Atmospheric Modeling with Interactive Chemistry

Presented by Simone Tilmes ACOM/CGD

- Running with fully-coupled chemistry, different chemical mechanism versions
- Description of secondary organic aerosols as parameterized in CAM-chem
- Evaluation
- Other applications of CAMchem

Tropospheric Chemistry and Aerosols

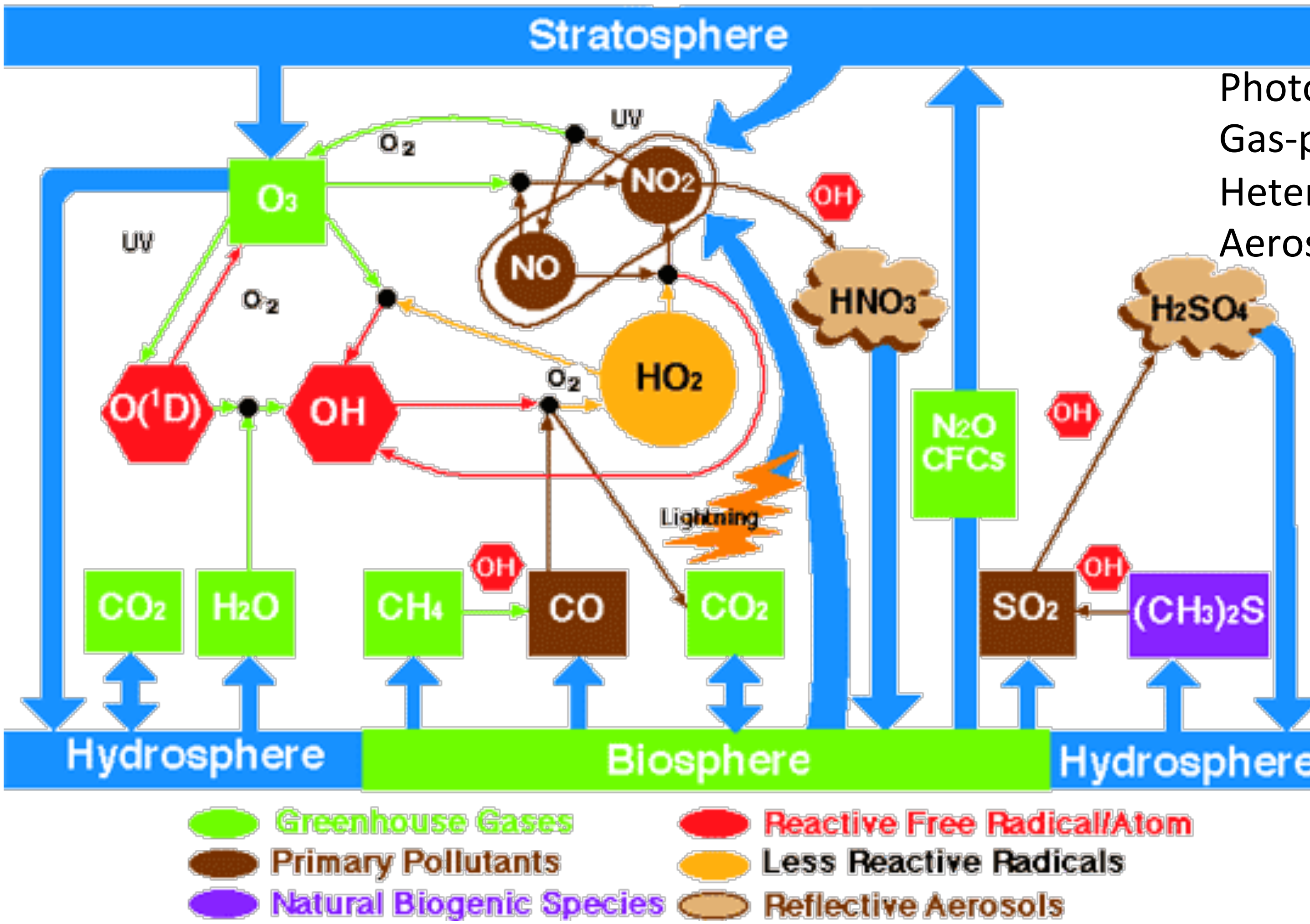


Photo-chemistry
Gas-phase chemistry
Heterogeneous chemistry
Aerosol formation

OH determines the lifetime of Methane

Modeling with Chemistry

Available chemical mechanisms in CAM-Chem

Superfast Chemistry (CAM4/5):

12 species, simple chemistry mechanism, CH_4 prescribed
LINOZ + Cariolle in stratosphere, fully coupled

Bulk Aerosol Model (BAM) (CAM4/5):

Includes Black Carbon, Organic Carbon, Sea Salt, Dust
(prescribed monthly fields of CO_2, CH_4, O_3, OH, HO_2, NO_2, N_2O, SO_2/SO_4)

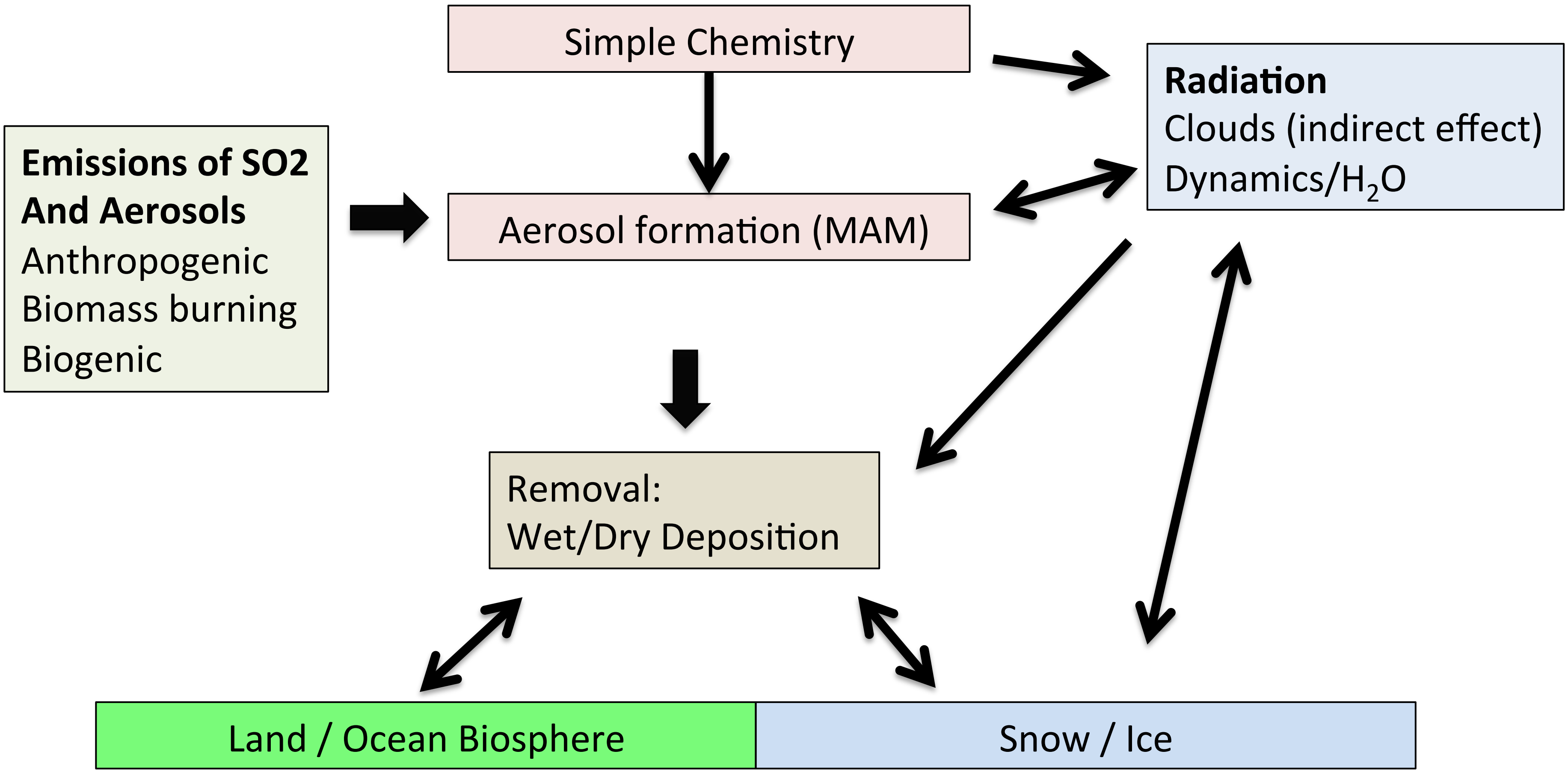
Tropospheric chemistry (trop_mozart) (CAM4/5):

Tropospheric mechanism, over 100 species (MOZART: *Emmons et al., 2010*)
Stratospheric chemistry is prescribed about 50 hPa: (O_3, HNO_3, CH_4, CO)
Emissions, Dry/Wet Deposition
Secondary Organic aerosols

Plus stratospheric chemistry (trop-strat mozart) (CAM4/5):

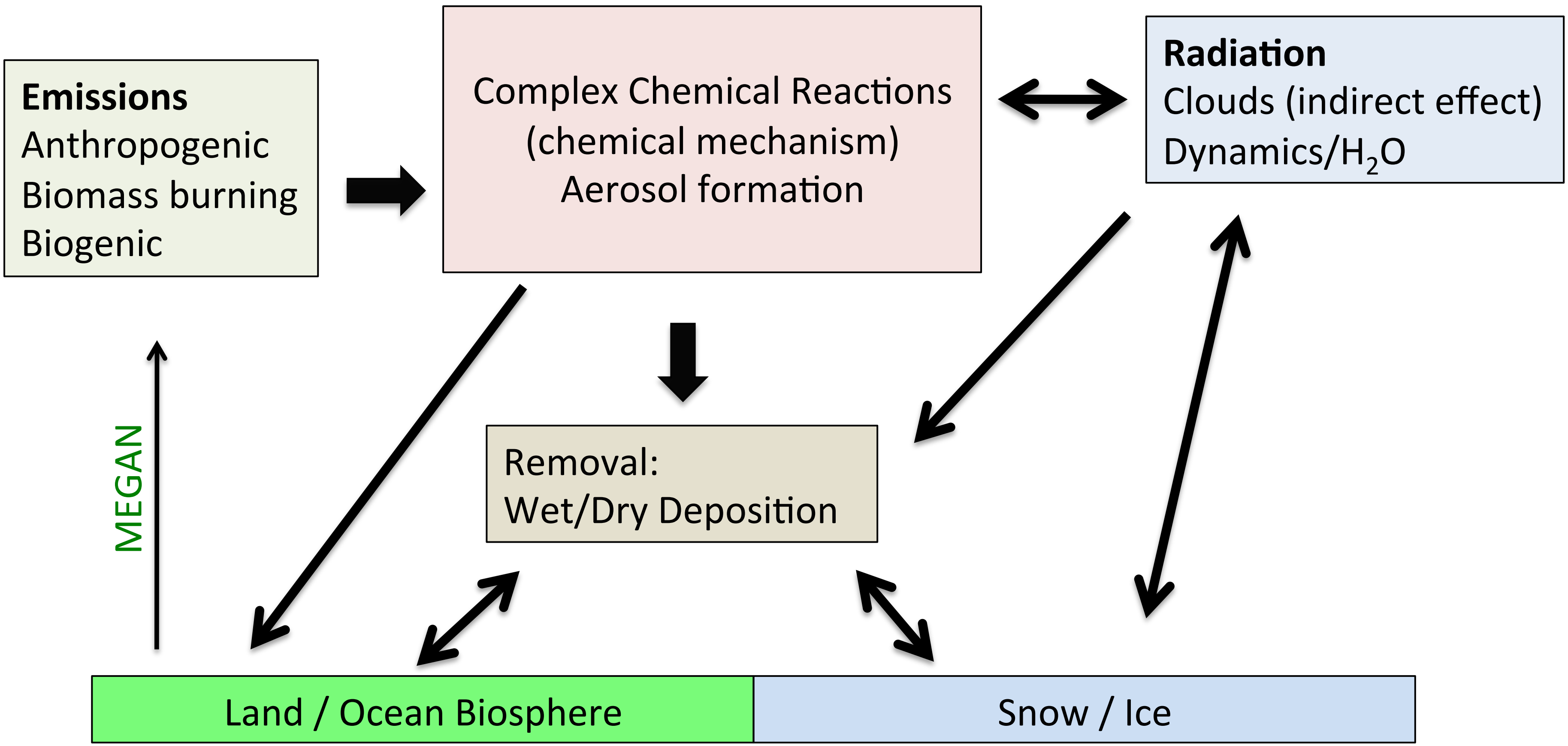
Tropospheric and Stratospheric mechanism (~122 species) including stratospheric heterogeneous reactions, about 300 reactions (similar to WACCM) (Lamarque et al., 2012, Tilmes et al., 2015)

Chemistry in CESM CAM5



Chemistry in CESM CAM5-Chem

CAM4-chem does not include coupling between aerosols and clouds



Modeling with Chemistry

Chemical Mechanism: includes set of equations
The chemistry preprocessor: tool that generates CAM Fortran source code; numerically solve a set of differential equations which represent the chemical reactions -> temporal evolution of the chemical tracers

1. Solutions: lists all chemical constituencies and defines what they are, e.g.
 `ISOP -> C5H8`, BIGENE -> C4H8, BIGALK -> C5H12, MEK -> C4H8O

- Includes Fixed Species: lists of chemical species that do not change
- And Non-transported Components (very short lifetime)

2. Solution classes, divides solution species into explicit and implicit (shorter timestep in the solver)

4. Chemistry:

- Photolysis: [jo3_a] O3 + hv -> O1D + O2
- Gas-phase chemistry:
  [O_O3] O + O3 -> 2*O2 ; 8.00e-12, -2060.
  rates (temperature dependence etc.)
- Heterogeneous Reaction
  [usr_N2O5_aer] N2O5 -> 2 * HNO3

User defined reactions: are defined in the model code: mo_usrrxt.F90

Emissions

Emissions: are defined in the user_nl_cam namelist variable

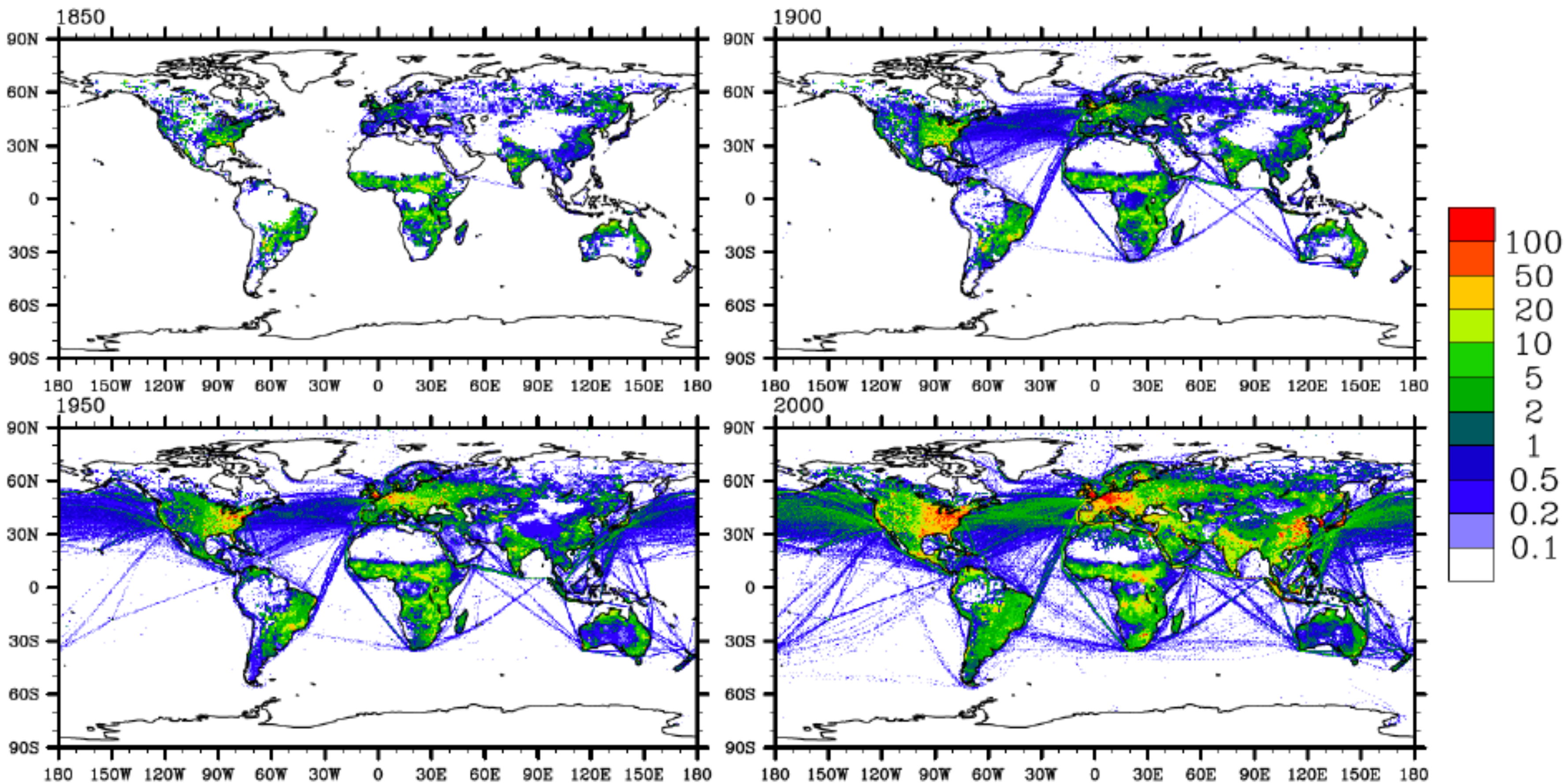
- Depending on mechanism, different species need to be emitted

```
srf_emis_specifier          = 'CH2O    -> /glade/p/cesmdata/cseg/inputdata/atm/ca
6.nc',
         'CO       -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'NO       -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'BIGALK   -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'BIGENE   -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'C2H2     -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'C2H4     -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'C2H5OH   -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'C2H6     -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'C3H6     -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'C3H8     -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'CH3CHO   -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'CH3OH    -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'MEK      -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'TOLUENE  -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'XYLENES  -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'BENZENE -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_21
         'HCN      -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'CH3CN    -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'CH3COCH3 -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'CH3COOH  -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'HCOOH    -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/emis/ccmi_1950_2
         'DMS       -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
         'SO2       -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
         'SOAG      -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
         'bc_a4     -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
         'num_a1    -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
         'num_a2    -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
         'num_a4    -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
         'pom_a4    -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
         'so4_a1    -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
         'so4_a2    -> /glade/p/cesmdata/cseg/inputdata/atm/cam/chem/trop_mozart_aer
```

- Chemical components are currently emitted at the surface.
- Include anthropogenic, biomass burning and fire emissions.
- **Biogenic emissions** can be calculated by MEGAN (make sure to not double-count)
- **Coming soon**: fire emissions may be calculated by the land model

-> Careful if changing emissions, to match your model setup

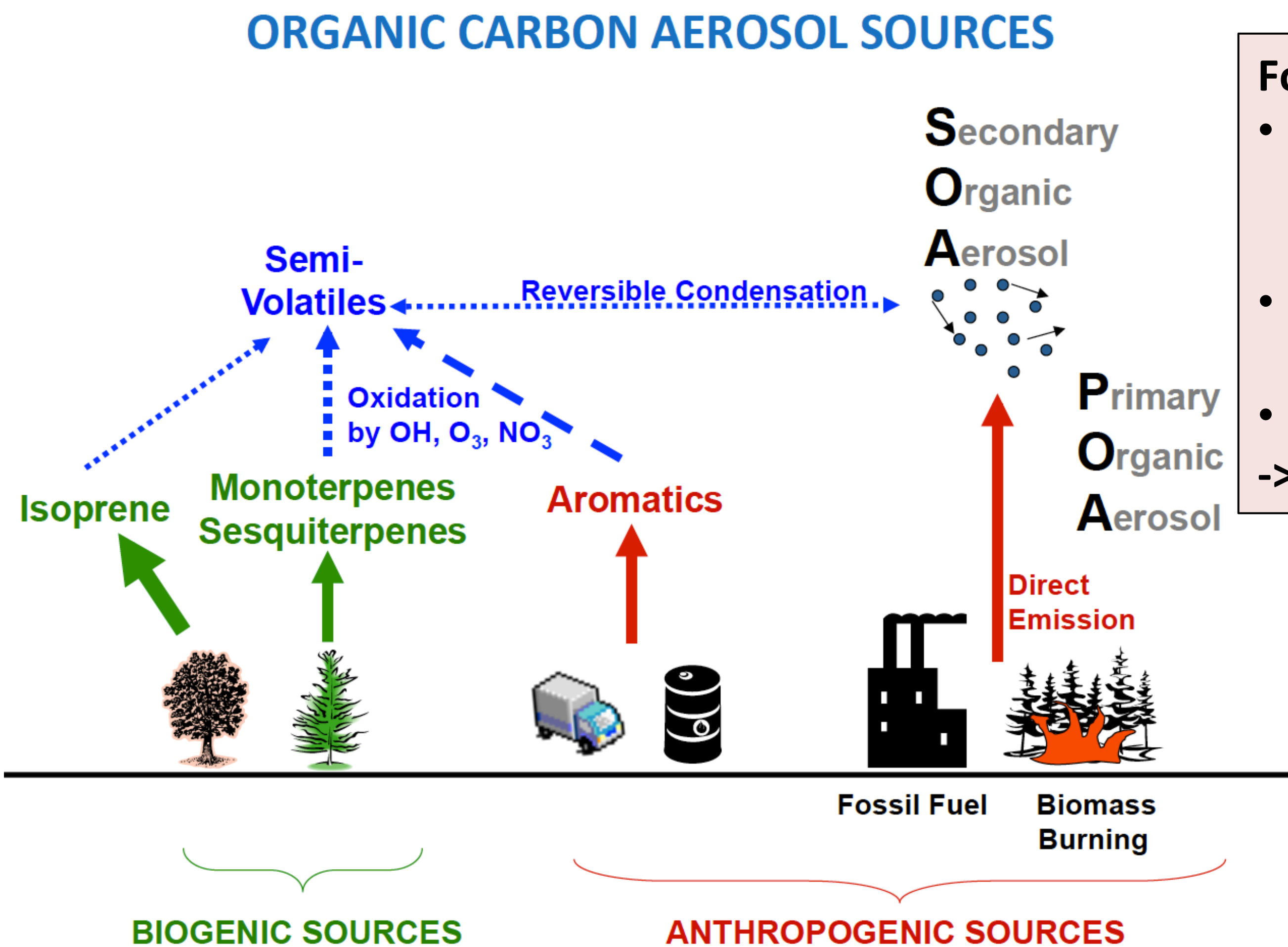
Example: NO_x emissions



Lamarque et al., 2010

Anthropogenic + biomass burning + ships: kg(N)/year

Organic Aerosols (simulated in CAM4-Chem)



Formation of SOA

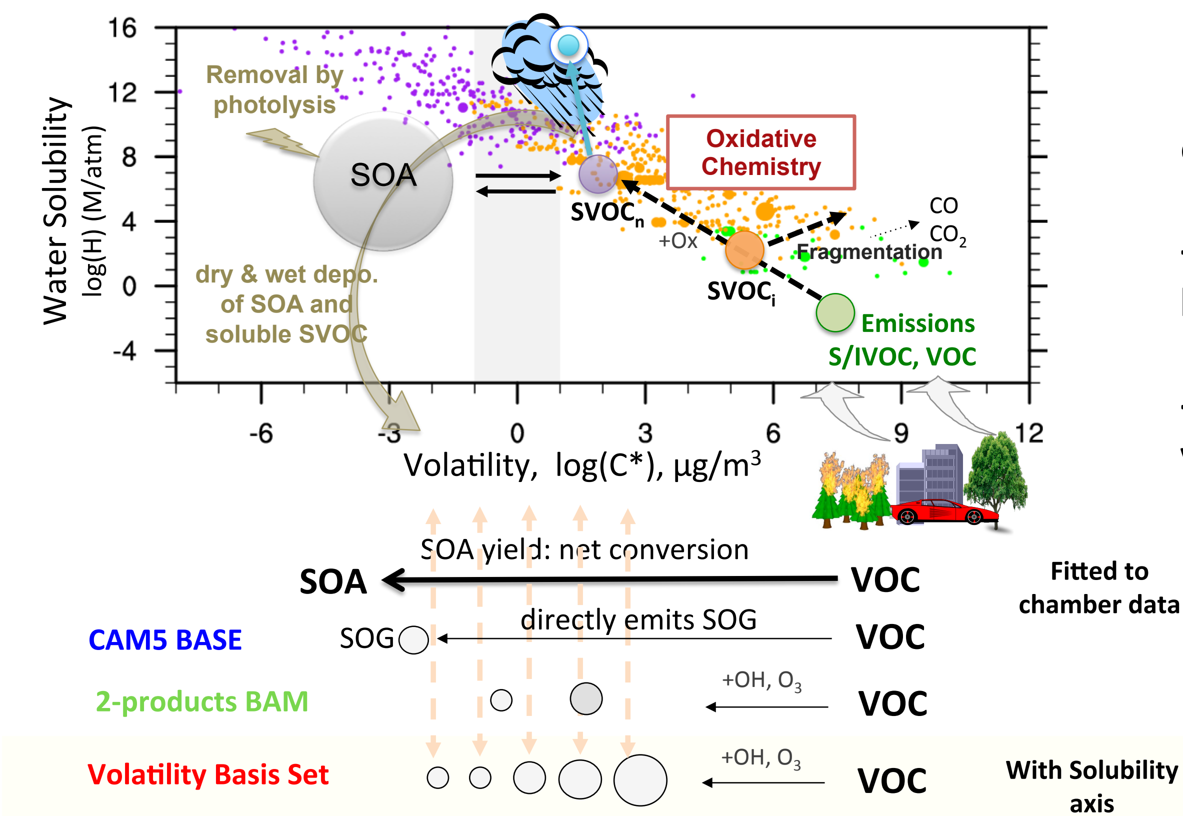
- Emissions of volatile organic carbons
- Formation of Semi-Volatiles
- Emissions of POM

-> SOA

From C. Heald, MIT Cambridge

New SOA approach in CESM2 CAM5-Chem/ WACCM (next year)

Simplistic ways of treating the complex SOA lifecycle

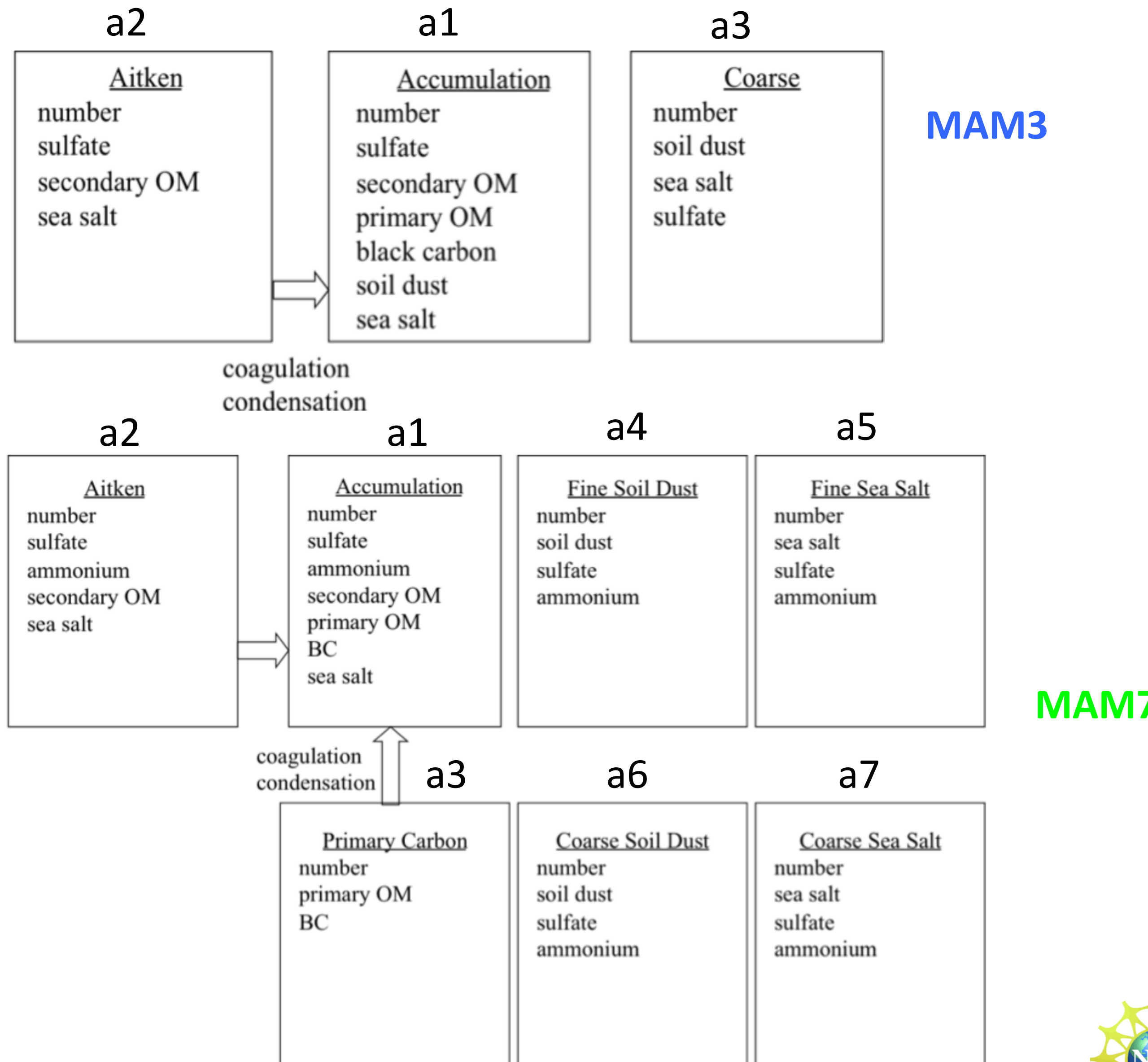


More physical approach
Direct coupling to biogenic emissions changes from MEGAN

-> couples SOA formation to land use and climate change

-> only works in full chemistry version at this point

Aerosols: CAM5 Modal Aerosol Model (MAM3/7)



Mode	σ_g	Size range (μm)
MAM3		
Aitken	1.6	0.015–0.053
Accumulation	1.8	0.058–0.27
Coarse	1.8	0.80–3.65
MAM7		
Aitken	1.6	0.015–0.052
Accumulation	1.8	0.056–0.26
Primary Carbon	1.6	0.039–0.13
Fine Sea Salt	2.0	0.095–0.56
Fine Dust	1.8	0.14–0.62
Coarse Sea Salt	2.0	0.63–3.70
Coarse Dust	1.8	0.59–2.75

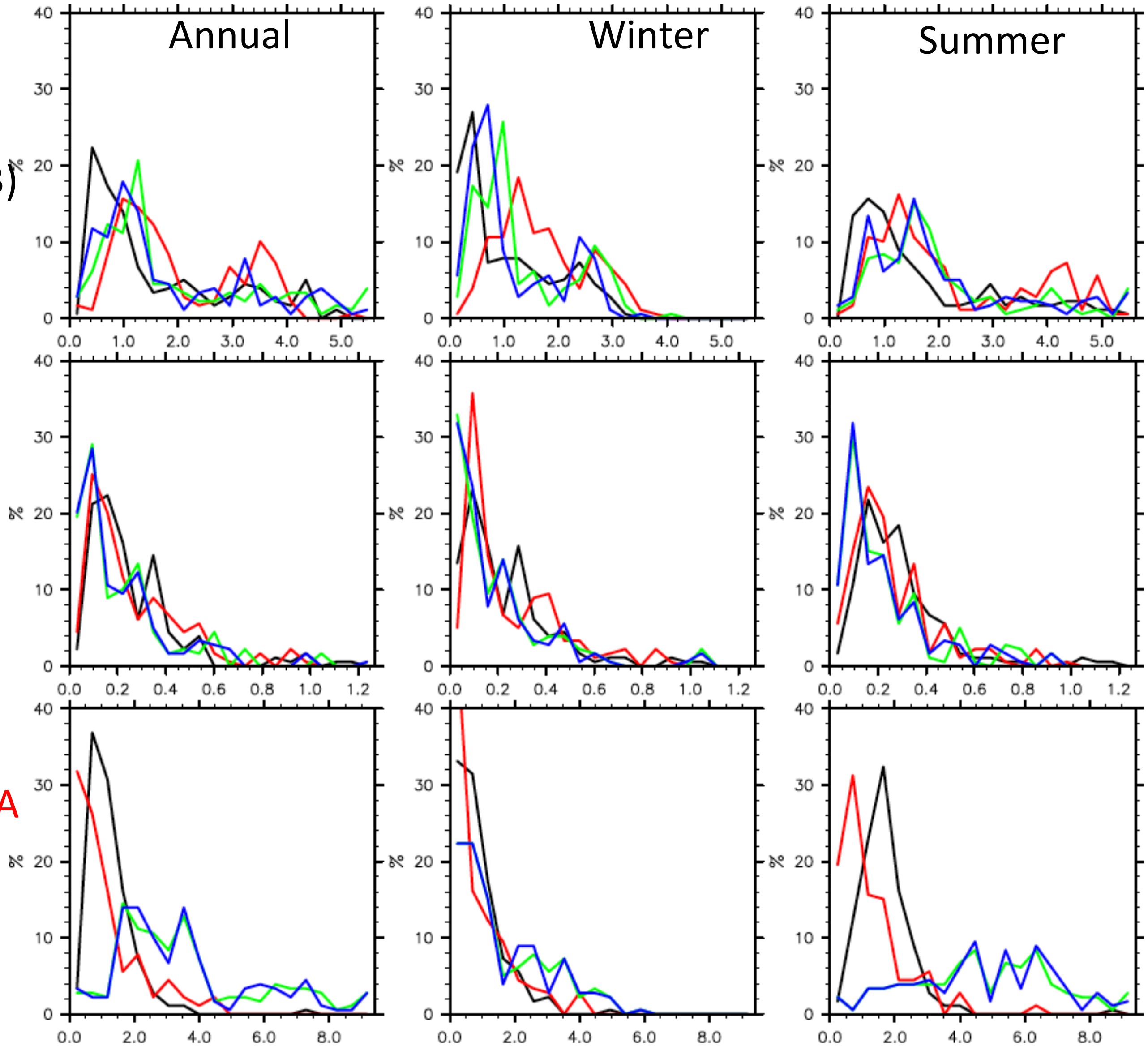
Liu et al., 2011

Differences in Aerosols, CAM4 and CAM5

Sulfate:
SO_4
SO_4 (a1,a2,a3)
SO_4 (a1,a2, a4-7)

BC:
CB1, CB2
BC (a1)
BC (a1, a3)

OC:
CB1, CB2, SOA
pom (a1, a3), soa (a1, a2)
pom (a1, a3), soa (a1, a2)



IMPROVE
CAM4-BAM
CAM5-MAM3
CAM5-MAM7

Surface layer concentration (mg/m^3)

Scientifically Validated Chemistry Versions

http://www.cesm.ucar.edu/models/scientifically-supported.html

Tilmes, S et al., 2015: Description and evaluation of tropospheric chemistry and aerosols in the Community Earth System Model (CESM1.2), Geosci. Model Dev., 8, 1395-1426, doi:10.5194/gmd-8-1395-2015, 2015. (http://www.geosci-model-dev.net/8/1395/2015/gmd-8-1395-2015.html)

CAM-CHEM SIMULATIONS

Brief Description	Case Details	Diagnostics				Length of Run Diagnostics	
FSTRATMAM3 **Case Name:** f2000.e122_mam4.STRATMAM3.f19.f19.003	Details	Atm	Ice	Land	Ocean	---	Ocean Timeseries
FSDSMAM **Case Name:** fmerra.e12_mam4.FSDSMAM.19.19.001	Details						
FSSOA **Case Name:** f2000.e122_mam4.C4SSOA_L40.f19.f19.so4	Details	Atm	Ice	Land	Ocean	---	Ocean Timeseries
FSDSSOA **Case Name:** fmerra.e12_mam4.FSDSSOA.19.19.so4	Details						
FSTRATMAM4 **Case Name:** f2000.e122_mam4.STRATMAM4.f19.f19.002	Details	Atm	Ice	Land	Ocean	---	Ocean Timeseries

Evaluation of the Model

AMWG Diagnostic Package includes Chemistry Evaluation

Chemistry Set Description
1 Tables / Chemistry of ANN global budgets
2 Vertical Contour Plots contour plots of DJF, MAM, JJA, SON and ANN zonal means
3 Ozone Climatology Comparisons Profiles, Seasonal Cycle and Taylor Diagram
4 Column O3 and CO lon/lat Comparisons to satellite data
5 Vertical Profile Profiles Comparisons to NOAA Aircraft observations
6 Vertical Profile Profiles Comparisons to Emmons Aircraft climatology
7 Surface observation Scatter Plot Comparisons to IMROVE

Evaluation of the Model

AMWG Diagnostic Package includes Chemistry Evaluation

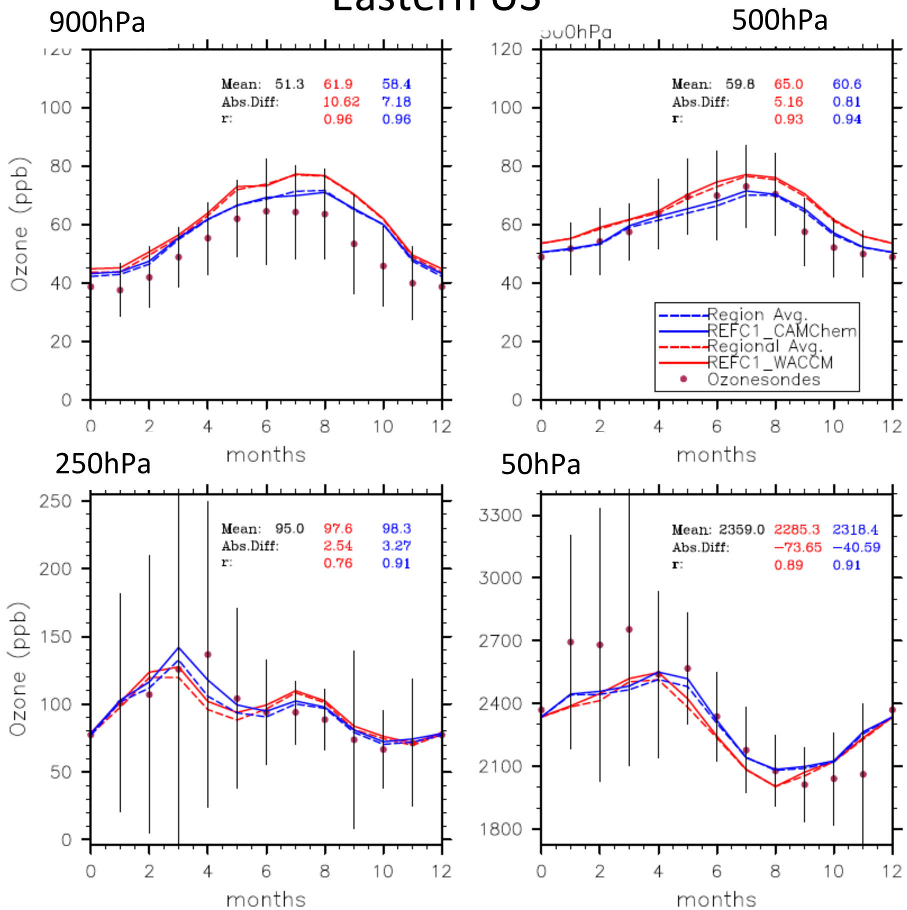
Variable	SD-CAM5-chem	CAM5-chem	SD-CAM5-chem-CAM5-chem
missing			
CH4_BURDEN (Tg)	4063.844	4102.330	-38.485
CH4_EMIS (Tg/yr)	0.000	0.000	0.000
CH4_TDEP (Tg/yr)	0.000	0.000	0.000
CH4_CHEM_LOSS (Tg/yr)	519.159	497.392	21.767
CH4_LIFETIME (yr)	7.828	8.248	-0.420
CH3CCL3_BURDEN (Tg)	1.067	1.083	-0.016
CH3CCL3_EMIS (Tg/yr)	0.000	0.000	0.000
CH3CCL3_TDEP (Tg/yr)	0.000	0.000	0.000
CH3CCL3_CHEM_LOSS (Tg/yr)	0.231	0.000	0.231
CH3CCL3_LIFETIME (yr)	4.626	0.000	4.626
CO_BURDEN (Tg)	282.893	288.537	-5.644
CO_EMIS (Tg/yr)	1053.287	1053.329	-0.042
CO_TDEP (Tg/yr)	127.022	0.000	127.022
CO_CHEM_LOSS (Tg/yr)	2234.106	2176.794	57.312
CO_LIFETIME (yr)	0.120	0.133	-0.013
O3_BURDEN (Tg)	313.246	313.950	-0.705
O3_EMIS (Tg/yr)	0.000	0.000	0.000
O3_TDEP (Tg/yr)	842.397	893.748	-51.351
O3_CHEM_LOSS (Tg/yr)	4156.022	4032.642	123.380
O3_LIFETIME (yr)	0.063	0.064	-0.001
O3_CHEM Prod (Tg/yr)	4715.190	4586.144	129.046
O3_NET_CHEM_CHANGE (Tg/yr)	479.835	499.257	-19.421
O3_STE (Tg/yr)	362.562	394.491	-31.930
O3 Strat BURDEN (Tg/yr)	2807.742	2854.809	-47.067
ISOP_EMIS (Tg/yr)	524.502	524.493	0.009
Monoterpene_EMIS (Tg/yr)	97.098	97.096	0.001
Methanol_EMIS (Tg/yr)	169.857	169.857	0.000
Aceton_EMIS (Tg/yr)	32.076	32.076	0.000
LNO_PROD (TgN/yr)	4.315	4.832	-0.000
Total optical depth	0.153	0.143	0.517
DUST optical depth	0.000	0.037	-0.010

CCMI Simulations in Comparison to Ozonesonde Data: Mid-Latitudes, 500hPa

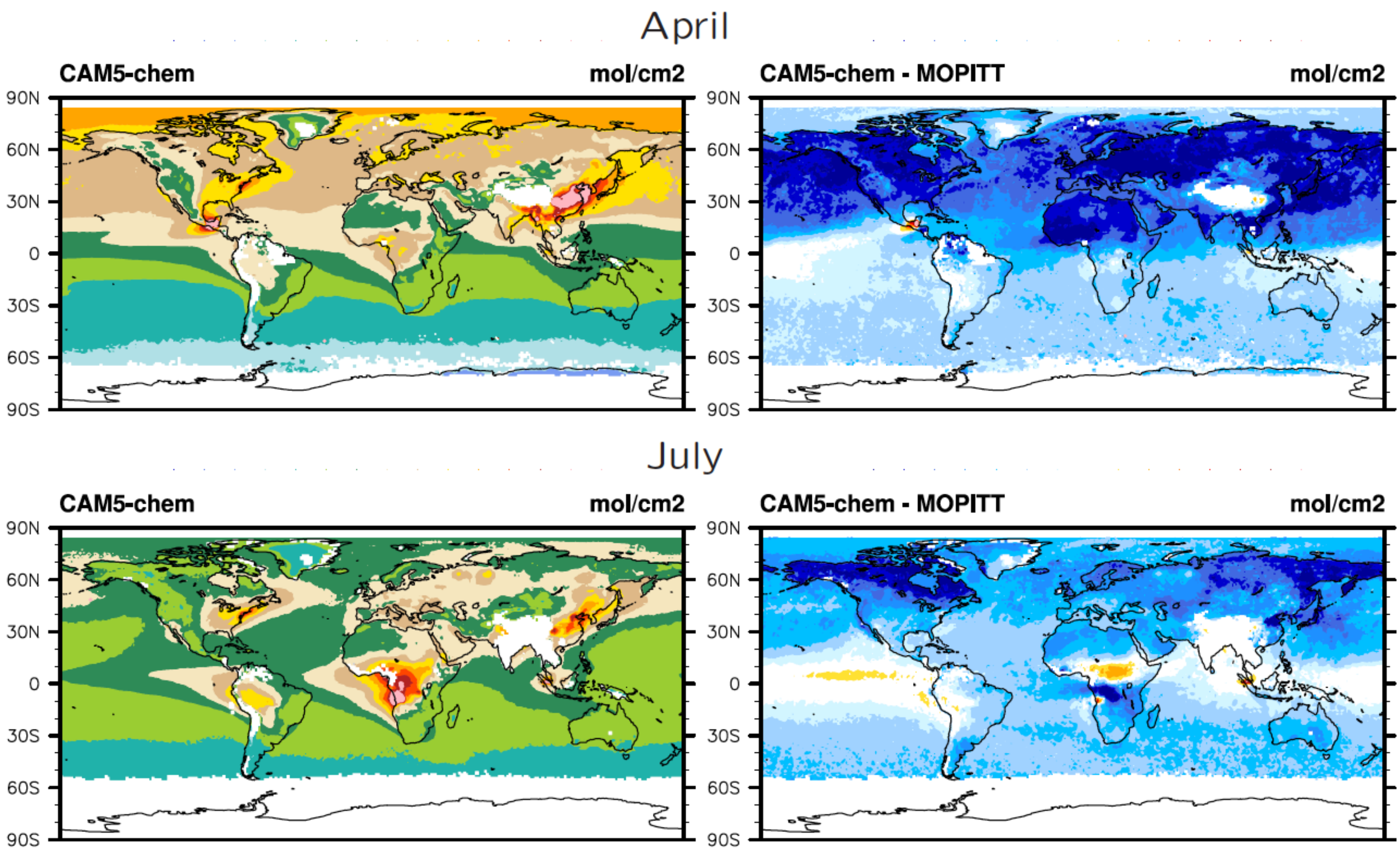
WACCM REFC1
CAM-Chem REFC1

1995-2004 average

Eastern US



Performance of the Models: Carbon Monoxide in Comparison to MOPITT



Changing Chemistry

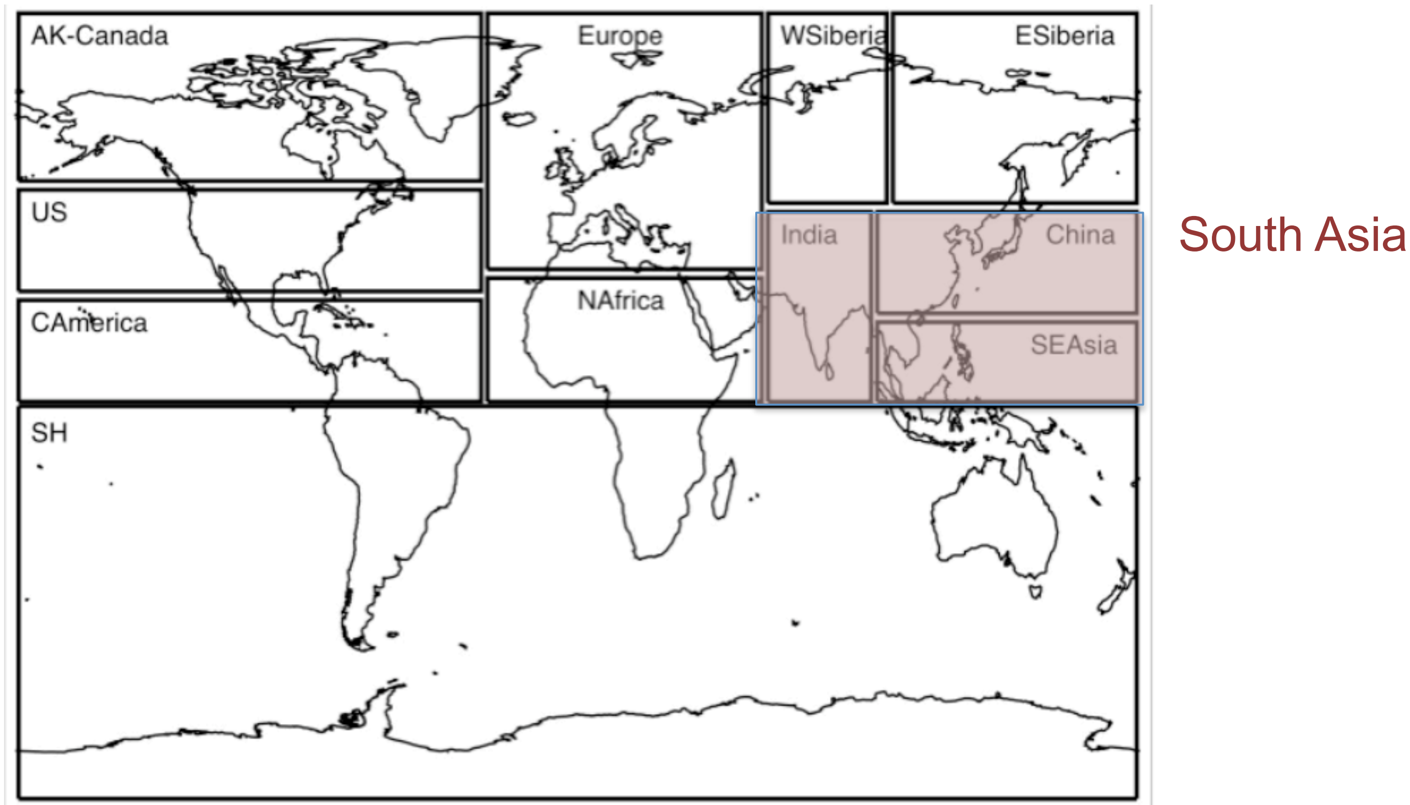
Chemical Mechanism: add or change tracers and reactions (e.g. Tagging of tracers)
Emissions: include required emissions
Deposition: add dry and wet deposition components to the model code

Running with MEGAN Emissions:
http://www.cesm.ucar.edu/working_groups/Chemistry/running_CESM1_MEGANNv0408.pdf

Roadmap to run and change chemistry (CESM 1.2.0)
http://www.cesm.ucar.edu/working_groups/Chemistry/roadmap_cesm120.pdf

O_3, CO, BC tags with Offline Meteorology

Emmons et al., 2012, GMD



The Model for Ozone and Related chemical Tracers (MOZART4)

Emissions: Streets ARCTAS emissions + daily fires (C. Wiedinmyer)

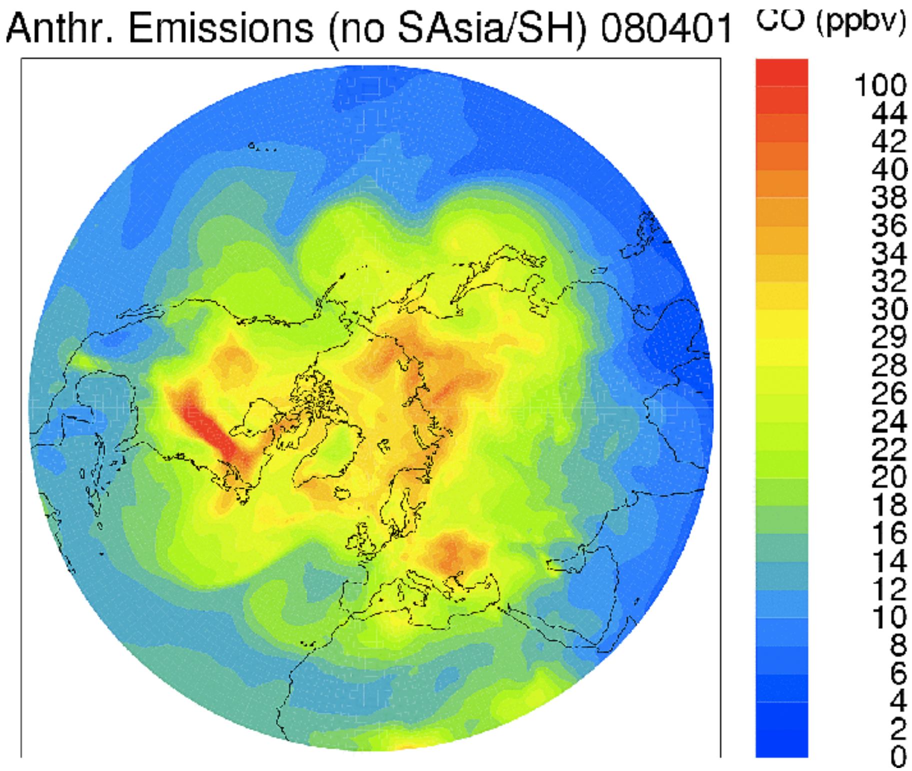
Vertical Injection of Fire Emission between 0-6 km

Importance of Anthropogenic CO Emissions

April

without South Asia and SH

South Asia and SH only



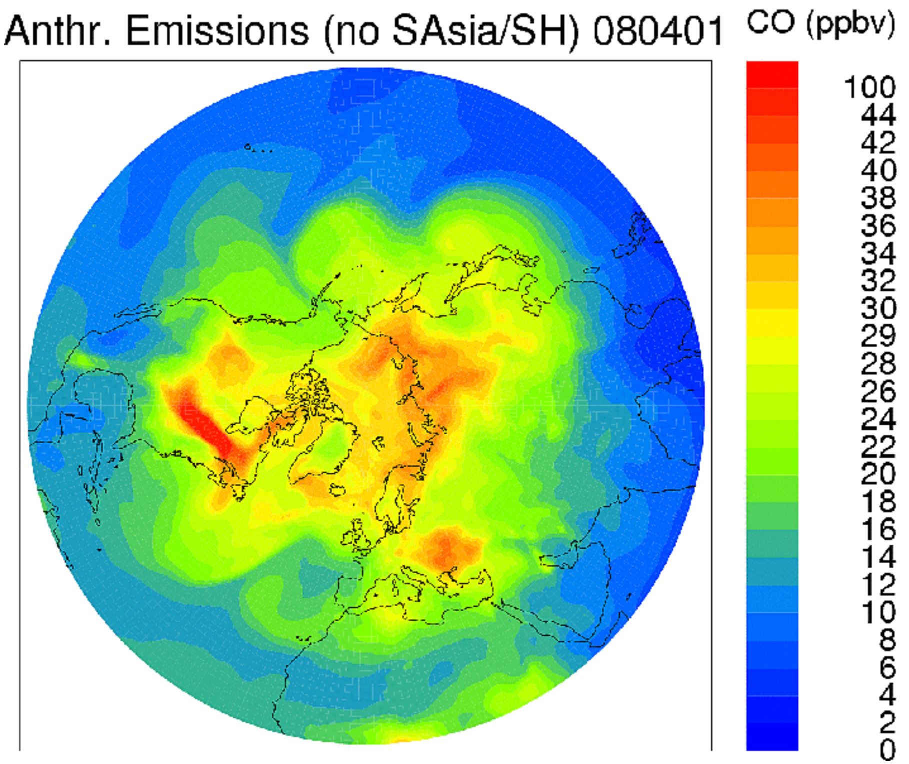
CO averaged column between surf. and 200 hPa

Importance of Anthropogenic CO Emissions

April

without South Asia and SH

South Asia and SH only

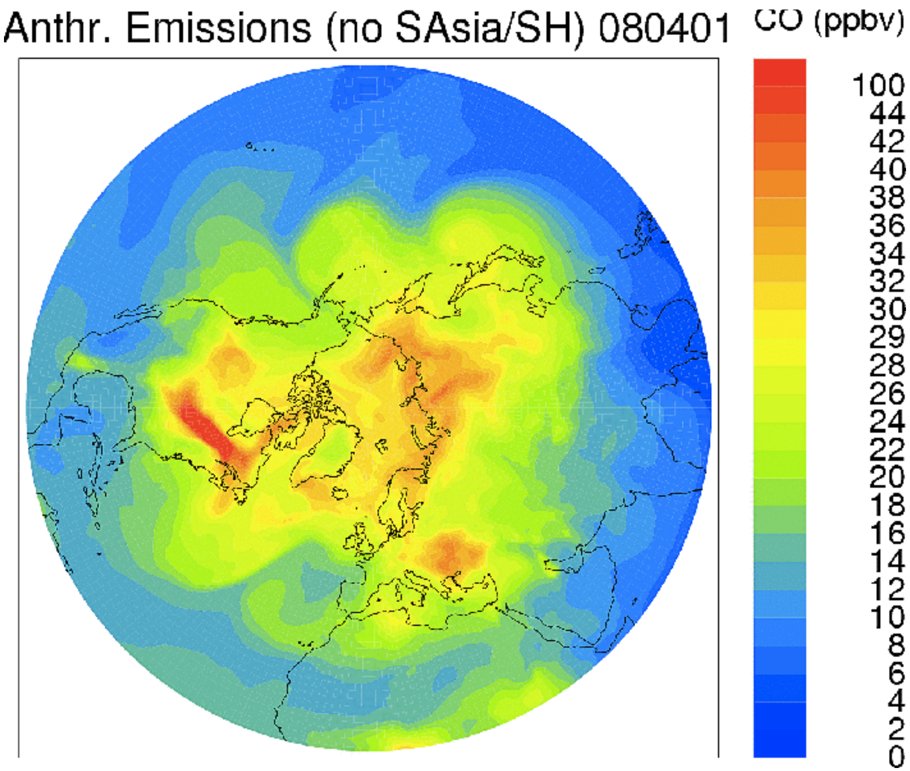


CO averaged column between surf. and 200 hPa

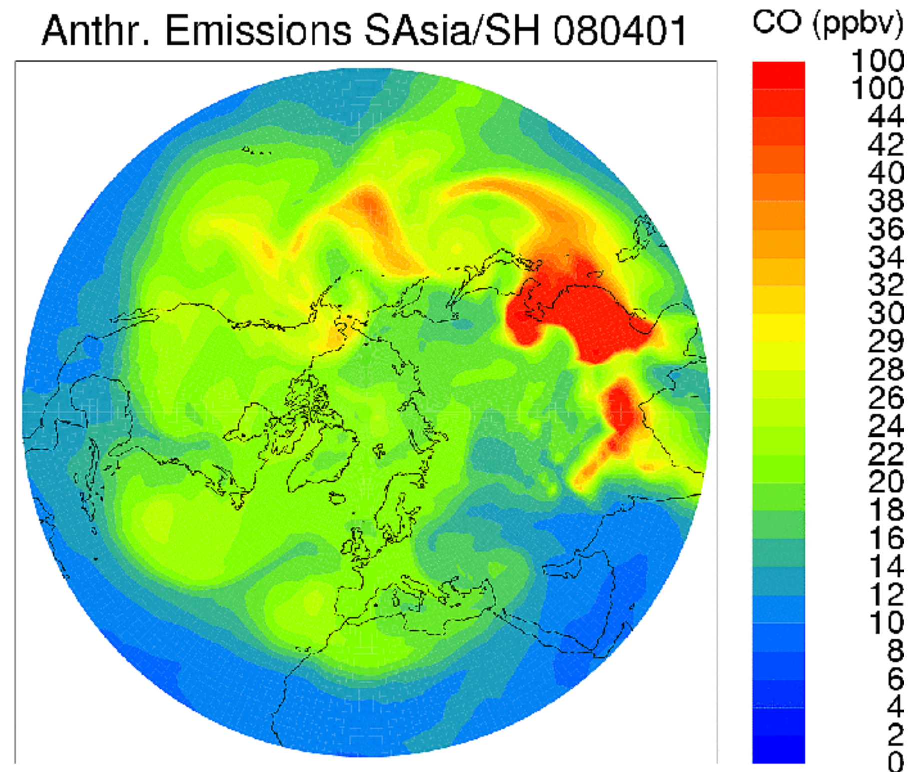
Importance of Anthropogenic CO Emissions

April

without South Asia and SH



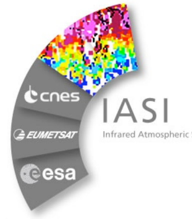
South Asia and SH only



CO averaged column between surf. and 200 hPa

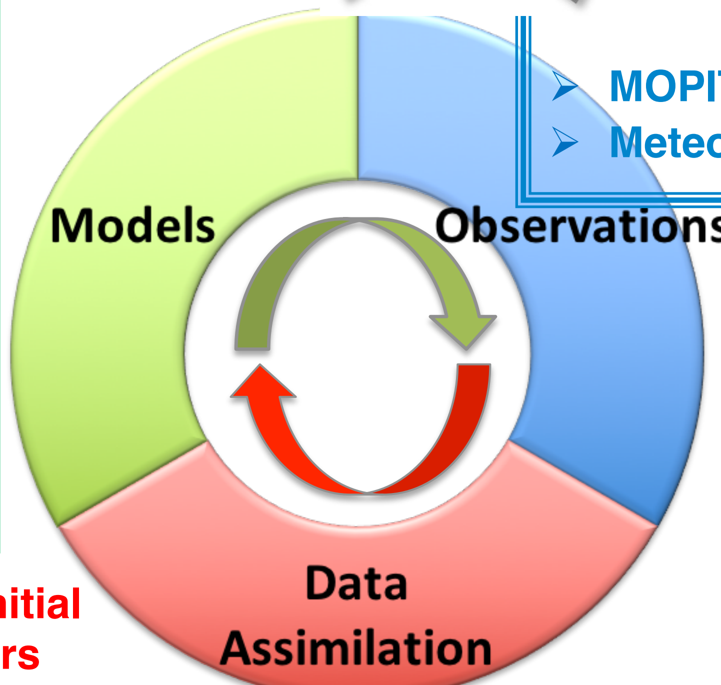
CESM
Community Atmosphere Model (CAM and CAM-Chem)
Ensemble of atmospheric state with chemistry

- Ensemble of emissions (+CO tags)
- Ensemble of transport
- Ensemble of deposition (land model)
- Ensemble of Chemistry



Observations

- MOPITT-CO, IASI-CO, MODIS AOD
- Meteorological observations



Observations, plus errors

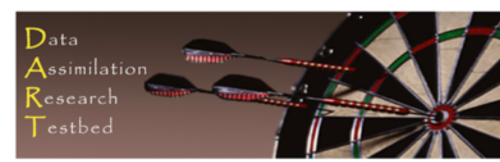
Ensemble of optimized initial conditions every 6 hours

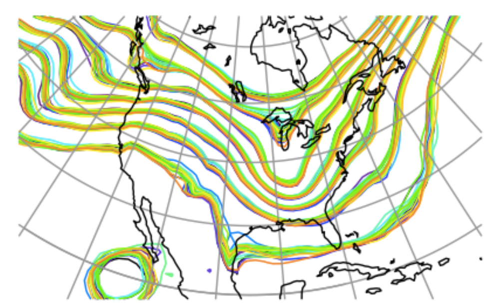
DART

Assimilation

-> update CO concentration
And Meteorology

Weighted mean of observations and model knowing respective errors





NESL

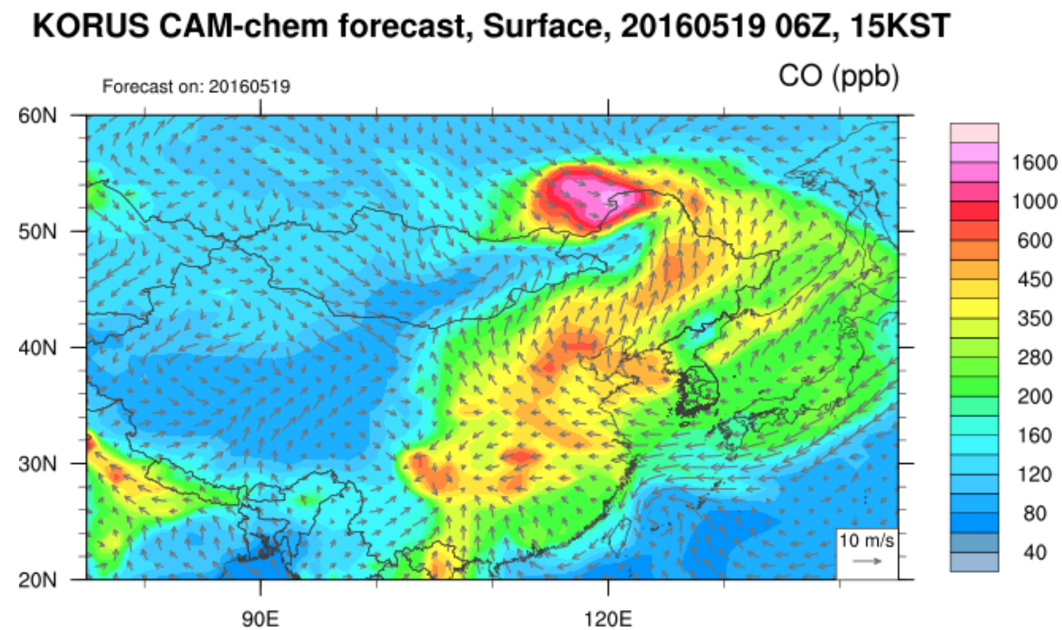
CAM-chem forecasting

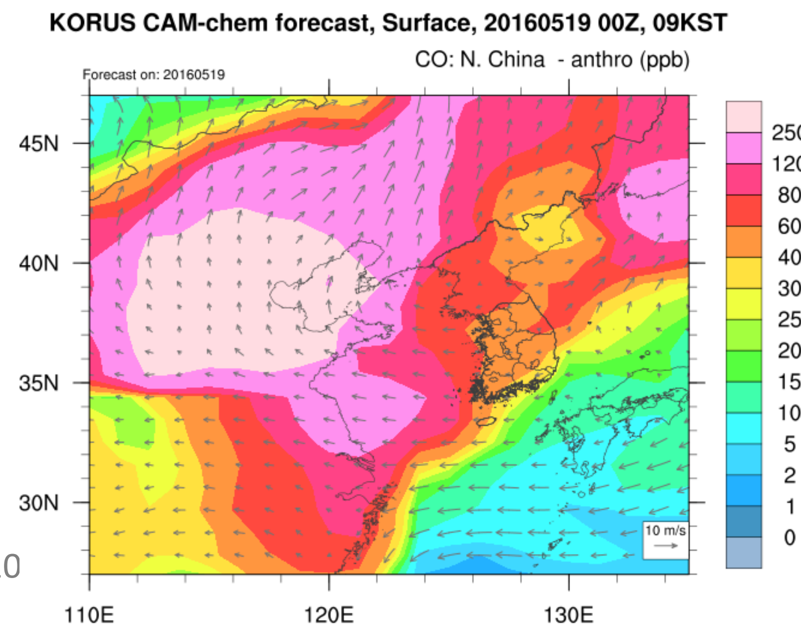
For the NASA KORUS-AQ experiment, CAM-chem/DART forecasts were run

MOPITT CO retrievals were assimilated each day (30-member ensemble)

GEOS-5 meteorology was used to drive a single CAM-chem forecast simulation

Tagged CO tracers were included to track source contributions to Korea





http://www.acom.ucar.edu/acresp/korus-aq/

WACCM and CAM-Chem Customer Support

CGD Forum: http://bb.cgd.ucar.edu/

Mike Mills
WACCM Liaison
mmills@ucar.edu
(303) 497-1425

Simone Tilmes
CAM-Chem Liaison
tilmes@ucar.edu
(303) 497-1445