Expanded chemical tagging for CAM-Chem

Attribution of ozone production to both NOx and VOC emissions

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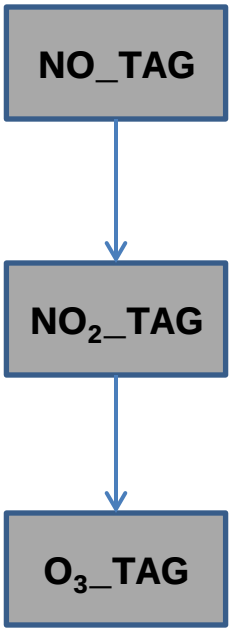
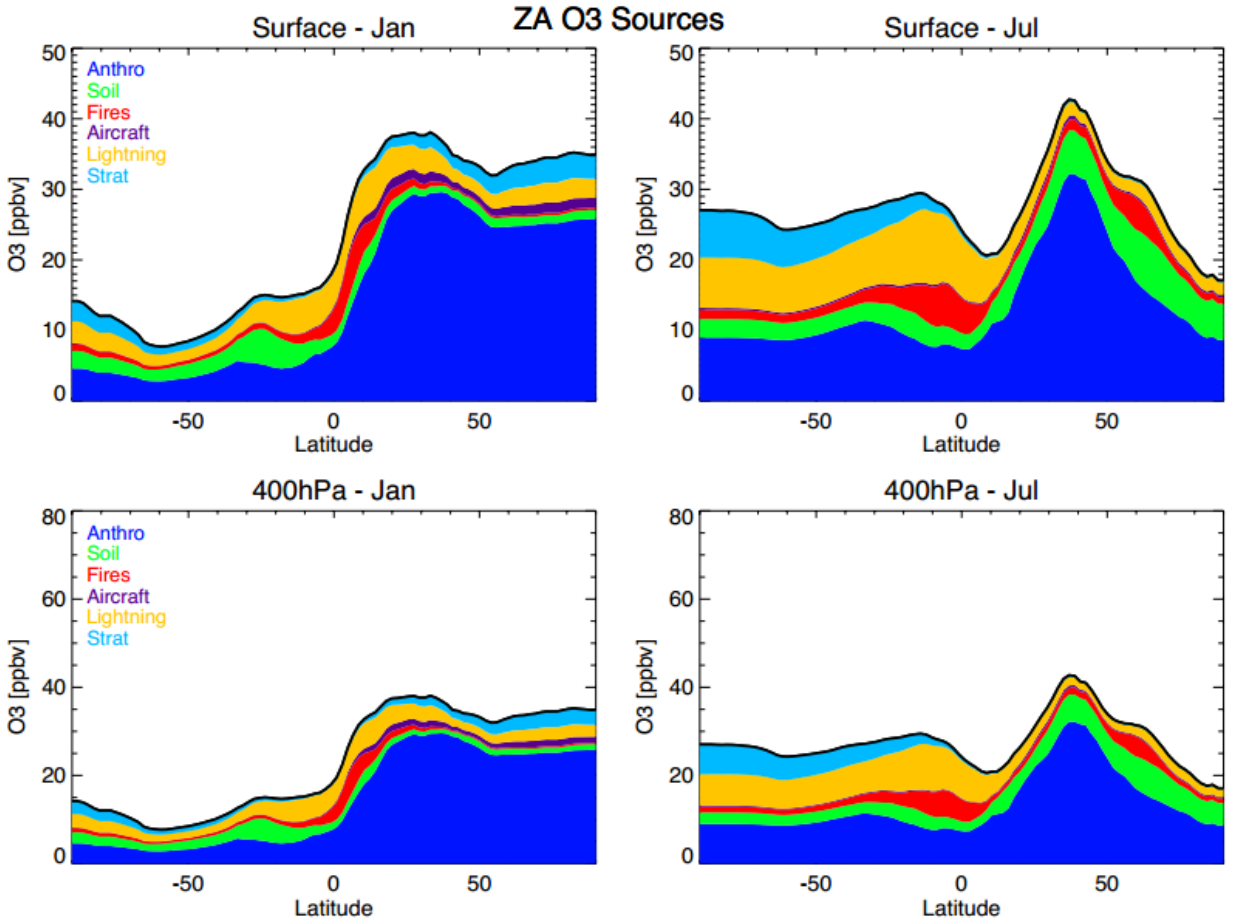
Established tagging in CAM-Chem: NO_x-based



New: multiple values of “TAG” possible in a single run

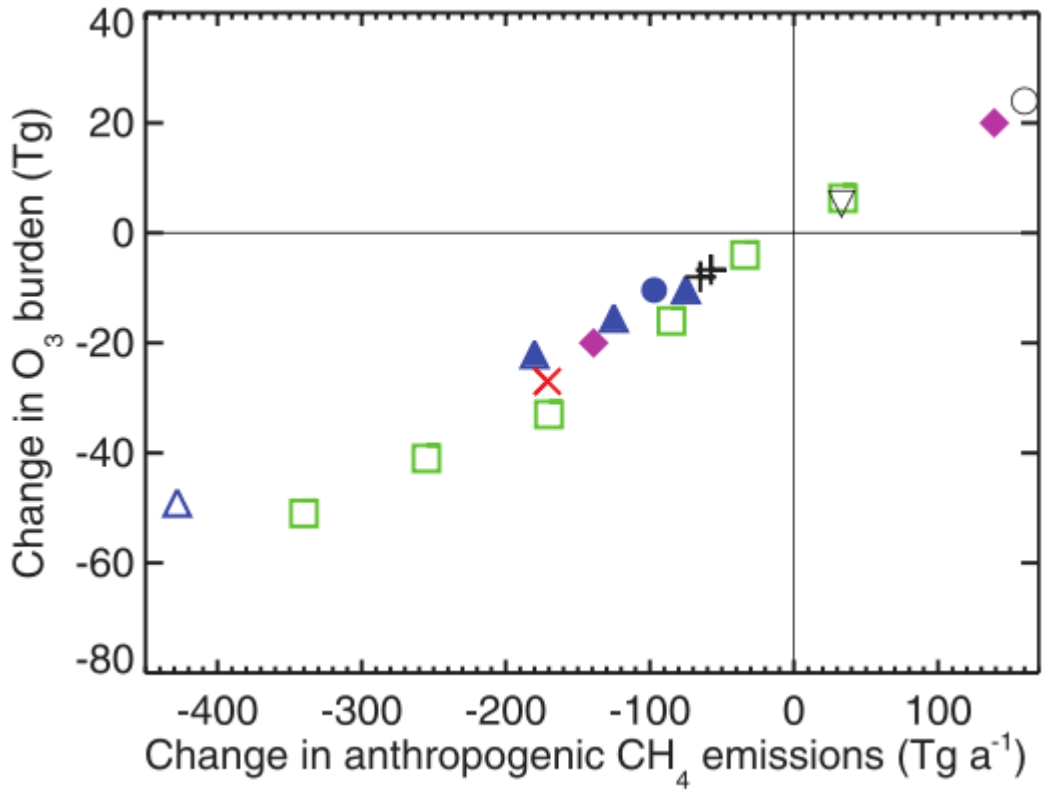


Emmons et al. (2012)

Null cycles

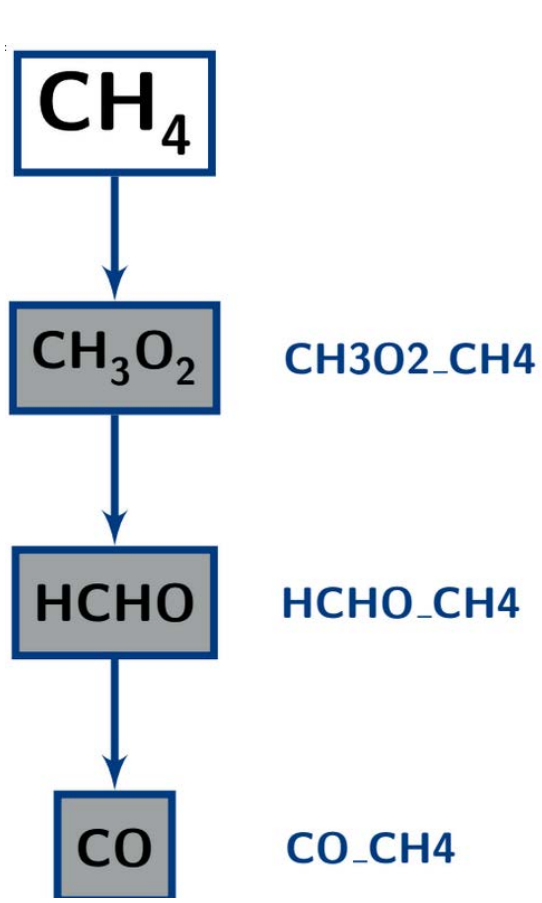
- O3 _A + NO_B -> NO2_B -> O3_B + NO_B
  - Tag is replaced by the O3-NO-NO2 null cycle!
- Solution: separation of NOx and Ox tags:
- O3_XA + NO_B -> NO2_XA + NO2_B -> O3_XA + NO_B
  - NOx tags represent emitted NOx
  - Ox tags represent chemically produced ozone

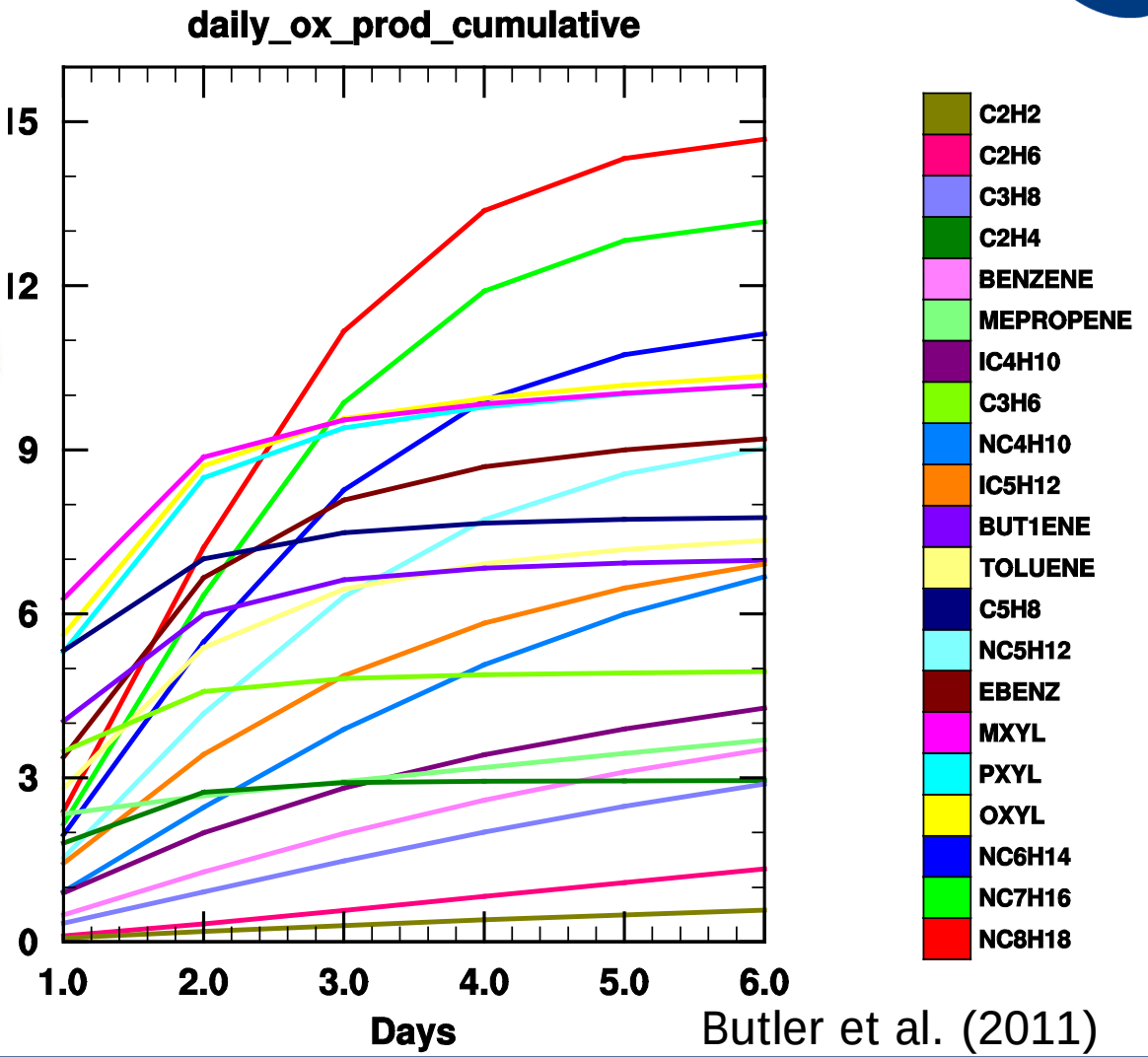
VOC sensitivity of tropospheric background ozone



Fiore et al. (2008)

Ozone production potential of VOC





Butler et al. (2011)

Implementation

- CESM 1.1.1 CCMI23 tag
  - Only works with troposphere-only mechanism adapted from Emmons et al. (2012)

- Predominantly a text processing problem
  - Perl scripts

- Preprocessing of the chemical mechanism file
  - Specify a list of tags to apply (eg. “TAG”, “FOO”, “BAR”)
  - Rewrite the mechanism file
    - XNO -> NO_TAG, NO_FOO, NO_BAR
    - Each tagged reaction is repeated for each additional tag

Implementation

- Original code:

```
if( jno2a_ndx > 0 .and. jno2_ndx > 0 ) then
      photos(:,:,jno2a_ndx) = photos(:,:,jno2_ndx)
end if
```

- Manually modified “template” code:

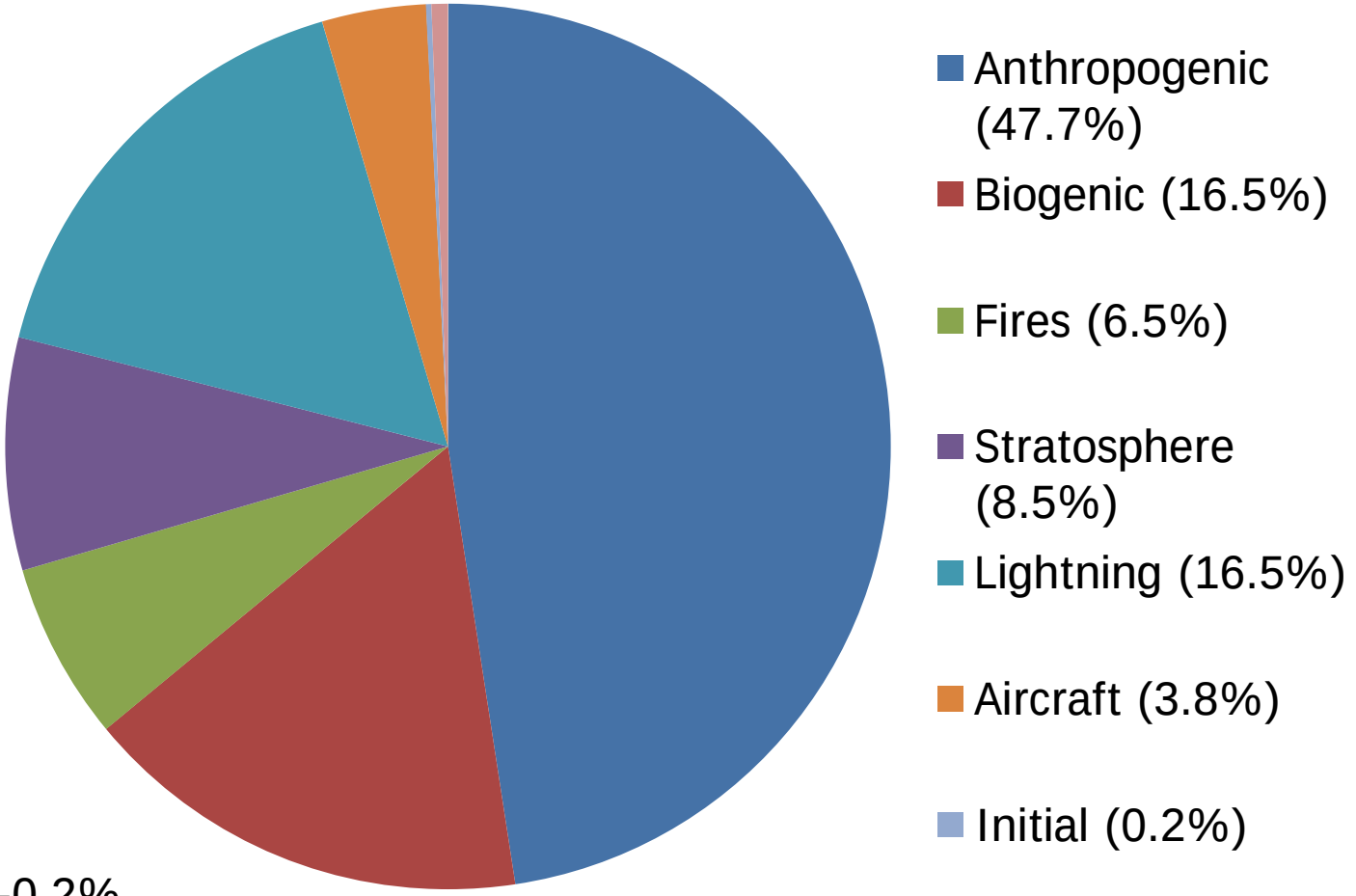
```
! BEGIN TAGGING CODE
if( jno2_tag_ndx > 0 .and. jno2_ndx > 0 ) then
      photos(:,:,jno2_tag_ndx) = photos(:,:,jno2_ndx)
end if
! END TAGGING CODE
```

- Template code is then automatically processed to produce compiler-ready code.

Model Setup

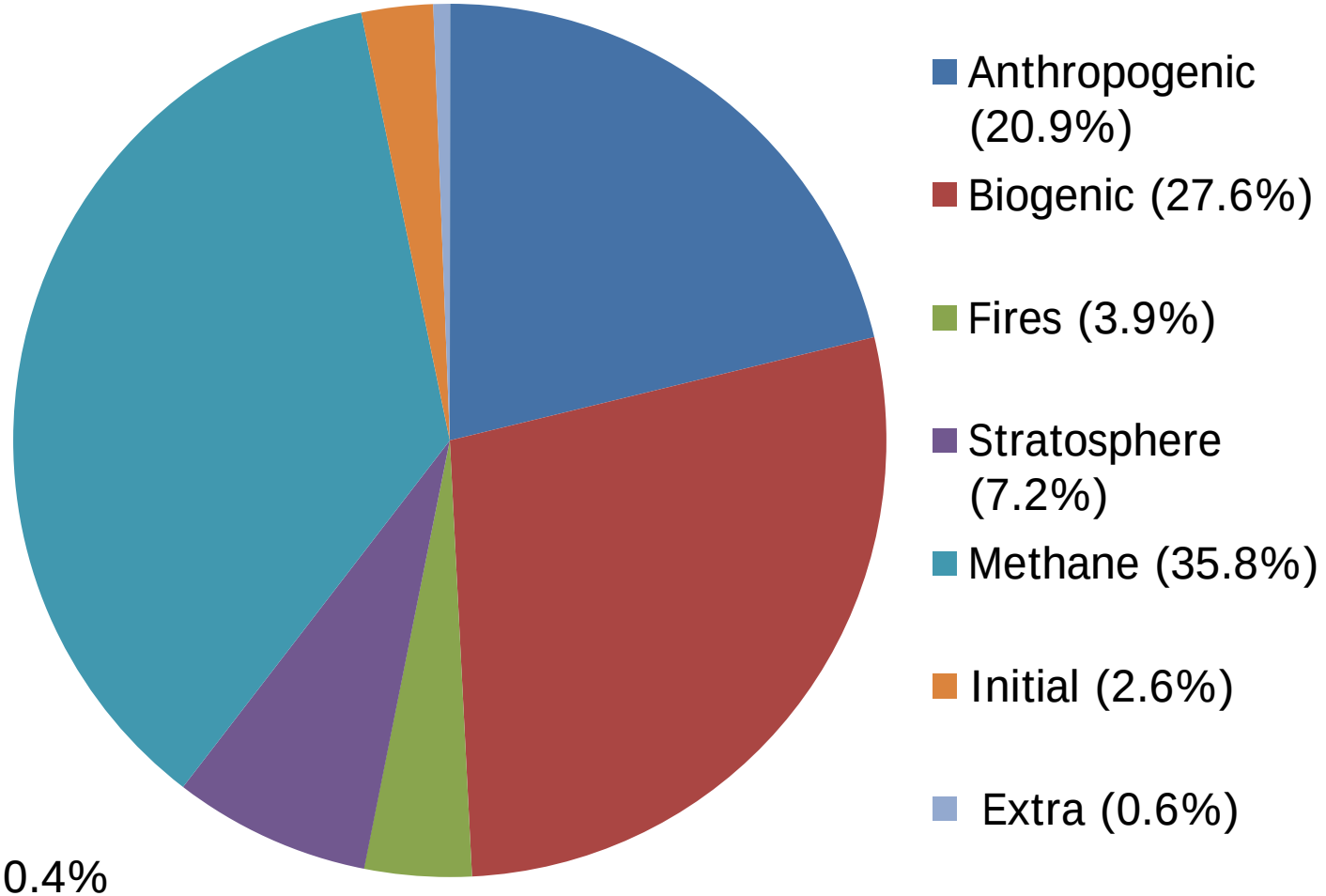
- **Two simulations**: tagged NOx and tagged VOC(+CO)
- Common tags:
  - ANT: anthropogenic
  - BIO: biogenic
  - BMB: fires
- NOx tags
  - AIR: aircraft
  - LGT: lightning
  - STR: stratosphere
- VOC tags
  - CH4: methane
  - INI: initial conditions
- Ox tags:
  - INI: initial ozone
  - STR: stratospheric ozone
  - XTR: difficult to classify

Results (surface ozone)



Residual: -0.2%

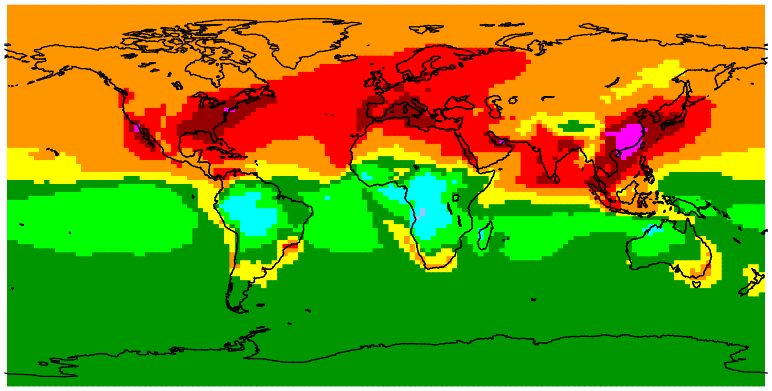
Results (surface ozone)

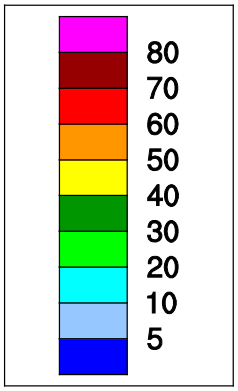


Residual: 0.4%

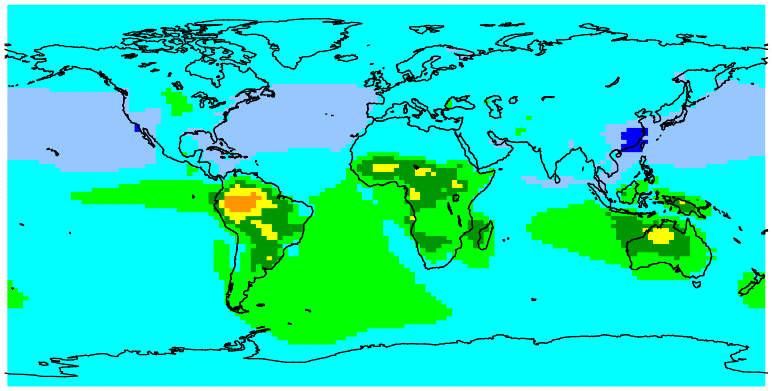
Ozone attributed to NOx

ccmi23_nox.O3_X_ANT



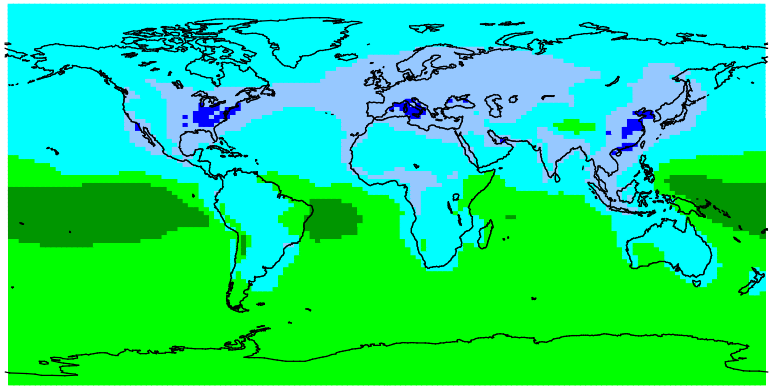


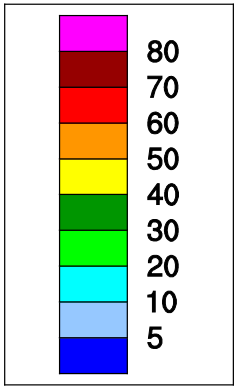
ccmi23_nox.O3_X_BIO



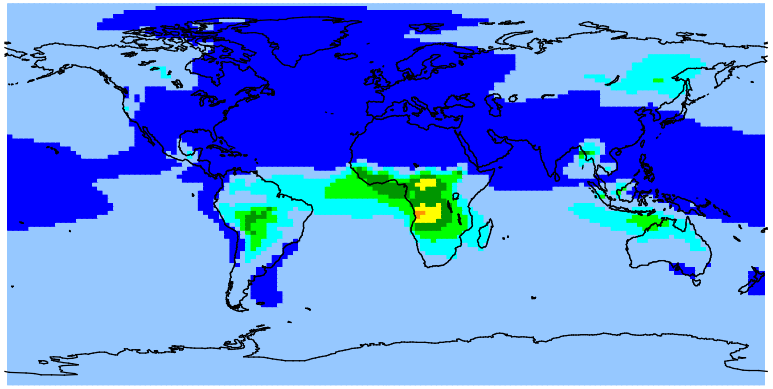
Percentage

ccmi23_nox.O3_X_LGT



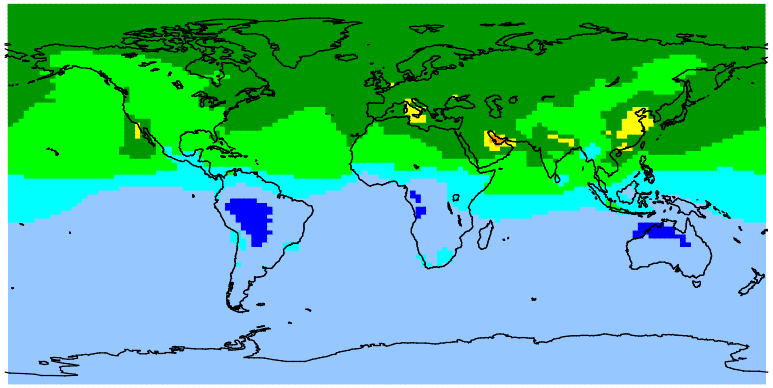


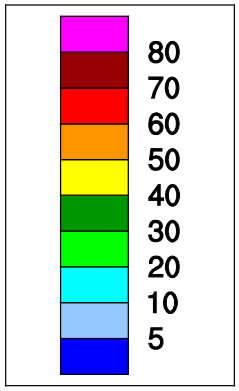
ccmi23_nox.O3_X_BMB



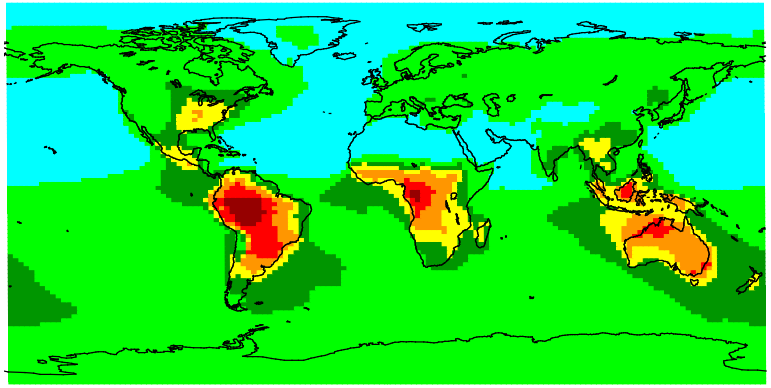
Ozone attributed to VOC+CO

ccmi23_voc.002.O3_X_ANT



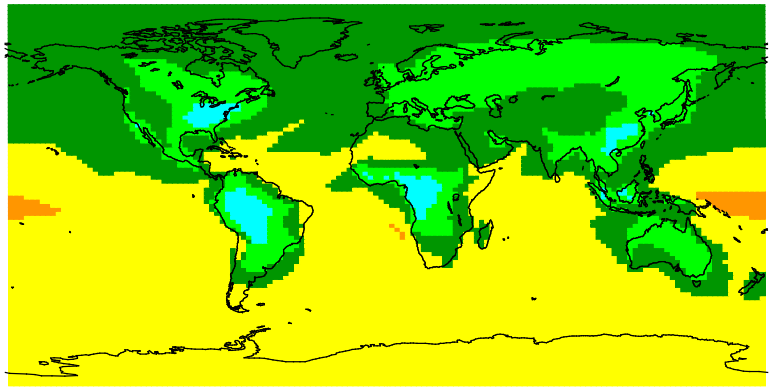


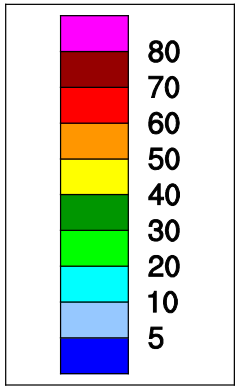
ccmi23_voc.002.O3_X_BIO



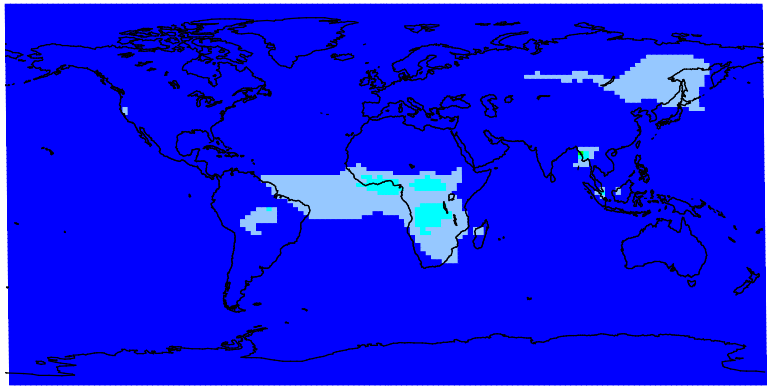
Percentage

ccmi23_voc.002.O3_X_CH4



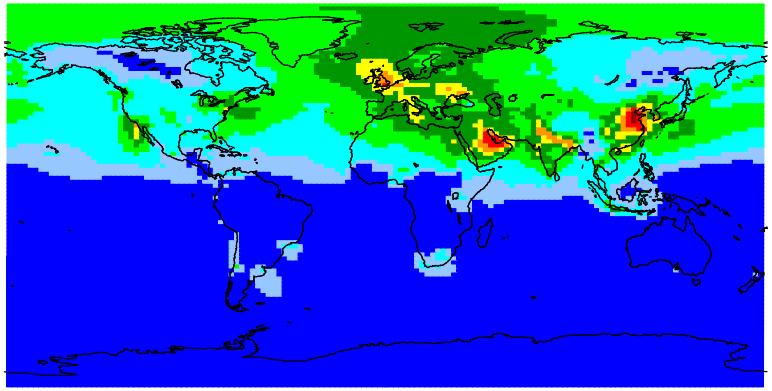


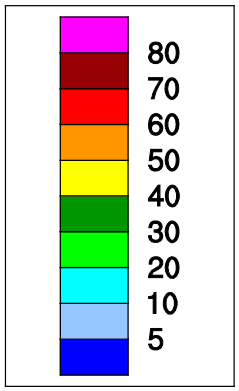
ccmi23_voc.002.O3_X_BMB



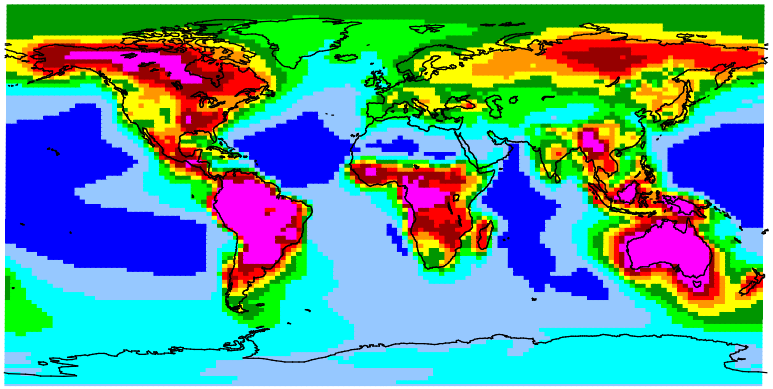
Formaldehyde attributed to VOC

ccmi23_voc.002.CH2O_ANT



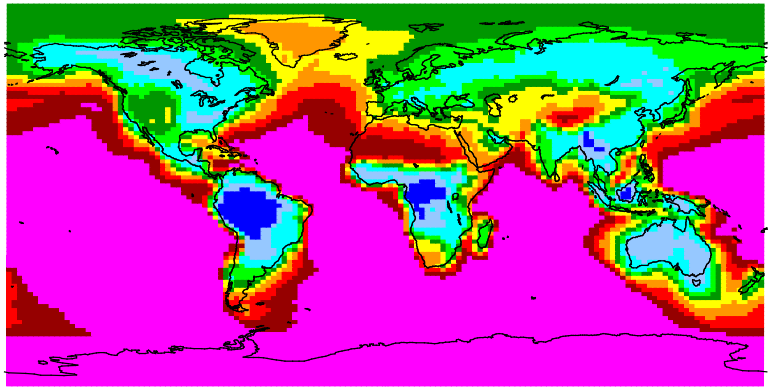


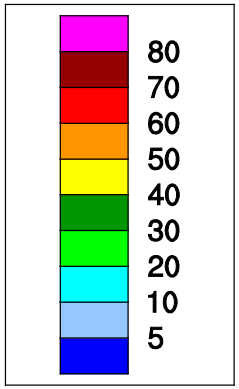
ccmi23_voc.002.CH2O_BIO



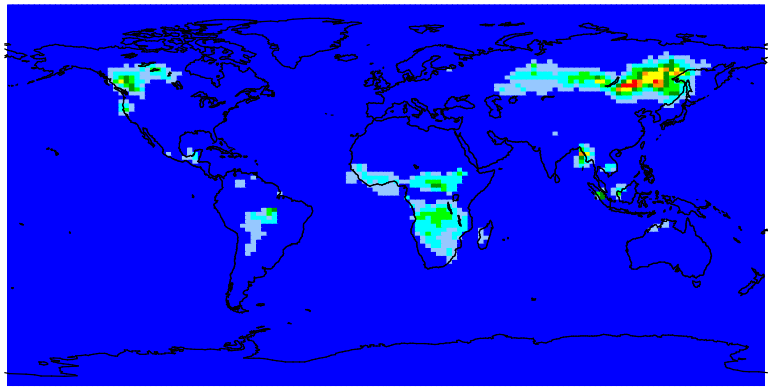
Percentage

ccmi23_voc.002.CH2O_CH4





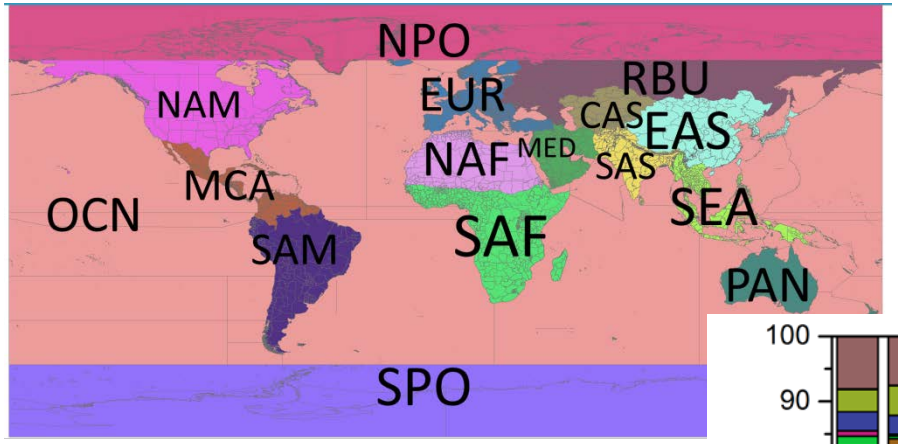
ccmi23_voc.002.CH2O_BMB

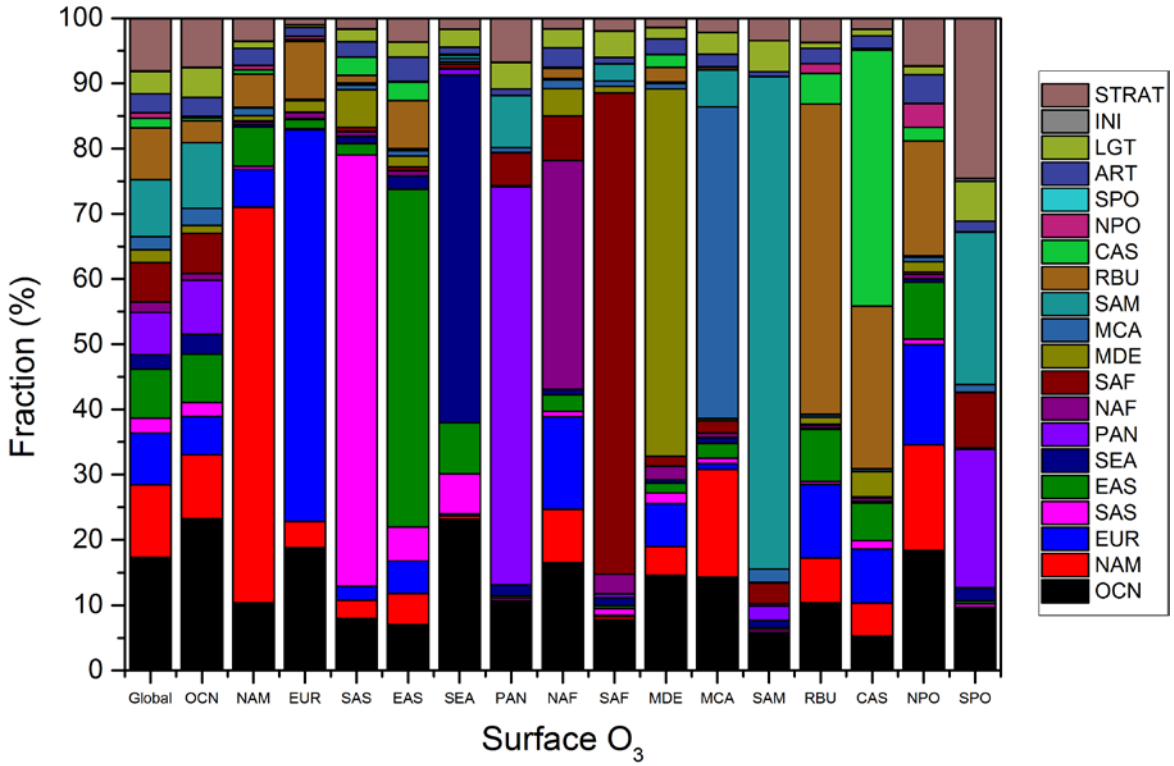


Model performance (yellowstone)

Run	Tags	Species	Reactions	PE-hours / Year	Seconds / Day
Standard	0	111	212	880	33
NOx tagged	8	287	1298	2740	105
VOC tagged	7	398	1354	2980	115

Application: Long Range Transport of Air Pollution (HTAP)





Next steps

- Write this up for GMD
- Application to HTAP simulations
- Increase automation
- Implement fully in the CCMI model version
- Comparison of different chemical mechanisms in CAM-Chem?
- Merge into a future version of CESM?
- (Somehow) combine NOx and VOC tagging?
- ...?