Modeling and tagging CO and CO_2 in CAM-chem: A case study during the KORUS-AQ campaign

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Motivation

Modeling CO_2 and CO in CAM-chem

Tagging CO_2 and CO in CAM-chem

In-situ measurements of co-emitted species are useful to study the sources of pollution and combustion efficiency

China 2015

Derived CO/CO_2 ratios from field campaigns and ground sites

Location	CO/CO_2 (ppbv/ppmv)	Reference
Pasadena, CA (2008)	11	Wunch et al., 2009
China (TRACE-P; 2001)	50-100	Suntharalingam et al., 2004
Japan (TRACE-P; 2001)	12-17	Suntharalingam et al., 2004
SoCAB, CA (2010)	14	Brioude et al., 2013
near Beijing (2008)	22	Wang et al., 2010
near Beijing (2005)	34-42	Wang et al., 2010
Tae-Ahn Peninsula (2009/2010)	13	Turnbull et al., 2011
Seoul (2010)	9	Turnbull et al., 2011

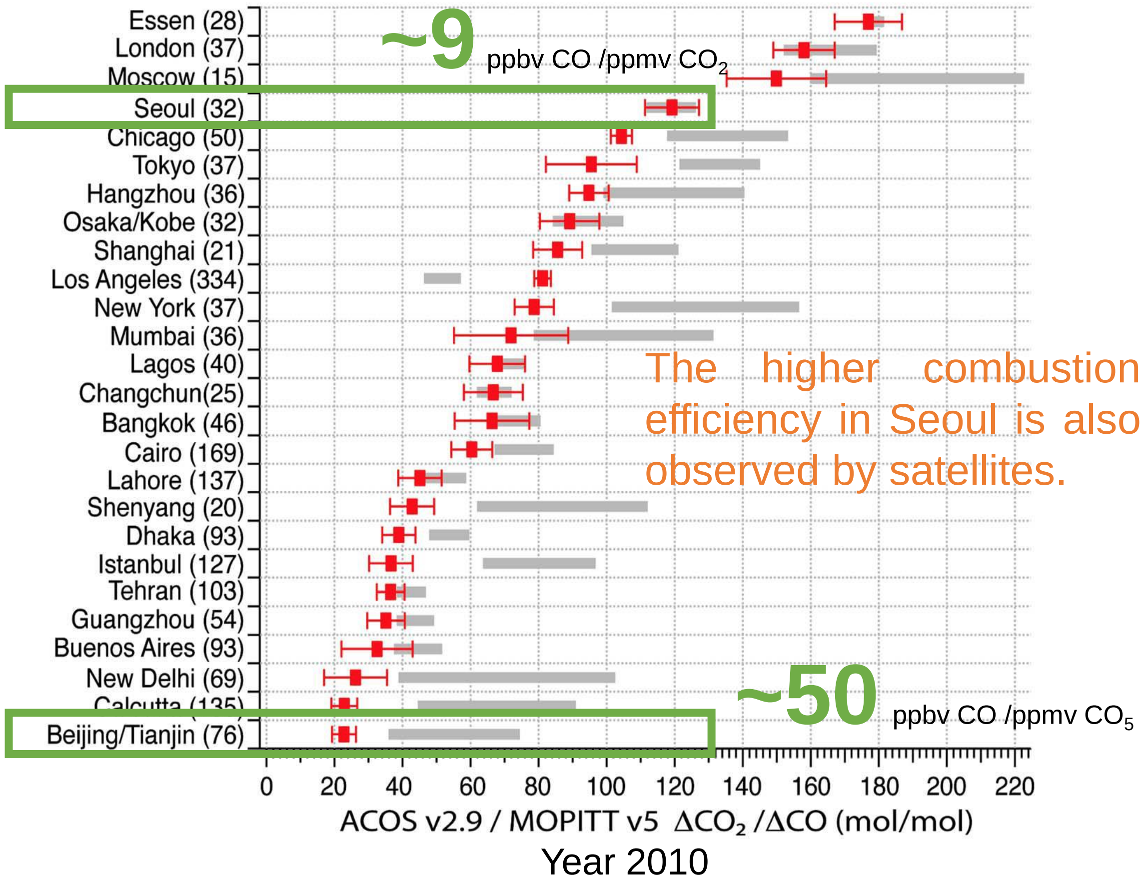
These measurements show that air samples observed from Seoul are more efficient (lower CO/CO_2 ratio) than air from Beijing.

Satellite measurements of co-emitted species are also useful to study the sources of pollution

Geophysical Research Letters

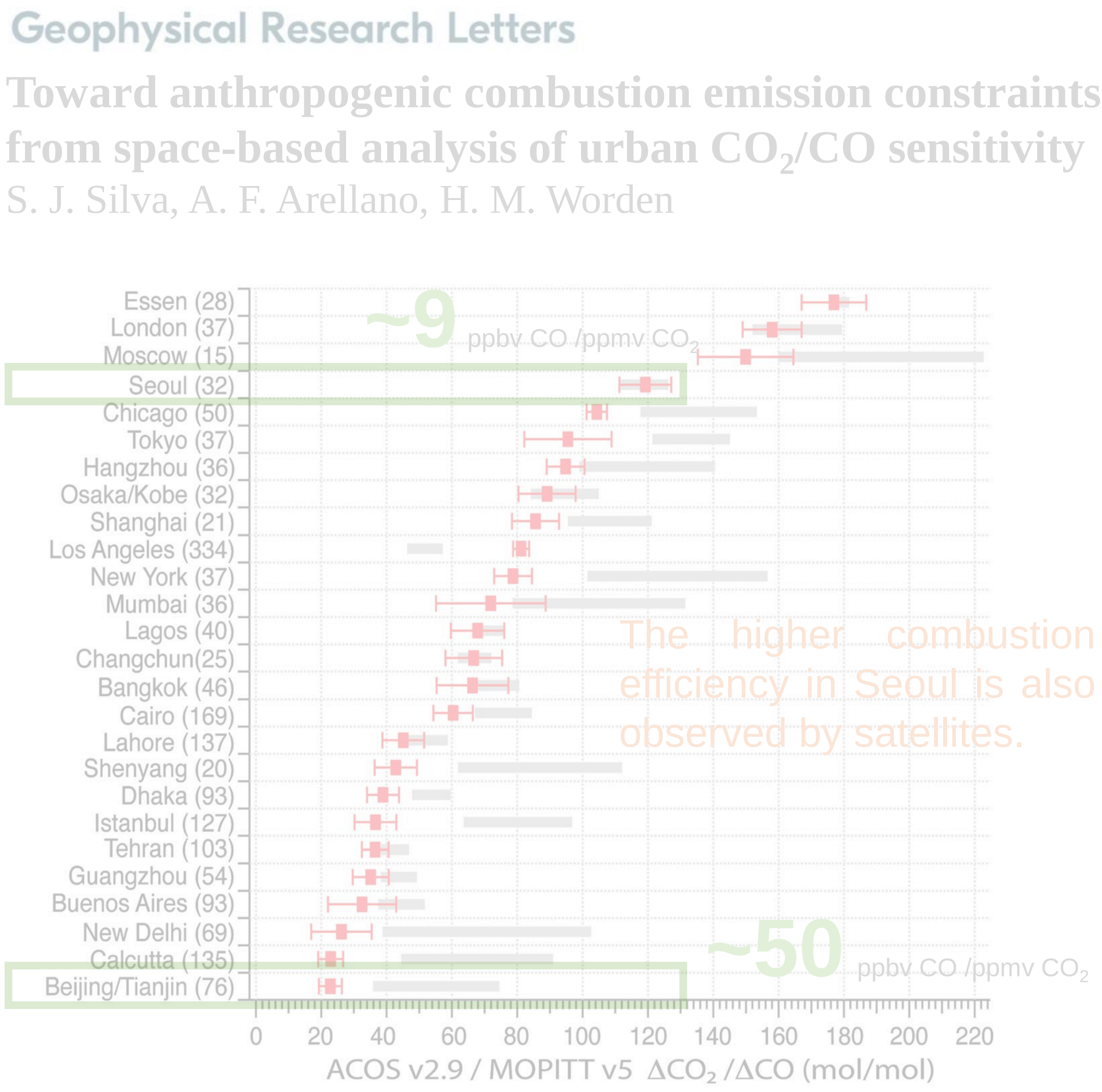
Toward anthropogenic combustion emission constraints from space-based analysis of urban CO_2/CO sensitivity

S. J. Silva, A. F. Arellano, H. M. Worden



The higher combustion efficiency in Seoul is also observed by satellites.

Satellite measurements of co-emitted species are also useful to study the sources of pollution



Unprecedented spatial, temporal and spectral resolution from new generation of satellite instruments (e.g., TROPOMI, GOSAT2, and TEMPO)

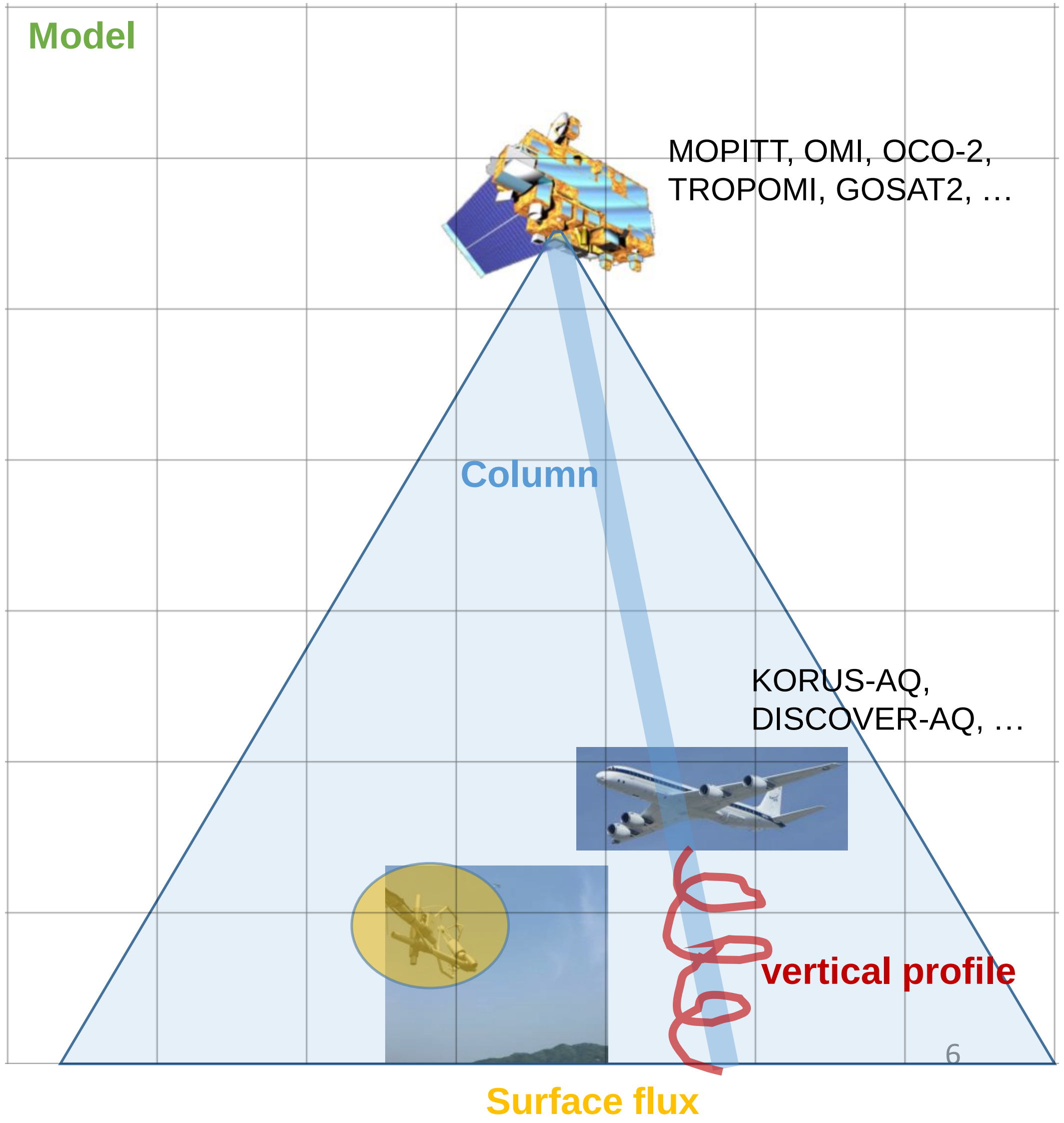
➢Allows us to **simultaneously retrieved greenhouse gases and air pollutants** at various spatial and temporal scales

➢Points to the need to understand the relationship between surface fluxes and column measurements through **a unique modeling system combining comprehensive chemistry, greenhouse gases, and aerosols**

Research Opportunities and Needs

- Goal 1: Develop a **modeling system** that simulates tropospheric chemistry (e.g., CO, NO_2, O_3) and greenhouse gases (e.g. CO_2, CH_4) simultaneously.

- Goal 2: Assess the relationship between **surface flux**, **vertical profile** and the resulting **column**, by using the model, as well as surface, aircraft, and satellite measurements.



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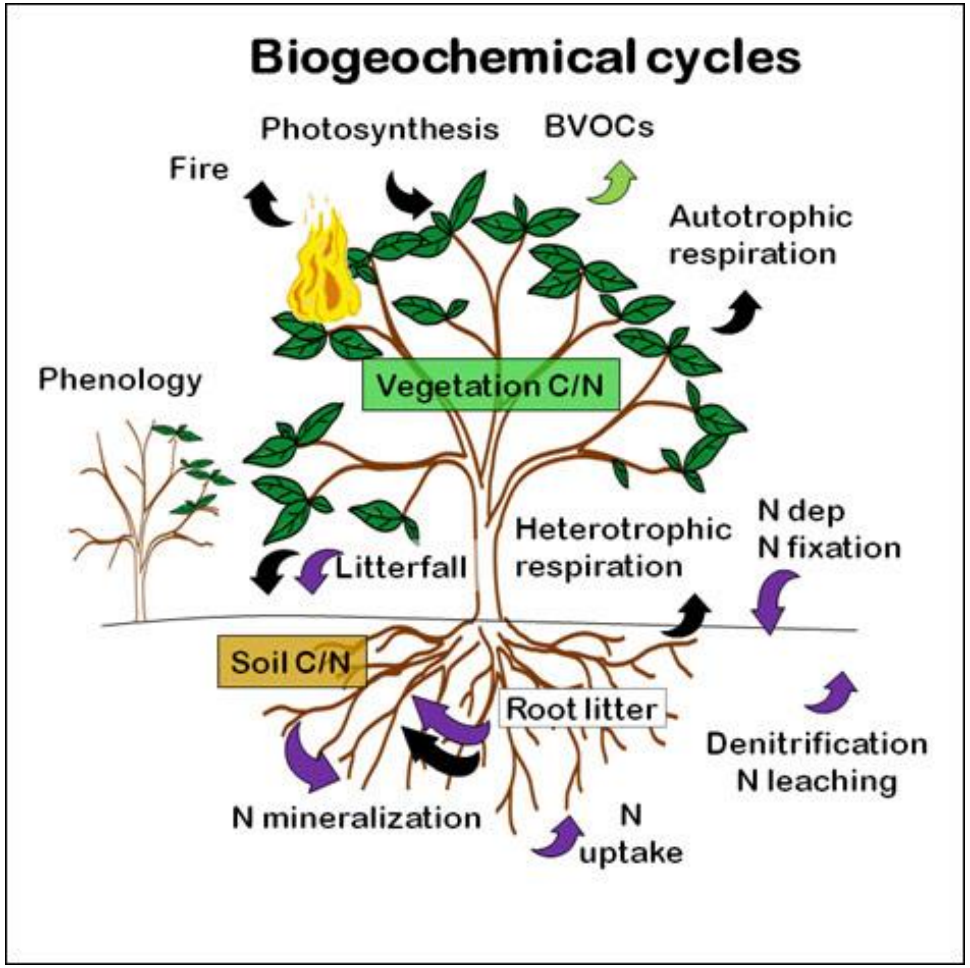
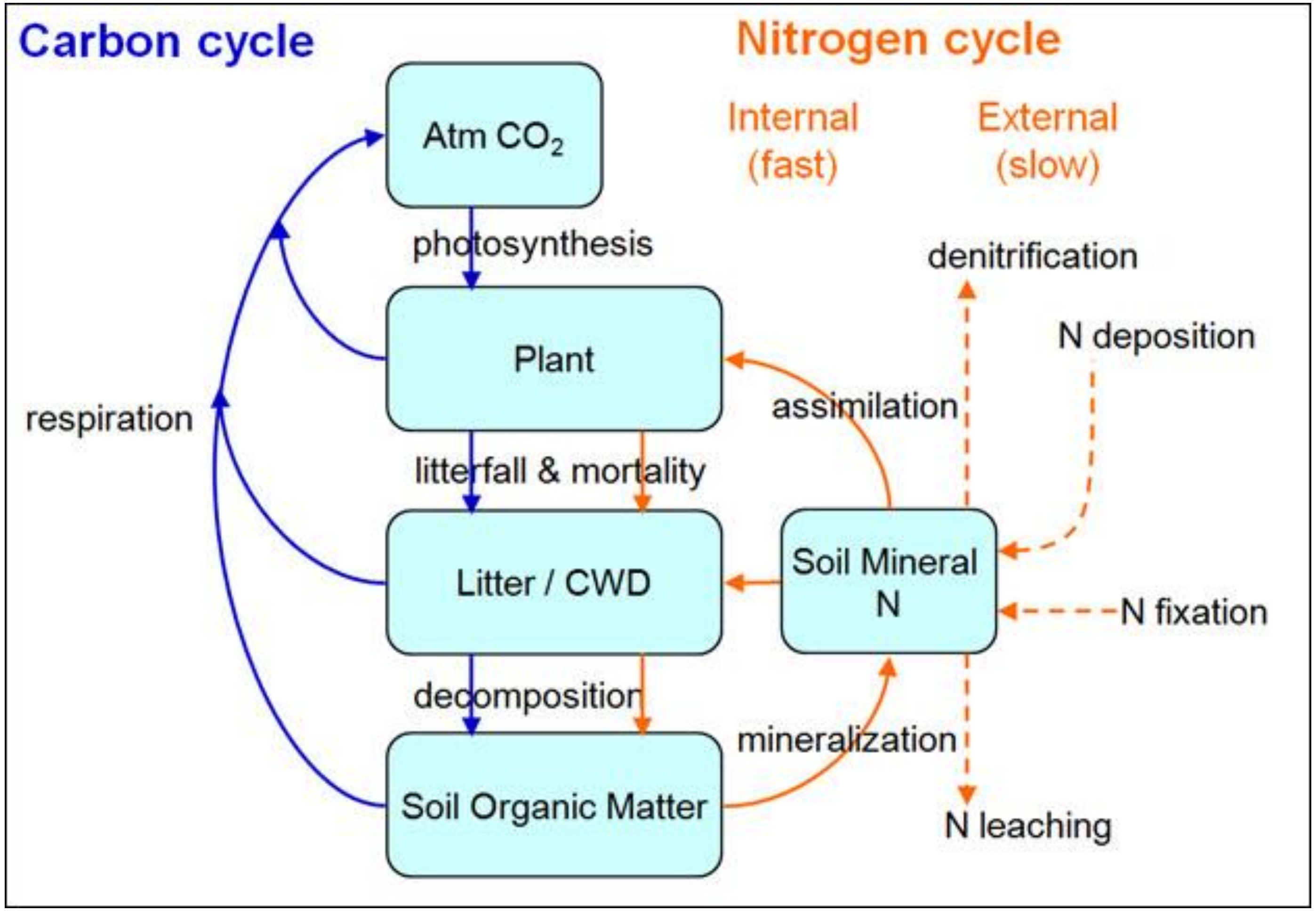
Existing biogeochemistry version in CESM





http://www.cesm.ucar.edu/models/clm/biogeochemistry.html

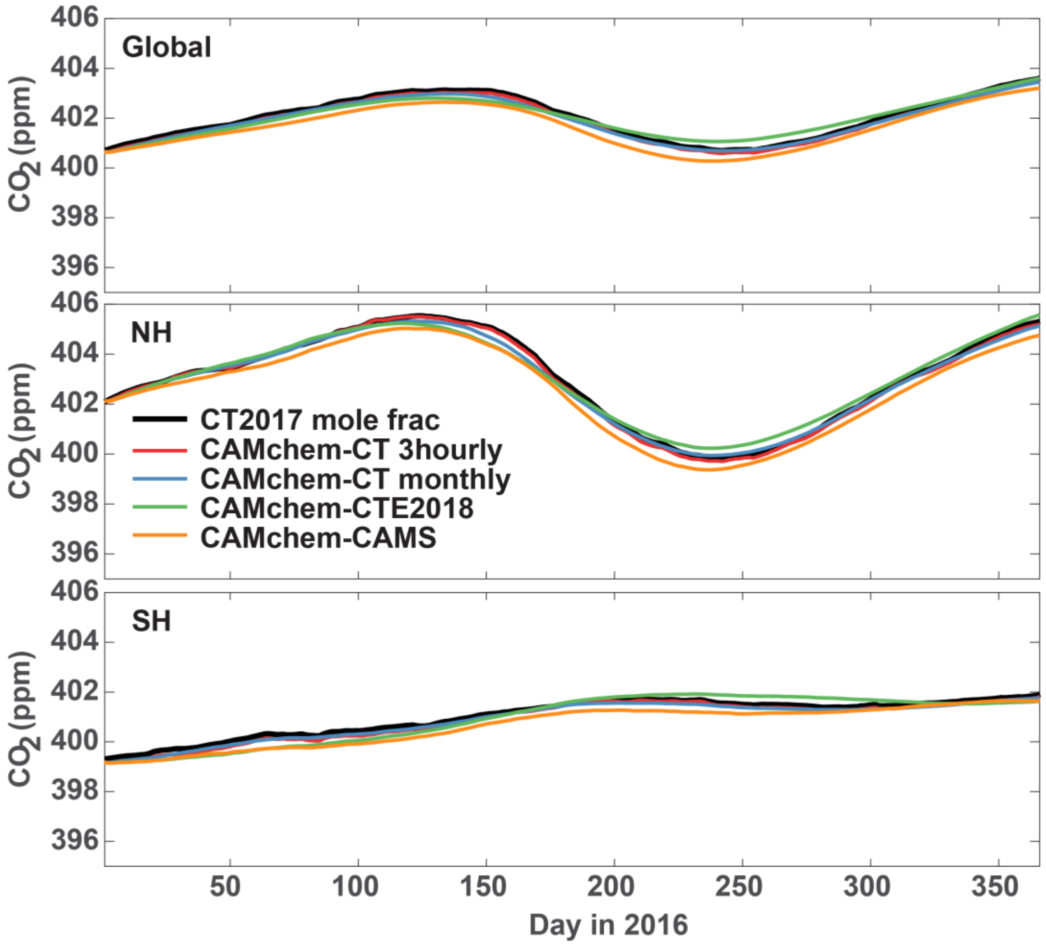
Modeling CO_2 in CAM-chem using optimized CO_2 fluxes

Optimized CO_2 fluxes we used in CAM-chem (CESM2)

CO_2 fluxes	Spatial Resolution	Temporal resolution	Available period	Transport model	Fossil Fuel Priors	Biosphere and Fires Priors	Ocean Priors	Reference
CAMS (v17r1)	3.75x1.875	3-hourly	1979-2017	Laboratoire de Météorologie Dynamique with “z” standing for zoom capacity	EDGAR scaled to CDIAC	ORCHIDEE (climatology) + GFEDv4	Landschüster et al. (2014)	Chevallier et al. (2018)
CT2017	1x1	3-hourly & monthly	2000-2017	TM5 model	“Miller" (EDGAR scaled to CDIAC) and "ODIAC"	Carnegie-Ames Stanford Approach (CASA) biogeochemical model, with GFED 4.1s and GFED_CMS	Jacobson et al. (2007) and Takahashi et al. (2009)	Peters et al. (2007)
CTE2018	1x1	monthly	2000-2016	TM5 model	EDGAR+IER, scaled to CDIAC	SiBCASA-GFED4	Jacobson et al. (2007)	van der Laan-Luijkx et al. (2017)

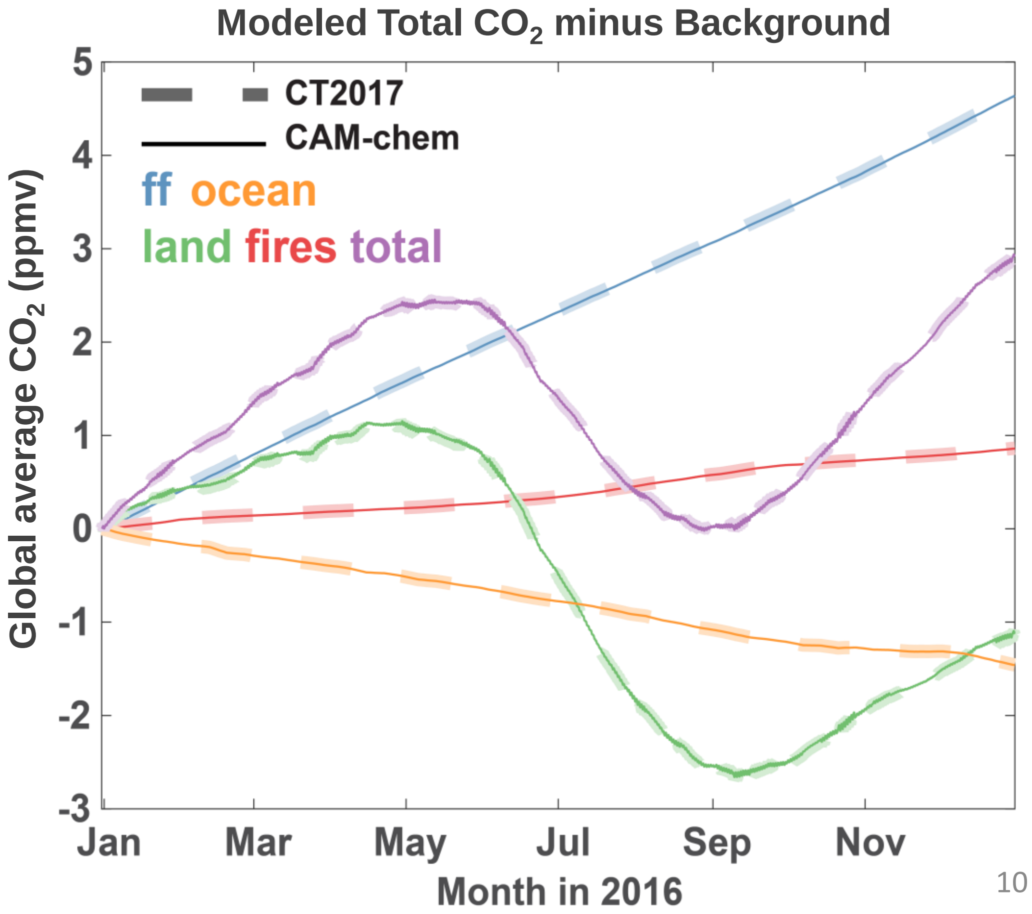
CT2017 and CTE2018 provides CO_2 fluxes as components: **fossil fuel emissions**, **land biosphere NEE excluding fires**, **wildfire emissions**, and **air-sea exchange**.

CO_2 global budget from CAM-chem



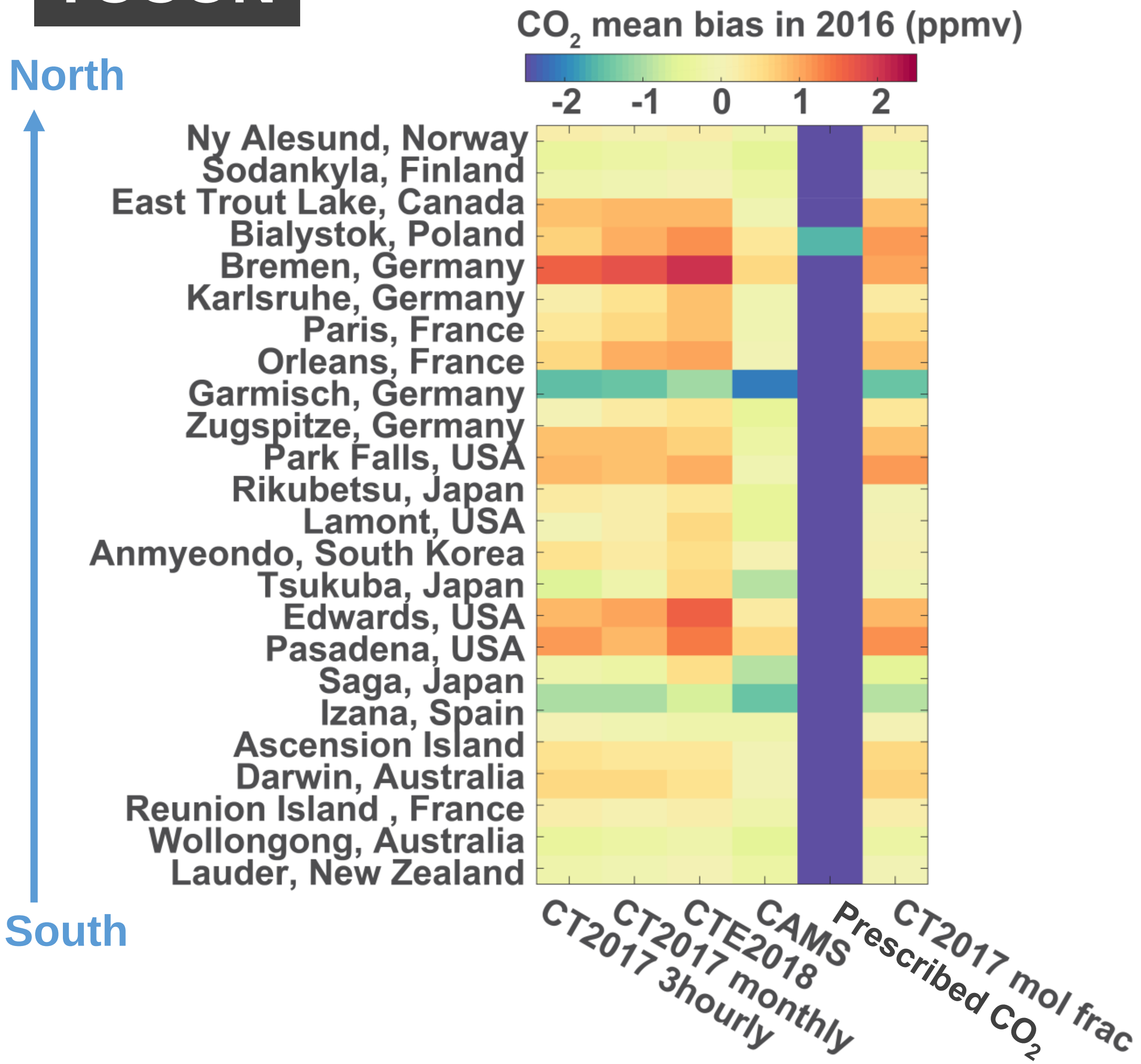
CAM-chem simulations of total CO_2 using different fluxes overall agree with CT2017 CO_2 mole fraction fields.

CAM-chem simulation of CO_2 using CT2017 fluxes agree well with CT2017 CO_2 mole fraction fields in terms of components.

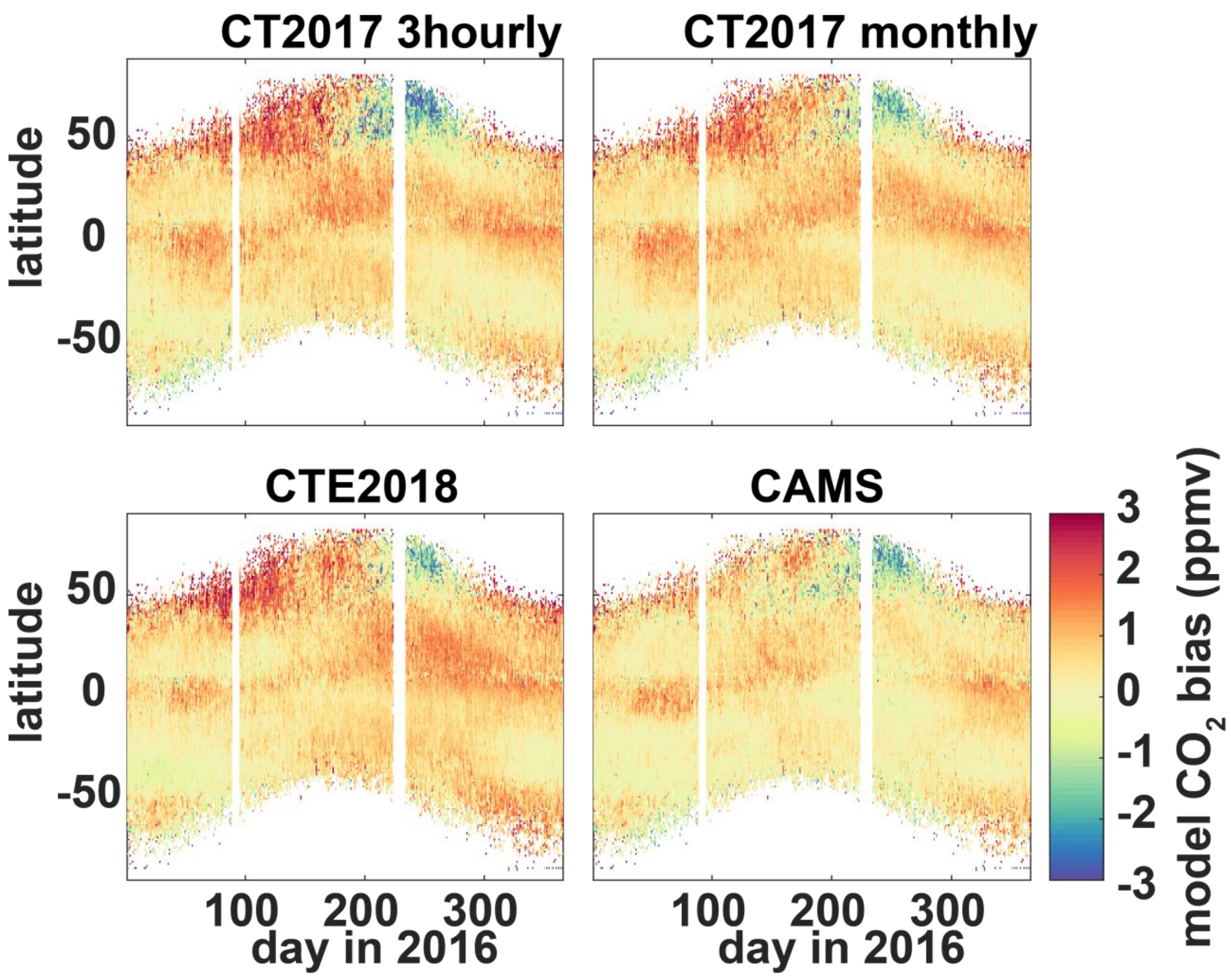


CAM-chem simulated CO_2 generally agrees with Observations

TCCON



OCO-2 v8 Lite



Motivation

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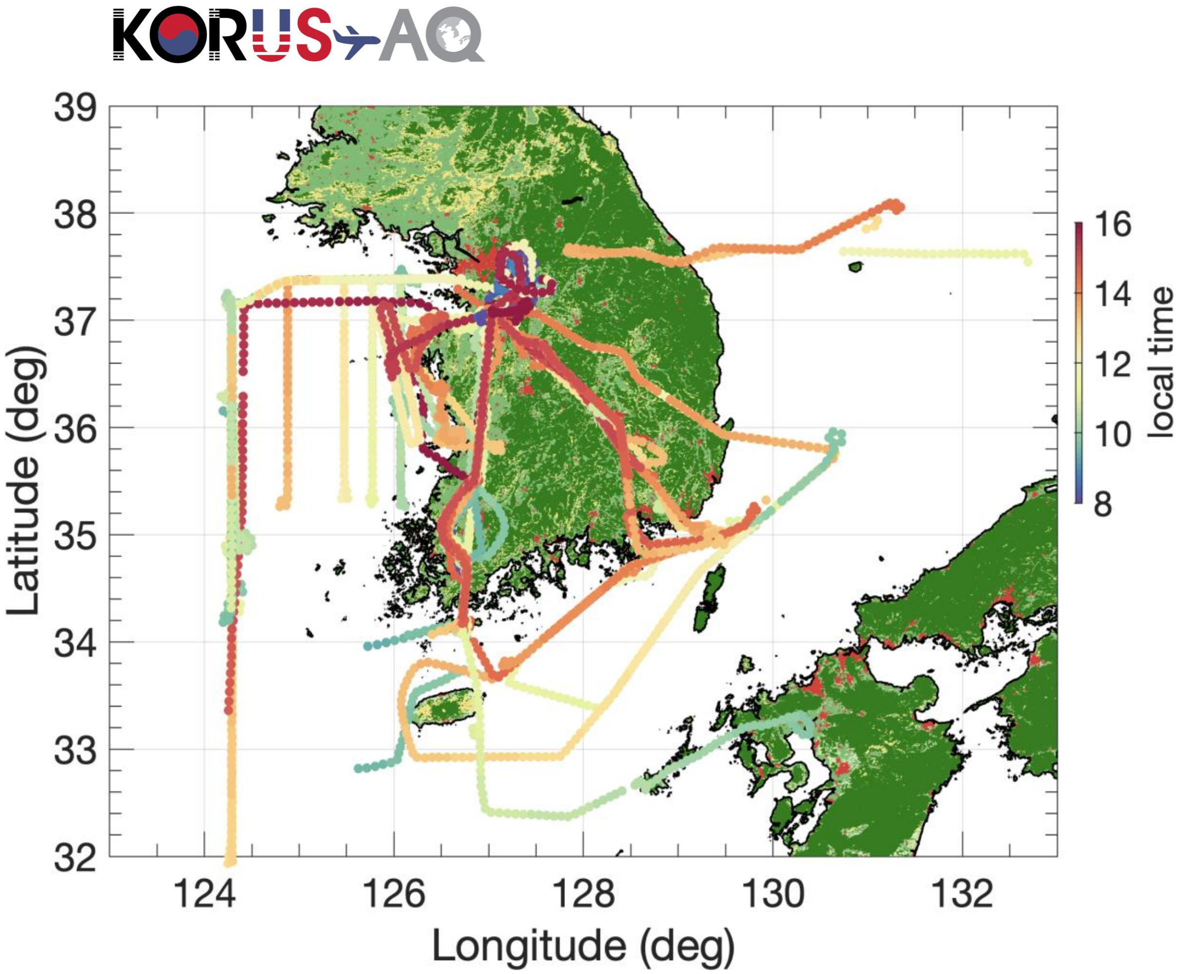
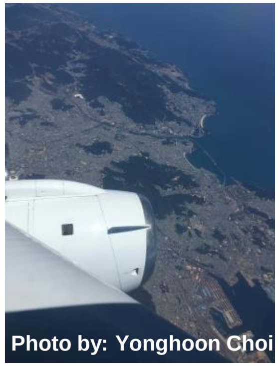
KORUS-AQ Campaign

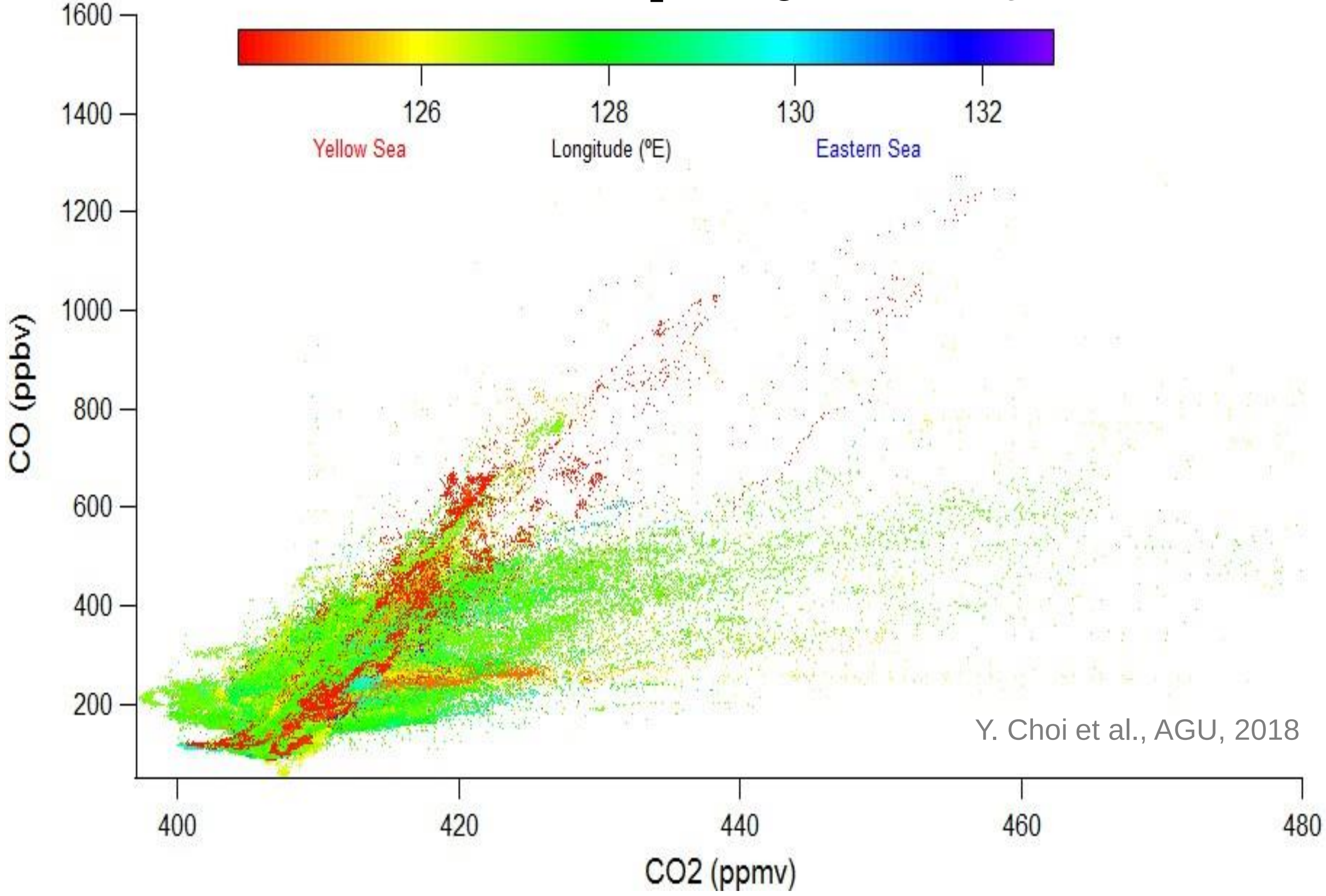




KORUS-AQ was conducted over South Korea and its surrounding waters from May to June 2016. During the campaign, observations from **aircrafts**, **ships**, **ground sites**, and **satellites** were integrated with **models** to help understand **air quality** and factors controlling air quality in the region.

Why is CO_2 and CO tagging needed?

Observed total CO vs CO_2 during KORUS-AQ



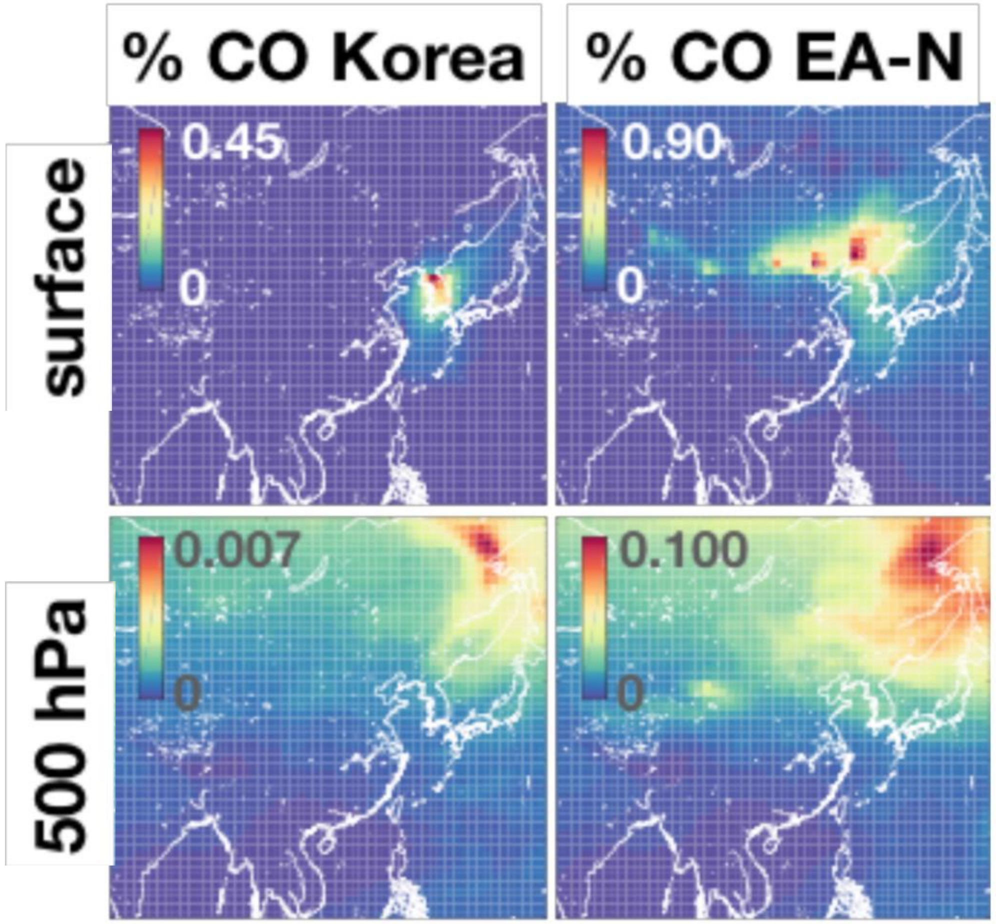
Y. Choi et al., AGU, 2018

When dividing the observations by longitude, differences in CO-CO_2 relationships pops up indicating different sources.

CO tagging capability in CAM-chem

What's tagged CO tracers?

Each of these CO tracers are treated in the model in the same way as the default CO, but only taking into account specific emissions from a particular region or sector or chemical production. The change in the tracer abundance however does not affect the interactive chemistry in the model.



CO tags in CAM-chem have been used previously to study sources of pollution.

Tang et al., 2019, JGR

Adding CO_2 tagging in CAM-chem

We add tags for fossil fuel CO_2 emissions in CAM-chem.

How a tag CO_2 is calculated in CAM-chem:

$$\frac{\mathbf{dCO_2}^{\mathbf{itag}}}{\mathbf{dt}} = \mathbf{Source}^{\mathbf{itag}} - \mathbf{Sink}^{\mathbf{itag}} + \mathbf{Transport}^{\mathbf{itag}} + \mathbf{Chemical\ Production}^{\mathbf{itag}}$$

Source: Fossil fuel emissions from a **region of interest** (e.g., China)

Sink: Negative fluxes over Biosphere or Ocean **across the globe**

Chemical Production: Chemical production emissions of CO, CH_4 …from the **region of interest** (e.g., China)

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How a tag CO_2 is calculated in CAM-chem:

	Provided	Not provided	Calculated online	Calculated online
$\frac{dCO_2^{itag}}{dt} =$	$\mathbf{Source}^{itag}$	$- \ \mathbf{Sink}^{itag}$	$+ \ \mathbf{Transport}^{itag}$	$+ \ \mathbf{Chemical\ Production}^{itag}$
	Fossil fuel emissions from a **region of interest** (e.g., China)	Negative fluxes over Biosphere or Ocean **across the globe**		Chemical production emissions of CO, CH_4 …from the **region of interest** (e.g., China)

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	Fossil fuel emissions from a **region of interest** (e.g., China)	Negative fluxes over Biosphere or Ocean **across the globe**		Chemical production emissions of CO, CH_4 …from the **region of interest** (e.g., China)

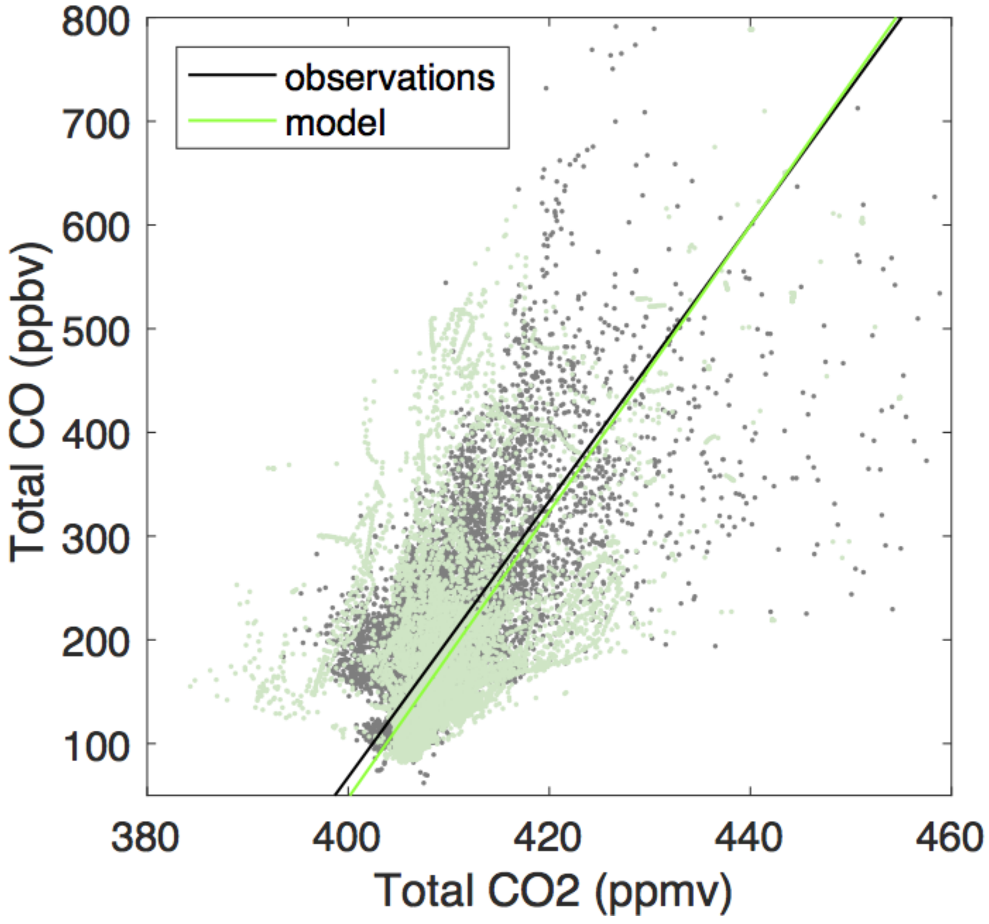
The deposition flux for the tag (itag) by ocean/biosphere at the grid (ilat, ilon) and at the time step (itime) is calculated online by:

$$\mathbf{Sink\ flux}_{\mathbf{ilat,ilon,itime}}^{\mathbf{itag}} = \mathbf{Flux}_{\mathbf{ilat,ilon,itime}}^{\mathbf{total\ CO2}} \times \frac{[\mathbf{CO2}_{\mathbf{surface}}]_{\mathbf{ilat,ilon,itime}}^{\mathbf{itag}}}{[\mathbf{CO2}_{\mathbf{surface}}]_{\mathbf{ilat,ilon,itime}}^{\mathbf{total}}}$$

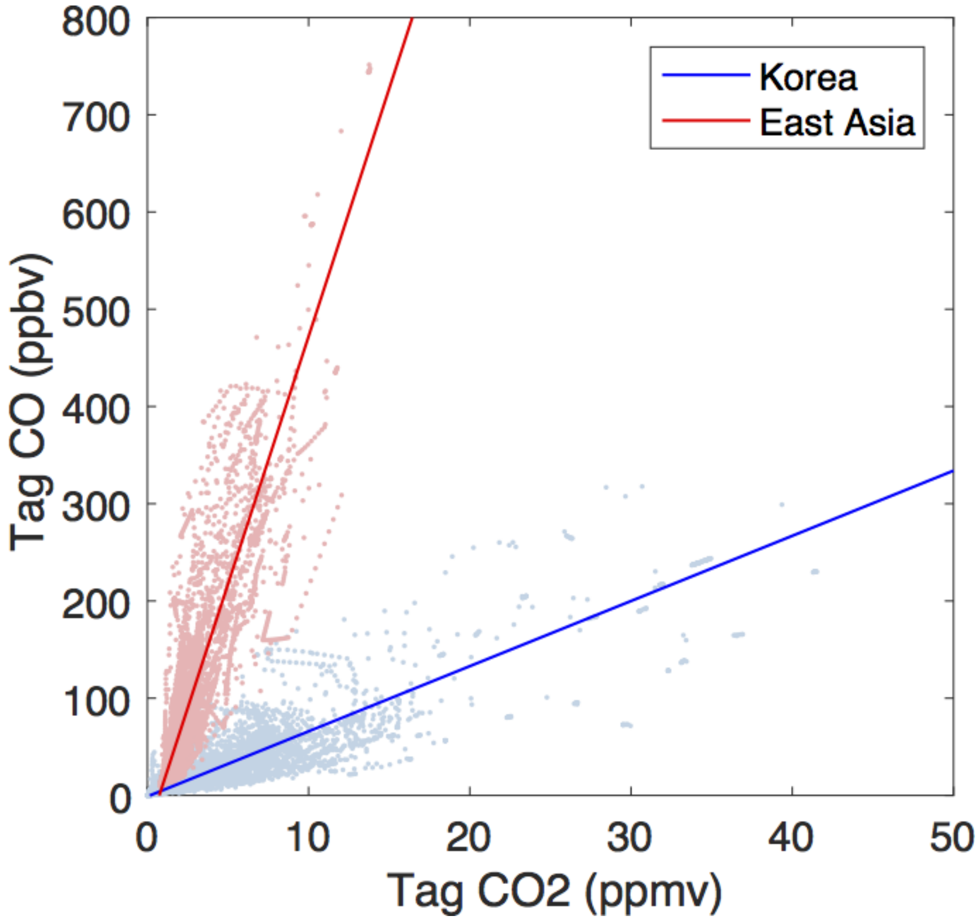
Changes are made to chem_mech.in, mo_srf_emissions.F90, and chemistry.F90.

Modeled and observed CO-CO_2 relationships during KORUS-AQ

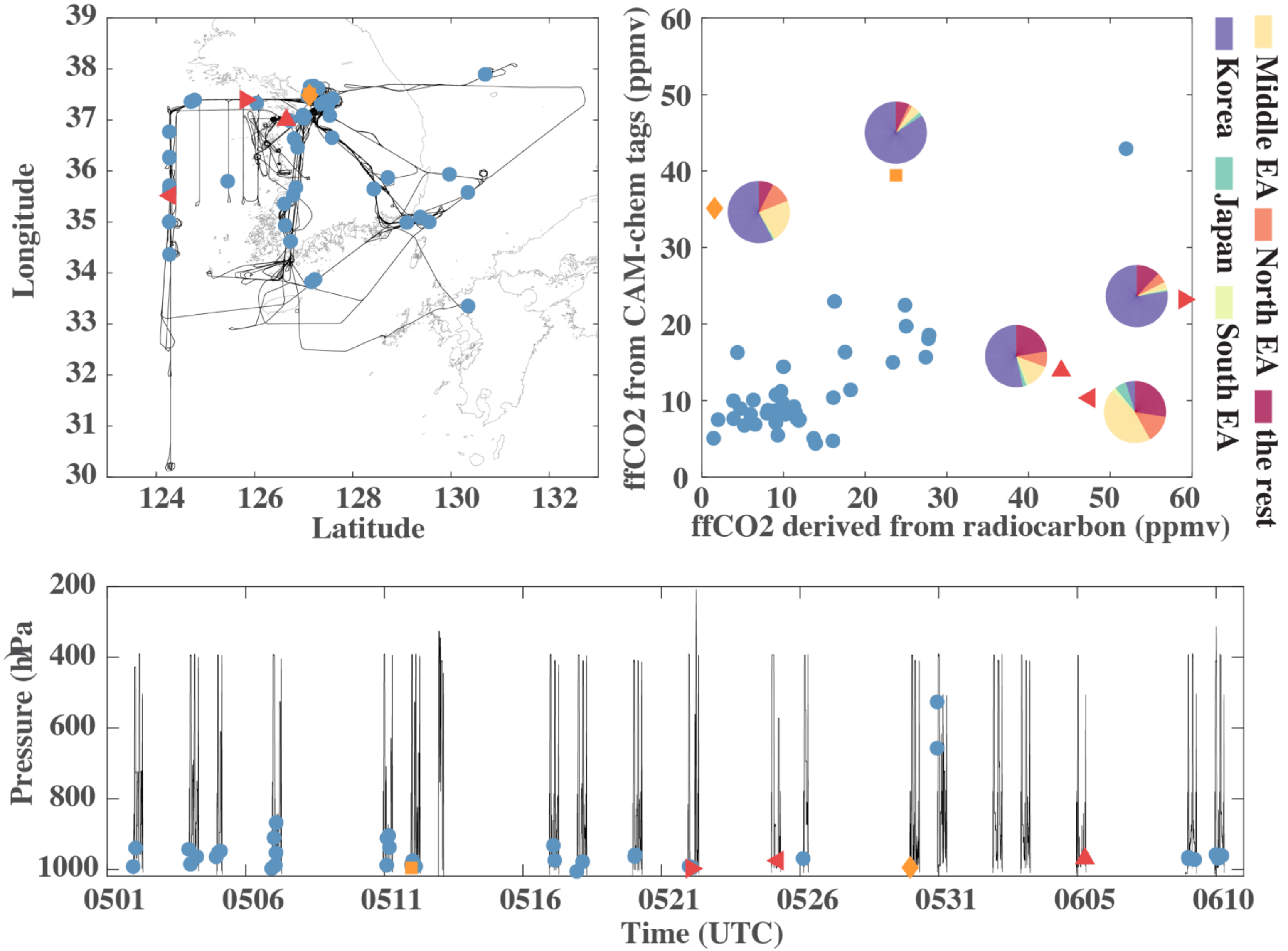
Model results of total CO_2 and CO overall agree well observations.



Distinct CO-CO_2 relationships can be seen from the CO and CO_2 tags of different regions.



fossil fuel CO_2 derived from CO_2 tags agree with fossil fuel CO_2 derived from radiocarbon



Take-home Messages

1. We added CO_2 simulations using 3 optimized CO_2 fluxes (CT2017, CTE2018, and CAMS) in CAM-chem, and the CO_2 simulation results are reasonably well matching the observations.

2. We add CO_2 tags in CAM-chem in addition to the existing CO tags. Temporal and spatial distributions of sinks for each $ffCO_2$ are calculated online. The atmospheric $ffCO_2$ concentrations derived from CAM-chem CO_2 tags agree well with the radiocarbon observations.

3. The CO and CO_2 tags in CAM-chem together can be used to track fossil fuel (as well as wildfire) emissions from the regions of interest, study combustion efficiency of the sources, and interpret the observed CO-CO_2 relationships from different measuring platforms (e.g., satellites, aircrafts, and ground sites).

Backup slides

Calculate ffCO$_2$ with radiocarbon

Radiocarbon

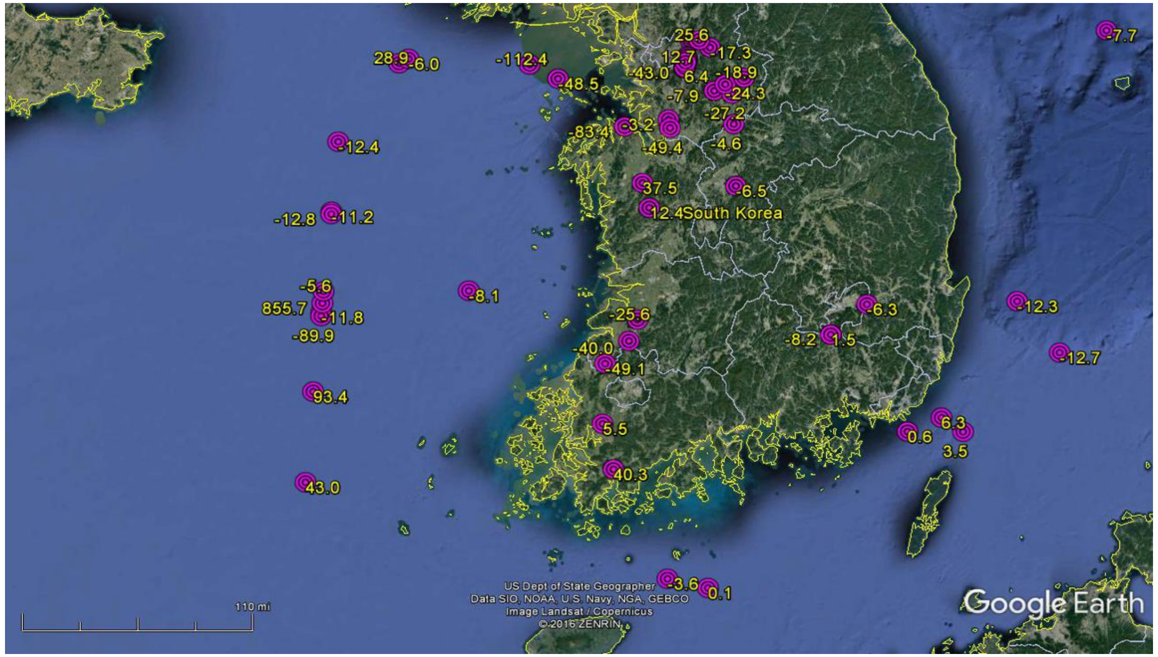
CO_2 Pool	$\Delta^{14}C$ Value	$\delta^{13}C$ Value
Fossil Fuels	-1000 ‰	~-28 ‰
Biosphere	~15 ‰	~(-14 to -26) ‰
Ocean	~15 ‰	~-10 ‰
Atmosphere	~15 ‰	~-8.8‰

$$CO_{2obs} = CO_{2bio} + CO_{2ff} + CO_{2bg}$$

$$\Delta_{obs}CO_{2obs} = \Delta_{bg}CO_{2bg} + \Delta_{ff}CO_{2ff} + \Delta_{bio}CO_{2bio}$$

$$CO_{2ff} = \frac{CO_{2obs}(\Delta_{obs} - \Delta_{bg})}{\Delta_{ff} - \Delta_{bg}} - \frac{CO_{2other}(\Delta_{other} - \Delta_{bg})}{\Delta_{ff} - \Delta_{bg}}$$

$$R_{CO} = \Delta CO / CO_{2ff}$$



Calculated FFCO$_2$

The background C-14 values here were used with 15 permil, which is comparable to Point Barrow, AK and NWR, CO values.

Taylor score

$$S = \frac{4(1+R)}{\left(\hat{\sigma}_f + 1/\hat{\sigma}_f\right)^2 (1+R_0)}$$

where $\hat{\sigma}_f$ is the ratio of σ_f (standard deviation of the model) and σ_r (standard deviation of observations), R is the correlation between model and observations, and R_0 is the maximum potentially realizable correlation (equivalent to 0.9 in this study).

Description of inversions: CAMS

- Copernicus Atmosphere Monitoring Service CAMS (V16r1)
- Model acronym: CAMS (V16r1)
- References: Chevallier et al., 2005; Chevallier et al., 2010
- Grid spacing: 3.75° x 1.875°,
- Number of vertical levels: 39
- Fossil Fuel Priors: EDGAR scaled to CDIAC
- Biosphere and Fires Priors: ORCHIDEE (climatology) + GFEDv4
- Ocean Priors: Landschüster et al. (2014)
- Transport model name: Laboratoire de Météorologie Dynamique with “z” standing for zoom capacity (Hourdin et al., 2006, 2012)
- Meteorological fields: European Centre for Medium-Range Weather Forecasts (ECMWF)
- Time period (provided): 1979 to 2016
- Observations: 119 measurement sites over the globe have been used. Observations were assimilated at their sampled times.

Description of inversions: CT2016

- Model acronym: CT2016
- References: Peters et al., 2007 with updates documented at http://carbontracker.noaa.gov Grid spacing: 3° x 2° resolution with a zoom at 1° x 1° over the United States.
- Number of vertical levels: 25
- Fossil Fuel Priors: “Miller" (EDGAR scaled to CDIAC) and "ODIAC"
- Biosphere and Fires Priors: Carnegie-Ames Stanford Approach (CASA) biogeochemical model, with GFED 4.1s and GFED_CMS
- Ocean Priors: Jacobson et al. (2007) and Takahashi et al. (2009)
- Transport model name: TM5 model (Krol et al., 2005)
- Meteorological fields: ERA-Interim (ECMWF, Reanalysis-Interim) Time period (provided): 2004 to 2015
- Observations: 66 surface in-situ and a total of 254 number of assimilated observations. hourly average observations are assimilated for continuous measurements, otherwise at their sampled time.

Description of inversions: CTE2017-FT

- Model acronym: CTE2017-FT
- References: Van der Laan-Luijkx et al., 2017 Grid spacing: 1° x 1°
- Number of vertical levels: 25
- Fossil Fuel Priors: EDGAR+IER, scaled to CDIAC
- Biosphere and Fires Priors: SiBCASA-GFED4
- Ocean Priors: Jacobson et al. (2007)
- Transport model name: TM5 model (Krol et al., 2005)
- Meteorological fields: ERA-Interim (ECMWF, Reanalysis-Interim)
- Time period (provided): 2004 to 2015, 2016 for 2017-FT
- Observations: 96 sites are assimilated, with hourly averages for continuous measurements