Updates to CAM-chem

Jean-François Lamarque

National Center for Atmospheric Research
(on leave at NOAA)

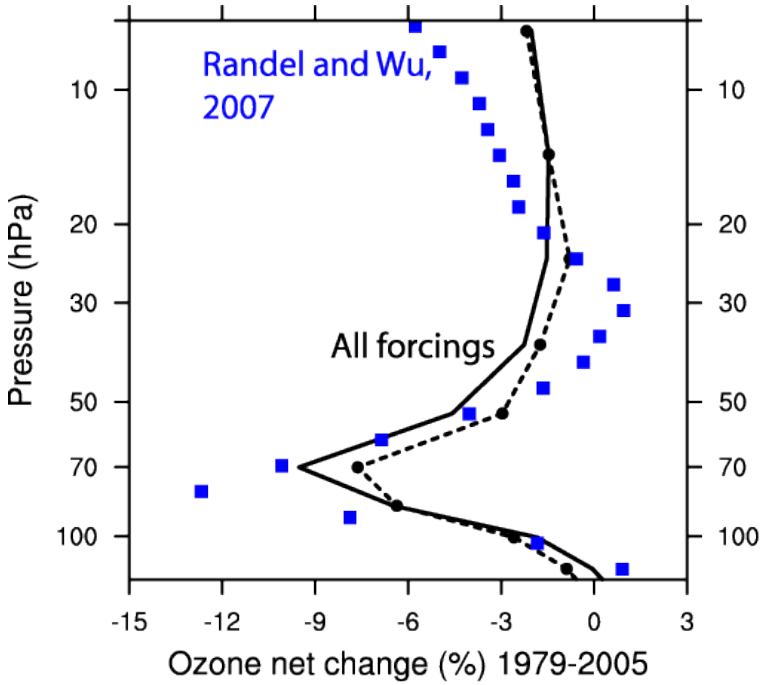
Who is using it?

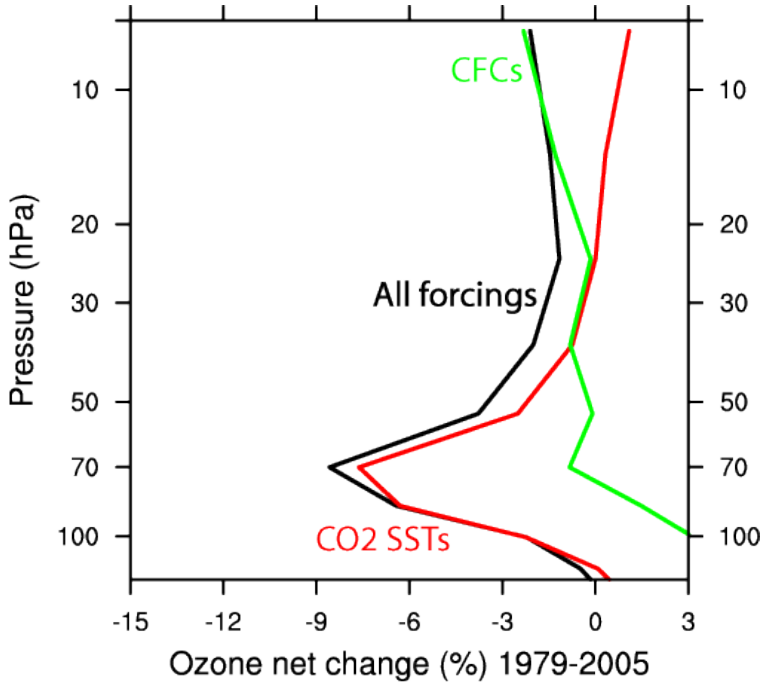
1. NCAR: Louisa, Simone, Ave, Doug, Andrew G., S. Massie
2. PNNL (Washington): S. Ghan, X. Liu
3. LLNL: P. Cameron-Smith
4. ORNL: J. Hack, D. Erickson
5. CU: B. Toon's group
6. UC Irvine: M. Prather, J. Neu
7. Cornell: P. Hess
8. CSU: C. Heald
9. UIUC: D. Wuebbles' group
10. NOAA: P. Young
11. University of Leeds: S. Arnold
12. Spain: A. Saiz-Lopez

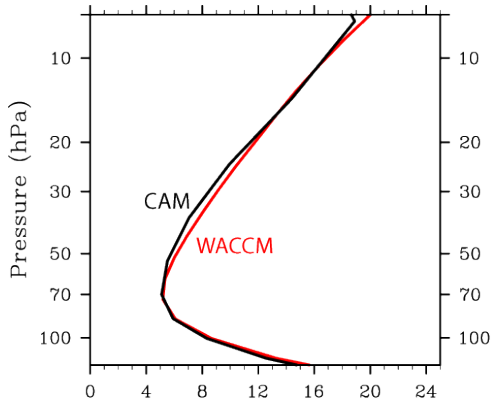
Status of CAM-chem

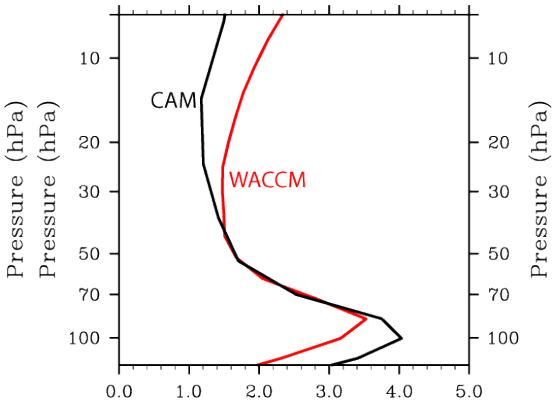
- Updated to latest version of CAM (coupling with MG microphysics and new modal aerosol scheme); now part of the trunk. Needs some update for full functionality with modal scheme (reaction on aerosols, OD).
- Merge with WACCM almost complete: stratospheric chemistry available for all configurations
- Mapping of photolysis (See Francis' talk)
- Merge with CLM for MEGAN/dry deposition in review
- Offline version (most problems fixed?) used for high-resolution MIRAGE and START08 simulations (see Simone/Louisa's presentation)
- Extension for halogen chemistry (with D. Kinnison, J. Orlando and A. Saiz-Lopez)
- Testing of variety of chemical mechanisms (P. Cameron-Smith)

Application to tropical LS trends









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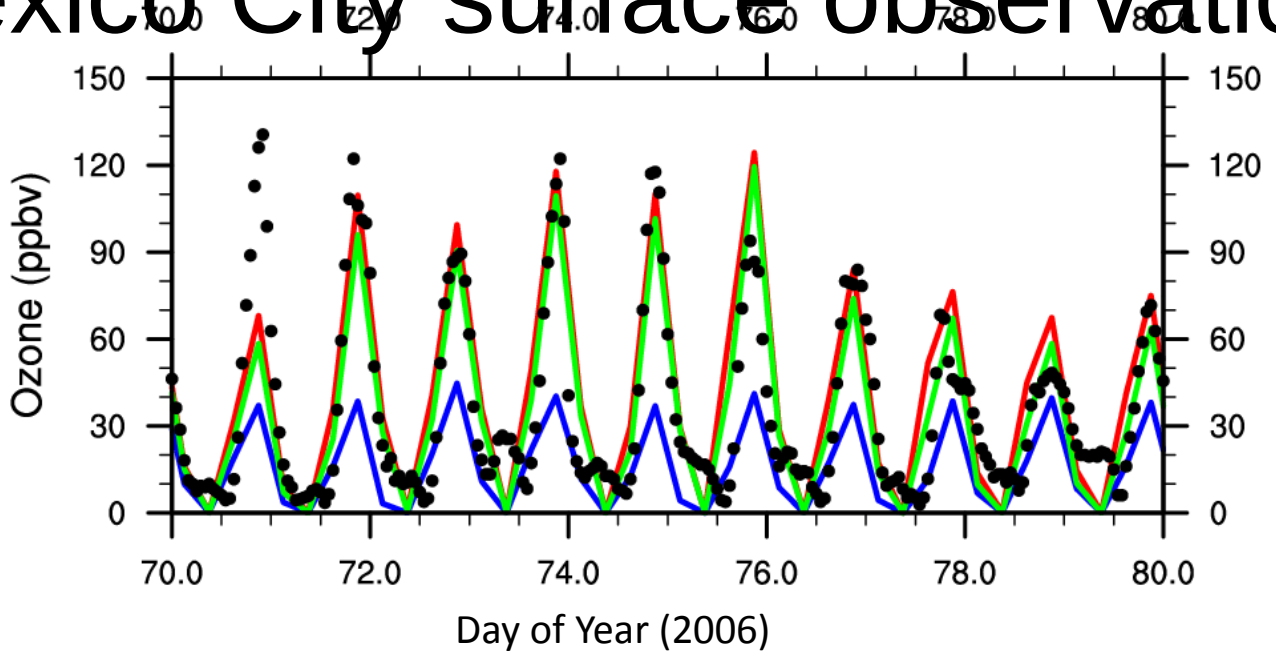
Air quality: Comparison with Mexico City surface observations



Red: Full mechanism

Green: Intermediate mechanism

Blue: Fast mechanism

Dots: observations

On most days, full and intermediate capture well the diurnal cycle and amplitude; the fast mechanism is much lower

Update to building CAM-chem

Francis Vitt

Improvements to CAM configure

- Easier to customize the chemistry
- Configure invokes preprocessor
- Determines the number advected tracers
- Ability to easily configure CAM with bulk aerosol/GHG packages (separately or combined)
- Ability to configure with non-transported chemical tracers

Configure options

Predefined chemistry packages:

```
-chem trop_mozart | trop_ghg | trop_bam | trop_mam3 |
      trop_mam7 | waccm_mozart | waccm_ghg |
      super_fast_llnl | none
```

Predefined bulk aerosol/GHG packages:

```
-prog_species  SO4 | DST | SSLT | OC | BC | GHG | CARBON16
```

Configure will generate a preprocessor input file for any combination of these predefined prognostic aerosol and GHG packages.

Example:

```
$cfgdir/configure -prog_species OC,BC,DST ...
```

```
 SPECIES

    Solution
   OC1 -> C, OC2 -> C
   CB1 -> C, CB2 -> C
   DST01 -> AlSiO5, DST02 -> AlSiO5, DST03 -> AlSiO5, DST04 -> AlSiO5
    End Solution

    Fixed
   M, N2, O2
    End Fixed

    Col-int
O3 = 0.
O2 = 0.
    End Col-int

  End SPECIES

  Solution Classes
    Explicit
    End Explicit
    Implicit
   CB1, CB2
   OC1, OC2
   DST01, DST02, DST03, DST04
    End Implicit
  End Solution Classes

  CHEMISTRY
    Photolysis
    End Photolysis

    Reactions
   CB1 -> CB2    ; 1.006e-05
   OC1 -> OC2    ; 1.006e-05
    End Reactions

    Heterogeneous
    End Heterogeneous

    Ext Forcing
    End Ext Forcing

  END CHEMISTRY
```

- **`-usr_mech_infile $mechanism_file`**
  - Allow user to specify a customized preprocessor input file
  - Determines the number of advected tracers
- **`-edit_chem_mech`**
  - Default vi
  - CAMCHEM_EDITOR environment variable to specify another editor (e.g. emacs)
  - Allows user to edit the mechanism file before it is processed

Preprocessor input file

List solution species

List prescribed species

List species not transported

Longer lived species

Shorter lived species

Photolysis reactions

Gas phase reactions

Gas phase wet removal

Prescribed prod/loss rates

```
SPECIES

  Solution
  End Solution

  Fixed
  End Fixed

  Not-transported
  End Not-transported

END SPECIES

SOLUTION CLASSES

  Explicit
  End Explicit

  Implicit
  End Implicit

END SOLUTION CLASSES

CHEMISTRY

  Photolysis
  End Photolysis

  Reactions
  End Reactions

  Heterogeneous
  End Heterogeneous

  Ext Forcing
  End Ext Forcing

END CHEMISTRY
```

Non-transported chemical tracers

mechanism file:

```
SPECIES

   ...

   NOT-TRANSPORTED
     OH, ...
   END NOT-TRANSPORTED

END SPECIES
```

build script:

```
$cfgdir/configure \
     -chem trop_mozart \
     -usr_mech_infile $mechanism_file \
```

```
  SPECIES

     Solution
O3, O, O1D ->  O, N2O, NO, NO2, NO3, HNO3, HO2NO2, N2O5, H2, OH, HO2, H2O2,
CH4,CO, CH3O2, CH3OOH, CH2O, CH3OH, C2H5OH
C2H4, EO -> HOCH2CH2O, EO2 -> HOCH2CH2O2, CH3COOH, GLYALD -> HOCH2CHO
C2H6, C2H5O2, C2H5OOH, CH3CHO, CH3CO3, CH3COOOH
C3H6, C3H8, C3H7O2, C3H7OOH, PO2 -> C3H6OHO2, POOH -> C3H6OHOOH
CH3COCH3, RO2 -> CH3COCH2O2, ROOH -> CH3COCH2OOH
BIGENE -> C4H8, ENEO2 -> C4H9O3
MEK -> C4H8O, MEKO2 -> C4H7O3, MEKOOH -> C4H8O3
BIGALK -> C5H12, ALKO2 -> C5H11O2, ALKOOH -> C5H12O2
ISOP -> C5H8, ISOPO2 -> HOCH2COOCH3CHCH2, ISOPOOH -> HOCH2COOHCH3CHCH2
MVK -> CH2CHCOCH3, MACR -> CH2CCH3CHO
MACRO2 -> CH3COCHO2CH2OH, MACROOH -> CH3COCHOOHCH2OH
MCO3 -> CH2CCH3CO3,  HYDRALD -> HOCH2CCH3CHCHO, HYAC -> CH3COCH2OH
CH3COCHO, XO2 -> HOCH2COOCH3CHCHOH, XOOH -> HOCH2COOHCH3CHCHOH
C10H16, TERPO2 -> C10H17O3, TERPOOH -> C10H18O3
TOLUENE -> C7H8, CRESOL -> C7H8O, TOLO2 -> C7H9O3, TOLOOH -> C7H10O3
XOH -> C7H10O4, BIGALD -> C5H6O2, GLYOXAL -> C2H2O2
PAN -> CH3CO3NO2, ONIT -> CH3COCH2ONO2, MPAN -> CH2CCH3CO3NO2
ISOPNO3 -> CH2CHCCH3OOCH2ONO2, ONITR -> CH2CCH3CHONO2CH2OH
CB1 -> C, CB2 -> C, OC1 -> C, OC2 -> C, SOA -> C12
SO2, SO4, DMS -> CH3SCH3, NH3, NH4NO3
SSLT01 -> NaCl, SSLT02 -> NaCl, SSLT03 -> NaCl, SSLT04 -> NaCl
Rn, Pb, O3S -> O3, O3INERT -> O3, O3RAD -> O3, SYNOZ -> O3
DST01 -> AlSiO5, DST02 -> AlSiO5, DST03 -> AlSiO5, DST04 -> AlSiO5
NH4, H2SO4
     End Solution

     Fixed
M, N2, O2, H2O
     End Fixed

     Col-int
O3 = 0.
O2 = 0.
     End Col-int

     Not-transported
       OH
     End Not-transported

  End SPECIES
```

```
  Solution Classes
     Explicit
      CH4, N2O, CO, Rn, Pb, H2, O3INERT, O3S, SYNOZ, O3RAD
     End Explicit
     Implicit
      O3, O1D, O, NO, NO2, NO3, HNO3, HO2NO2, N2O5, OH, HO2, H2O2
      CH3O2, CH3OOH, CH2O, CH3OH, C2H5OH
      C2H4, EO, EO2, CH3COOH, GLYALD
      C2H6, C2H5O2, C2H5OOH, CH3CHO, CH3CO3, CH3COOOH
      C3H6, C3H8, C3H7O2, C3H7OOH, PO2, POOH, CH3COCH3, RO2, ROOH
      BIGENE, ENEO2, BIGALK, ALKO2, ALKOOH, MEK, MEKO2, MEKOOH
      ISOP, ISOPO2, ISOPOOH, MVK, MACR, MACRO2, MACROOH, MCO3
      HYDRALD, HYAC, CH3COCHO, XO2, XOOH
      C10H16, TERPO2, TERPOOH
      TOLUENE, CRESOL, TOLO2, TOLOOH, XOH, BIGALD, GLYOXAL
      PAN, ONIT, MPAN, ISOPNO3, ONITR
      CB1, CB2, SO2, SO4, DMS, NH3, NH4NO3, NH4, H2SO4
      OC1, OC2, SSLT01, SSLT02, SSLT03, SSLT04, SOA
      DST01, DST02, DST03, DST04
     End Implicit
  End Solution Classes

CHEMISTRY
     Photolysis
[jo2]                  O2 + hv -> 2*O
[jo1d]                 O3 + hv -> O1D + O2
[jo3p]                 O3 + hv -> O + O2
[jn2o]                 N2O + hv -> O1D + N2
[jno2]                 NO2 + hv -> NO + O
[jn2o5]                N2O5 + hv -> NO2 + NO3
[jhno3]                HNO3 + hv -> NO2 + OH
[jno3->,1.1236*jno3]   NO3 + hv -> .89*NO2 + .11*NO + .89*O3
[jho2no2]              HO2NO2 + hv -> .33*OH + .33*NO3 + .66*NO2 + .66*HO2
[jch3ooh]              CH3OOH + hv -> CH2O + HO2 + OH
 ...
[jpooh->,jch3ooh]      POOH + hv -> CH3CHO + CH2O + HO2 + OH
[jch3co3h->,.28*jh2o2] CH3COOOH + hv -> CH3O2 + OH  + CO2
 ...
     End Photolysis

     Reactions
[usr1]   O + O2 + M -> O3 + M
         O + O3 -> 2*O2                                              ; 8e-12, -2060
[o1d_n2] O1D + N2 -> O + N2                                          ; 2.1e-11, 115
[o1d_o2] O1D + O2 -> O + O2                                          ; 3.2e-11, 70
...
     End Reactions
```

Simple mechanism example

mechanism file:

```
 SPECIES

      Solution
        CO
      End Solution

      Fixed
        OH
      End Fixed

 END SPECIES

 CHEMISTRY

     Reactions
[usr8]  CO + OH -> CO2 + HO2
     End Reactions

     Ext Forcing
        CO<-dataset
     End Ext Forcing

 END CHEMISTRY
```

script file:

```
$cfgdir/configure \
      -chem trop_mozart \
      -usr_mech_infile $mech_file.in \

...

 $cfgdir/build-namelist -case $case -runtype $runtype -d $rundir \
   -namelist "&camexp  stop_n=$stop_n, stop_option='ndays' \
   srf_emis_specifier = 'CO ->
$emispath/emissions.CO.surface.T42LR.nc'\
   tracer_cnst_specifier = 'OH:OH_VMR_avrg'\
   tracer_cnst_file = '$datapath/oh_2004.nc'\
   tracer_cnst_type = 'CYCLICAL'\
   tracer_cnst_ymd = 20040101\
   tracer_srcs_file = '$datapath/oh_2004.nc'\
   tracer_srcs_specifier = 'CO:CO_PROD_avrg'\
   tracer_srcs_type = 'CYCLICAL'\
   tracer_srcs_ymd = 20040101\
  / "  || echo "build-namelist failed" && exit 1
```