC4RS emission inventory
- Package includes a sample namelist file mozcart.inp
- Creates wrfchemi* files in anthro_emis directory

**NO\textsubscript{x}, CO, AVOCs**
The spatial patterns look similar with both the nearest neighbor and mass conserving mapping but total emissions can be different by about 10%.

Domain total emissions:
Original Inventory : 203 Gg/year
Nearest-neighbor mapping : 229 Gg/year.
Mass Conserving Anthropogenic Emissions Preprocessor

- To **compile**: `make_anthro`
- To **run**: `anthro_emis < anthro_emis.inp > anthro_emis.out`
- Example namelist “mozcart.inp” (included in download)

```plaintext
&CONTROL
  anthro_dir = ''
  src_file_prefix = 'IPCC_emissions_'
  src_file_suffix = '_surface_1850-2000_1.9x2.5.nc'
  src_names = 'CO(28)', 'NO(30)', 'BIGALK(72)', 'BIGENE(56)', 'C2H4(28)', 'C2H5OH(46)',
               'C2H6(30)', 'C3H6(42)', 'C3H8(44)', 'CH2O(30)', 'CH3CHO(44)', 'CH3COCH3(58)',
               'CH3OH(32)', 'MEK(72)', 'SO2(64)', 'TOLUENE(92)', 'NH3(17)',
               'OC(12)', 'BC(12)', 'CH3COOH(60)'
  sub_categories = 'anthro'
  emis_map = 'CO->CO', 'NO->NO', 'BIGALK->BIGALK', 'C2H4->C2H4', 'C2H5OH->C2H5OH',
             'C2H6->C2H6', 'C3H6->C3H6', 'C3H8->C3H8', 'CH2O->CH2O', 'CH3CHO->CH3CHO',
             'CH3COCH3->CH3COCH3', 'CH3OH->CH3OH', 'MEK->MEK', 'SO2->SO2', 'TOLUENE->TOLUENE',
             'NH3->NH3', 'OC(a)->OC', 'BC(a)->BC', 'CH3COOH->CH3COOH'
  sub_categories = 'anthro'
  serial_output = .true.
  start_output_time = '2010-05-01_00:00:00'
  stop_output_time = '2010-10-31_00:00:00'
  output_interval = 86400
/
```
Biogenic Emissions Modeling: MEGAN

MEGAN:

*Model of Emissions of Gases and Aerosols from Nature*
- Guenther et. al., *Atmospheric Chemistry and Physics*, 2006
  - Version 2.1 is in preparation for WRF-Chem
- 134 emitted chemical species
  - Isoprene
  - Monoterpenes
  - Oxygenated compounds
  - Sesquiterpenes
  - Nitrogen oxide
- 1 km² resolution

Online version of MEGAN in WRF-CHEM currently *same* as offline version 2.04
MEGAN Framework: Calculation of emissions

\[ EM = \varepsilon \cdot \gamma_{CE} \cdot \gamma_{age} \cdot \gamma_{SM} \cdot \rho \]

\[ \gamma_{CE} = \gamma_{LAI} \cdot \gamma_{P} \cdot \gamma_{T} \]

EM: Emission (μg m\(^{-2}\) hr\(^{-1}\))

\(\varepsilon\): Emission Factor (μg m\(^{-2}\) hr\(^{-1}\))

\(\gamma_{CE}\): Canopy Factor

\(\gamma_{age}\): Leaf Age Factor

\(\gamma_{SM}\): Soil Moisture Factor

\(\rho\): Loss and Production within plant canopy

\(\gamma_{LAI}\): Leaf Area Index Factor

\(\gamma_{P}\): PPFD Emission Activity Factor (light-dependence)

\(\gamma_{T}\): Temperature Response Factor
Emissions increase as

- Temperature increases
- PPFD transmission (light) increases
- Leaf area index increase
Fig. 5. Monthly normalized isoprene emission rates estimated with MEGAN for 2003. Rates are normalized by the emission estimated for standard LAI ("5 m² 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.
MEGAN online biogenic emissions

In Summary:
• Estimate emissions of VOCs, NO\textsubscript{x} and CO from vegetation
• Driving variables include landcover, weather, and atmospheric chemical composition
• Note: currently land cover used in MEGAN differs from that used within WRF-Chem
• Plan: Update to MEGAN 2.1 (Guenther et al., 2012) and link to CLM land cover

from Guenther et al., 2012
**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*

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**Process 1:**
Calculation of Gamma Values

Read into WRF-chem simulation

**Temp @ 2m**

Downward Solar Radiation

Read in from model

**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
MEGAN preprocessor

- Static input fields needed to run with online MEGAN biogenic emissions: *Isoprene Emissions Factors, monthly LAI, Solar Radiation & Temperature, Fractional coverage of broadleaf and needeleaf 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 `wrbiochemi_d<domain>` file

[https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community](https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community)
MEGAN preprocessor

- **To compile:**
  
  \texttt{make\_util\_megan\_bio\_emis} - creates the executable \texttt{megan\_bio\_emiss}

- **megan\_bio\_emiss** is controlled by a namelist file (e.g. \texttt{megan\_bio\_emiss.inp})

  &\texttt{control}
  
  \begin{itemize}
  \item \texttt{domains = 3},
  \item \texttt{start\_lai\_mnth = 4},
  \item \texttt{end\_lai\_mnth = 6},
  \item \texttt{wrf\_dir = '/home/me/megan/wrf\_files'},
  \item \texttt{megan\_dir = '/home/me/megan/30sec'}
  \end{itemize}

  \begin{itemize}
  \item \texttt{creates wrfbiochemi\_dnn} for three domains (default: 1)
  \item \texttt{starting month for the monthly LAI} (default: 1)
  \item \texttt{ending month for the monthly LAI} (default: 12)
  \item \texttt{path to wrfinput\_dnn} (default: current)
  \item \texttt{path to MEGAN input files} (default: current)
  \end{itemize}

- **To run:** \texttt{megan\_bio\_emiss < megan\_bio\_emiss.inp > megan\_bio\_emiss.out}

- \rightarrow \texttt{creates wrfbiochemi\_d<domain> file}
Running WRF-Chem with MEGAN

- WRF-Chem output variables: EBIO_<species>
- namelist.input:

```plaintext
&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)
```
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
• Available for hindsight and forecast model applications

CO, NO$_x$, VOCs, SO$_2$, PM
Modeling Fire Emissions

\[ Emissions_i = f(A(x,t), B(x,t), E_{fi}) \]

**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
<table>
<thead>
<tr>
<th>Version 1 Model Drivers:</th>
</tr>
</thead>
<tbody>
<tr>
<td>MODIS Rapid Response fire detections</td>
</tr>
<tr>
<td>MODIS Vegetation Continuous Fields and Land Cover Type</td>
</tr>
<tr>
<td>Speciation of VOCs provided for MOZART-4, SAPRC99, GEOS-Chem</td>
</tr>
<tr>
<td>Plume rise option available- <em>but requires additional inputs</em></td>
</tr>
</tbody>
</table>
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
**FINN Fire Emissions Preprocessor**

- create WRF-Chem ready fire emissions from FINN inventory - `wrffirechemi_d<domain>_ <date>` for use with online plume rise (can also be merged into wrfchemi files)
  note: fire_emis also works to create global emission files for MOZART-4/CAM-Chem

- Works for different chemical schemes (namelist controlled)

- WRAP diurnal emission profile applied

- Processor and FINN inputs available on Web

- FINN inputs in MOZART-4, SAPRC99, and GEOS-Chem speciation

  [https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community](https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community)

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**Fire_Emis**

Fortran based preprocessor for creating fire emission inputs for WRF-Chem when running with plumerise and also for creating fire emission inputs for the MOZART-4 and CAM-Chem global models. The fire emissions inventory is based on the Fire Inventory from NCAR (FINN). Both software (fire_emis.tgz) and required FINN input data sets are available at the download page.

The fire_emis.tgz file when uncompressed `{tar -zxf fire_emis.tgz}` yields three directories `{data_files, src, and test}` and two readme files `{README.WRF.fire and README.GL.B.fire}`. The data_files directory is empty and is where users should put the FINN files and the wrfinput_d<domain> file(s). The test directory contains two test namelist input files, one for creating WRF inputs and another for creating global inputs. Users are highly advised to read the README files before using the fire emission utility.
FINN Fire Emissions Preprocessor

- To **compile**: `make_fire_emis`
- To **run**: `fire_emis < fire_emis.inp > fire_emis.out`
- `→ creates wrffirechemi_d<domain>_<date>`
- Example namelist “fire_emis.inp” for MOZCART

```
&control
  domains = 1,
  fire_directory = '',
  fire_filename = 'GLOB2012a_MOZ4_07242012.txt',
  wrf_directory = '',
  start_date = '2012-06-01',
  end_date = '2012-06-10',
  diag_level = 1,

  wrf2fire_map = 'co -> CO', 'no -> NO', 'so2 -> SO2', 'bigalk -> BIGALK', 'bigene -> BIGENE', 'c2h4 -> C2H4',
                 'c2h5oh -> C2H5OH', 'c2h6 -> C2H6', 'c3h8 -> C3H8', 'c3h6 -> C3H6', 'ch2o -> CH2O',
                 'ch3cho -> CH3CHO', 'ch3coch3 -> CH3COCH3', 'ch3oh -> CH3OH', 'mek -> MEK',
                 'toluene -> TOLUENE', 'nh3 -> NH3', 'no2 -> NO2', 'open -> BIGALD', 'c10h16 -> C10H16',
                 'ch3cooh -> CH3COOH', 'cres -> CRESOL', 'glyald -> GLYALD', 'mgly -> CH3COCHO',
                 'gly -> CH3COCHO', 'acetol -> HYAC', 'isop -> ISOP', 'macr -> MACR', 'mvk -> MVK',
                 'oc -> 0.24*PM25 + 0.3*PM10;aerosol', 'bc -> 0.01*PM25 + 0.08*PM10;aerosol',
                 'pm10_raw -> PM10;aerosol', 'pm25_raw -> PM25;aerosol',
                 'sulf -> -0.01*PM25 + 0.02*PM10;aerosol',
                 'pm25 -> 0.36*PM25;aerosol', 'pm10 -> -0.61*PM25 + 0.61*PM10;aerosol'
/
```
**FINN Fire Emissions Preprocessor**

Running WRF-Chem with FINN emissions and plumerise:

```
&time_control
    auxinput7_inname = 'wrffirechemi_d<domain>_<date>',
    auxinput7_interval_m = 60, 60, 60,
    io_form_auxinput7 = 2,
    frames_per_auxinput7 = 1, 1, 1,
&chem
    biomass_burn_opt = your choice
    plumerisefire_frq = your choice
    scale_fire_emiss = .true.
```
Fire INventory from NCAR (FINN)

Daily global emissions available from 01 January 2002 – 30 June 2014

https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community

Also available at:

http://www.acom.ucar.edu/acresp/forecast/fire-emissions.shtml
http://www.acom.ucar.edu/acresp/dc3/AMADEUS/finn/emis/
Lightning-NO$_x$ Emissions

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

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
  $\rightarrow$ 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
1) Predicting Lightning Flashrate

- Cloud-resolving parameterization: Barth et al., ACP, 2012
  \[ \text{Flashrate} = 5.7 \times 10^{-6} w_{\text{max}}^{4.5} \]  
  \[ \text{Flashrate} = 3.44 \times 10^{-5} H^{4.9} \]  
  \( H = \text{cloud top height of the 20 dBZ contour} \) 

- Convective-parameterized parameterization: Wong et al., GMD, 2011
  \[ \text{Flashrate} = 3.44 \times 10^{-5} H^{4.9} \]  
  \( H = \text{level of neutral buoyancy (from Grell convective parameterization)} \) 
  Can adjust \( H \) in namelist.input

\[ \text{Note:} \] 
These are highly non-linear estimates and are often wrong. 
\[ \rightarrow \text{flashrate Factor} \] for adjusting 
\[ \rightarrow \text{Active research} \] 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)
  \[
  \text{IC/CG} = 0.021 d^4 - 0.648 d^3 + 7.49 d^2 - 36.54 d + 63.09 \\
  \]
  \(d\) = depth of the “cold cloud”, from \(T=0^\circ\text{C}\) 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., 2012
  
  Placed throughout the grid cell
3) Determine where to put the NO emissions

Vertical Placement
3) Determine where to put the NO emissions

**Vertical Placement**

- 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
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

Note:
Ongoing research to find “a good number” to use. This number is often adjusted when evaluating model results with observations.
Running WRF-Chem with Lightning-NOx emissions

&physics
  lightning_option = 11, 1,
  iccg_method = 2, 2,
  lightning_dt = 75, 75,
  cellcount_method = 0, 1,
  lightning_start_seconds = 600, 600,
  flashrate_factor = 20., 1.,
  cldtop_adjustment = 0, 0,

&chem
  lnox_opt = 1, 2,
  N_IC = 125., 500.,
  N_CG = 125., 500.

See WRF-Chem Users Guide for option choices
Chemical Boundary Conditions

mozbc – set chemical initial and lateral boundary conditions

- chemical initial and boundary conditions are needed to account for initial concentrations and inflow
- fills the chemical fields in wrfinput_d<domain> and wrfbdy_d<domain> with global model output
- set-up for MOZART-4 and CAM-Chem global model output
- controlled by namelist file (e.g. define species mapping; mappings available for MOZART to RACM, RADM, CBMZ, MADE/SORGAM, MOSAIC, GOCART)
- Interpolation in time and space
- MOZART-4 output for past years and forecasts available on Web

https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community
Chemical Boundary Conditions

mozbc – set chemical initial and lateral boundary conditions

- *mozbc* operates on the most common map projections in WRF (Lambert, Mercator, Polar, Lat/Lon)

- To **compile**: *make_mozbc* -> will create the executable *mozbc*

- Package includes example namelist files ("mozbc.inp")

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

- to enable chemical IC and BC when running WRF-Chem set in namelist.input:  
  
  **have_bcs_chem = .true**
Chemical Boundary Conditions

Example namelist file for mozbc:

```plaintext
&control

do_bc = .true.          \text{defines if BC are set (default: .false.)}
do_ic = .true.          \text{defines if IC are set (default: .false.)}
domain = 2              \text{number of domains to work on (default: 1);}
                        \text{e.g. } d=2 \text{ sets BC for } d01 \text{ and IC for } d01 \text{ and } d02

dir_wrf = '/ptmp/me/WRF_chem/' \text{path to WRF-Chem files (met_em*, wrfinp*, wrfbdy*)}
dir_moz = '/ptmp/me/MOZBC/' \text{path to MOZART/CAM-Chem input files}
fn_moz = 'h0040.nc'      \text{initial MOZART/CAM-Chem file; mozbc increments filenames,}
                        \text{filenames must be of the form prefix<nnn>.nc}

moz_var_suffix = ' _VMR_avrg' \text{suffix string for MOZART/CAM-Chem variables (default: ‘_VMR_inst’)}
met_file_prefix = 'met_em' \text{prefix string for the WRF meterological files (default: ‘met_em’)}
                        \{standard WRF names: met_em.d<nn>.<yyyy-mm-dd_hh:mm:ss>.nc \}
met_file_suffix = '.nc' \text{suffix string for the WRF meterological files (default: ‘.nc’)}
met_file_separator = '.' \text{separator character for WRF meterological files (default: ‘.’)}

spc_map = 'o3 -> O3', 'o -> O', 'o1d_cb4 -> O1D', 'n2o -> N2O', 'no -> NO',
          \ldots
          'DUST_4 -> .2348*[DUST3]+.5869*[DUST4];1.e9', 'DUST_5 -> .5869*[DUST4];1.e9'
/

Note: Sometimes a species is not in the MOZART output. Just remove that species from the spc_map
namelist. (unless it is really important to include)
```
Chemical Boundary Conditions

ubc - upper chemical boundary conditions

- WRF-Chem does not have a stratosphere – possible issues when looking at UTLS or comparing to some satellite products (e.g. trop. O₃ retrievals)
- \( o₃, no, no₂, hₙ₂o₃, ch₄, co, n₂o, n₂o₅ \) are set to climatology above certain pressure level and relaxed to tropopause level below
- Same scheme as used in the global models, MOZART-4 and CAM-Chem
- Climatologies available for present and future times
- download climatologies from Web
- namelist.input (&chem):
  
  ```
  have_bcs_upper     = .true.
  fixed_upper_bc     = 50.
  fixed_ubc_inname   = "ubvals_b40.20th.track1_1996-2005.nc"
  ```

https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community

Upper Boundary Conditions

Download input files for running WRF-Chem V3.3.1 with Chemical Upper Boundary Conditions: UBC_inputs.tar
Contact the following people with your questions

NCAR Preprocessors:  Stacy Walters  stacy@ucar.edu  
                     Gabriele Pfister pfister@ucar.edu  
FINN emissions:      Christine Wiedinmyer  christin@ucar.edu  
MOZART data files:   Louisa Emmons  emmons@ucar.edu  
Lightning emissions: Mary Barth  barthm@ucar.edu  

BVOCs  
CO, NOx,  
VOCs, SO2, PM  
NO