An exploration of the discrepancy between observations and simulated atmospheric ethane emission inventories: underestimations in key source emission categories

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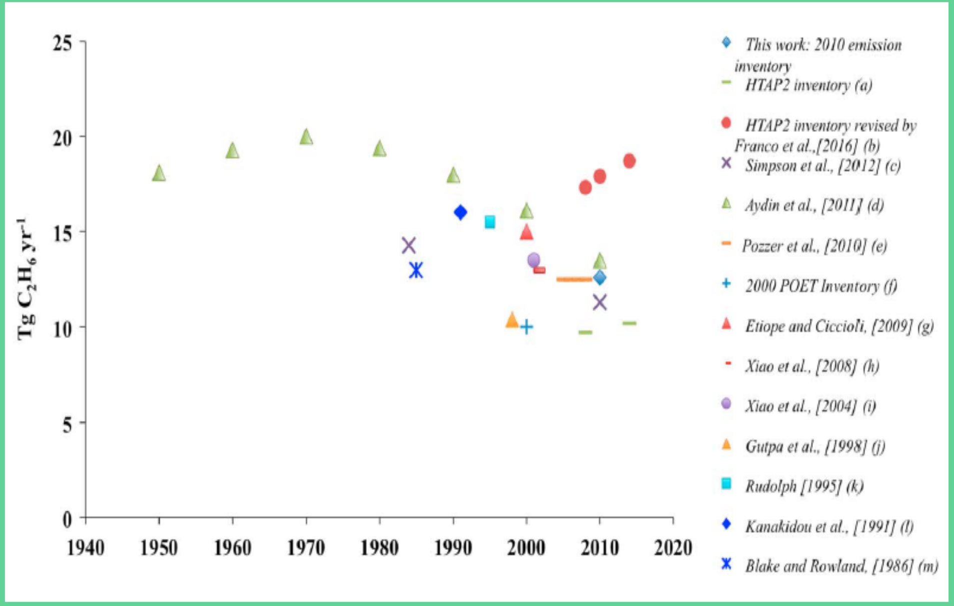
Introduction

Motivation & Characteristics of Ethane (C_2H_6):

This research seeks to:

- further explore the discrepancy between atmospheric observations and simulated atmospheric ethane emission inventories via contextualizing said discrepancy with varied emission scenarios.
- Our primary inquiry posits that the *existing discrepancy can be attributed to underestimations in key source emission categories coupled with the exclusion of biogenic, geologic, and oceanic emission sources.*
- By exploring more detailed emissions inventories we can better understand the recent trends in the global ethane budget.



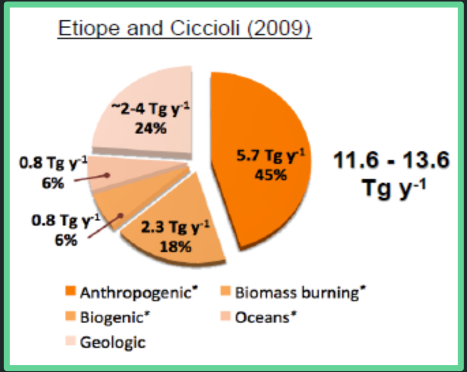
Key Characteristics:

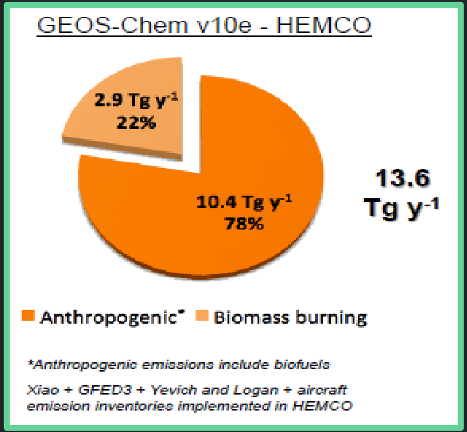
- Ethane (C_2H_6) is one of the most abundant NMHC within the atmosphere and is co-emitted with methane (CH_4) in key source categories.
- It has an ~2-month lifetime reacting with tropospheric hydroxyl radical (OH), and has a 100-year indirect global warming potential (GWP) of ~5.5. (**OH is primary sink and main contributor to seasonality**)
- Ethane has anthropogenic, pyrogenic, biogenic, oceanic, and geologic emission sources.
- Observations in atmospheric ethane concentrations show a negative trend of ethane mixing ratios from 1984 to 2010, while observations from 2010 and onward show a positive trend, particularly across the Northern Hemisphere. (**decoupling in co-emission of ethane and methane**)

Emission Categories and Inventories:

An emission inventory is an accounting of the amount of pollutants discharged into the atmosphere. An emission inventory usually contains the total emissions for one or more specific greenhouse gases, in this case, ethane (C_2H_6):

- C2H6 is primarily emitted during the production, processing, and transportation of natural gas sources. (**Tracer-Indicator for CH_4 emitted from anthropogenic fossil fuels**)
- The basis of inferring the relative C_2H_6 global budget based upon CH_4 emission estimates is from approximate $\frac{CH_4}{C_2H_6}$ emission ratio of $\sim\frac{2000\ ppbv}{2\ ppbv}$ [*Tzompa-sosa et al.*, 2017]. (**Baseline C_2H_6 emission inventory utilizes this method**)
- With about ~60% of global C_2H_6 emissions sourced from natural gas leakage events [*Xiao et al.*, 2008]—the remaining ~40% of global C_2H_6 emissions are commonly attributed to, in approximate equal partition, sources of biomass burning and biofuel consumption [*Rudolph et al.*, 1995]. (**Conventional Composition: ~0.6FF%: ~0.2BF%: ~0.2BB%)**
- In most **standard community emission inventories biogenic, geologic, and oceanic emissions are considered negligible on a global scale** [*Rudolph et al*, 1995], but research has contested this determination by **positing that key to the discrepancy between C_2H_6 observations and model simulations is the exclusion of geologic emissions** [*Etiope & Ciccioli*, 2009].
- The conventional global C_2H_6 budget has repeatedly yielded discrepancies between C_2H_6 observations and model simulations. **The inclusion of additional source emission inventories and/or scaling appears warranted, which will both serve evaluate the efficacy of conventional and non-conventional global C_2H_6 budget compositions.**



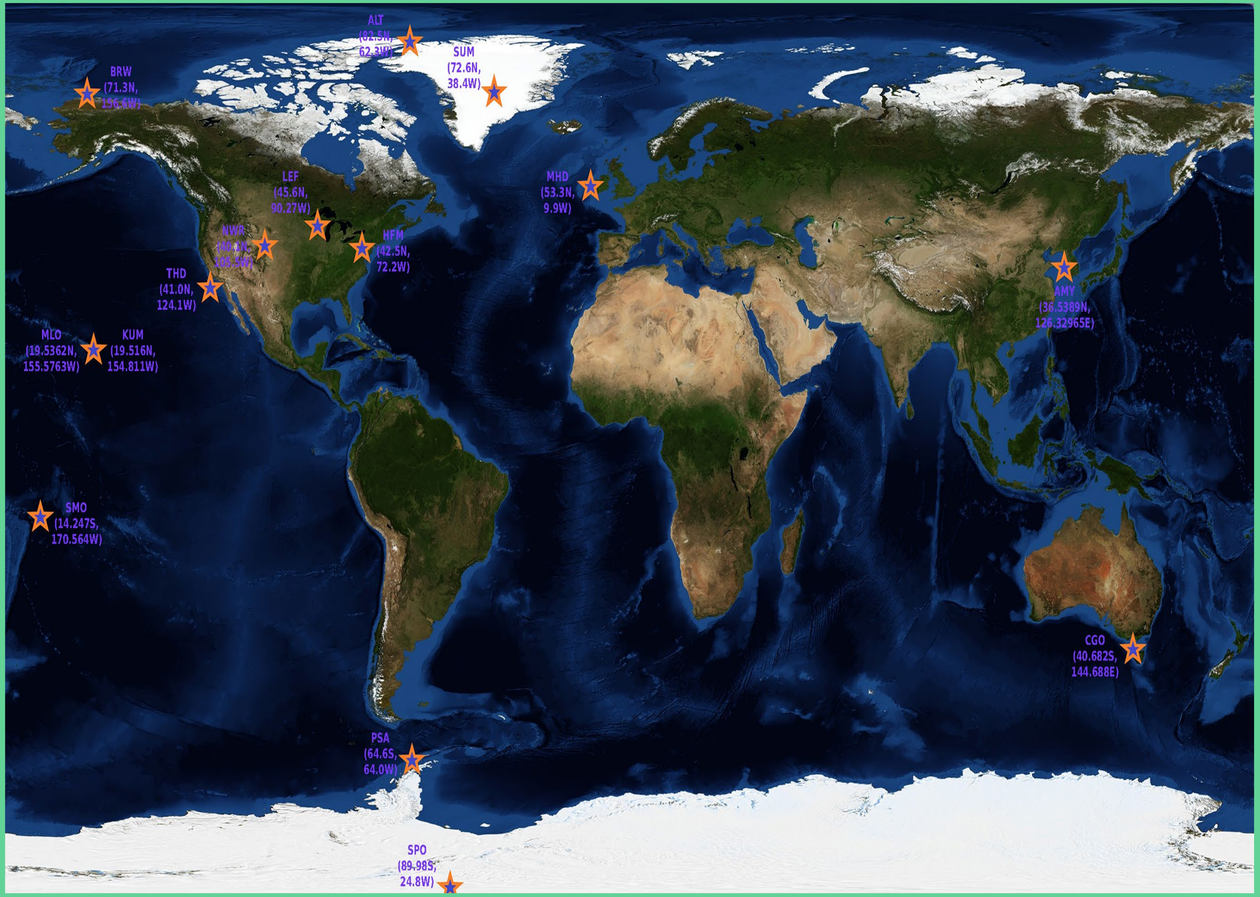


Methods

NOAA Observation Sites:

NOAA Observation Sites					
Site	Nearest Municipality	Country	Lat	Lon	Elevation
ALT	Alert	Canada	82.5 N	62.3 W	210 m asl
AMY	Anmyeon-do	South Korea	36.5389 N	126.3295 E	47.0 m asl
BRW	Barrow, AK	USA	71.3 N	156.6 W	8 m asl
CGO	Cape Grim	Australia	40.682 S	144.688 E	164 m asl
HFM	Harvard Forest	USA	42.5 N	72.2 W	340 m asl
KUM	Cape Kumukahi, HI	USA	19.516 N	154.811 W	3 m asl
LEF	NEAR Worcester, WI	USA	45.6 N	90.27 W	868 m asl
MHD	Mace Head	Ireland	53.3 N	9.9 W	42 m asl
MLO	Mauna Loa, HI	USA	19.5362 N	155.5763 W	3397 m asl
NWR	Niwot Ridge, CO	USA	40.1 N	105.5 W	3475 m asl
PSA	Palmer Station	Antarctica	64.6 S	64.0 W	10 m asl
SMO	NEAR Vaifanua	American Samoa	14.247 S	170.564 W	77 m asl
SPO	Not Specified	South Pole	89.98 S	24.8 W	2837 m asl
SUM	Summit	Greenland	72.6 N	38.4 W	3200 m asl
THD	Trinidad Head, CA	USA	41.0 N	124.1 W	120 m asl

- All C_2H_6 observations were made by NOAA's Global Monitoring Laboratory: Halocarbons & other Atmospheric Trace Species (*HATS*)
- Recorded from flasks by gas chromatography with mass spectrometry detection (*GCMS PERSEUS/M2*



Methods of Research: Compilation & Data Aggregation:

Compilation of GEOS-Chem GCHP (v13.0.2):

- GEOS-Chem is a global 3-D atmospheric chemistry model driven by meteorology data (**MERRA2**) sourced from the Goddard Earth Observing System (**GEOS**) of NASA's Global Modeling and Assimilation Office.
- This research utilizes GEOS-Chem GCHP (**v13.0.2**), which was compiled on the COEUS High-Performance Computing Cluster hosted through the Portland Institute for Computational Science and Portland State University. (**Linux-Terminal *cluster* of computation focused computers**)
- Implemented within GEOS-Chem is the Harvard-NASA Emission Component (**HEMCO**), which is a stand-alone software component for computing emissions within global atmospheric models.
- HEMCO determines emissions from a variety of different sources, regions, and species on a user-defined grid and can combine, overlay, and even update a set of data inventories with scale factors—as all specified by the user through the HEMCO configuration file (**HEMCO_Config.rc**).

Aggregation of Additional Source Emission Inventories:

- All additional source emission inventories, such as: MEGAN-MACC, MEGANv2, POET, RETRO were accessed through Emissions of Atmospheric Compounds and Compilation of Ancillary Data (**ECCAD**).
- The global geological CH4 gridded emission inventory (**Etiope: GEOCH4 (2018)**) produced by Dr. Giuseppe Etiope and S. Schwietzke [Etiope et al., 2019].
- The global geologic data was explicitly for CH_4 emissions and was composed of several comma-separated value (**.csv**) datasets each corresponding to differing geologic emission sources—preprocessing in the form of scaling was necessary. ($\frac{CH_4}{C_2H_6}$ **emission ratio used in scaling**)
- Each sub-source: onshore seeps, micro-seeps, marine seeps, and geothermal seeps were scaled for C_2H_6 the new emission output values were reaggregated into a total geologic C_2H_6 emission inventory. (**Converted into .nc format with script written in Python**)

Methods of Research: Emission Scenarios & Observations:

Baseline Emission Scenario, Optimized Fossil Fuel Emission Scenario (OFF), and Optimized Biomass Burning Emission Scenario (OBB):

- Each emission scenario composition is detailed in the table to the right.
- In the Optimized Fossil Fuel Emission Scenario (OFF), scaling begins at approximately 1.4 due to what Tzompa-Sosa [2017] speaks to an ~1.4 scaling factor improving the correspondence of the GEOS-Chem simulation with observations in regions without major oil and gas operations.
- In the Optimized Biomass Emission Scenario (OBB), scaling begins at approximately 1.2 due to what Van der Werf [2010] speaks to an ~20% +/- uncertainty regarding global biomass emissions.

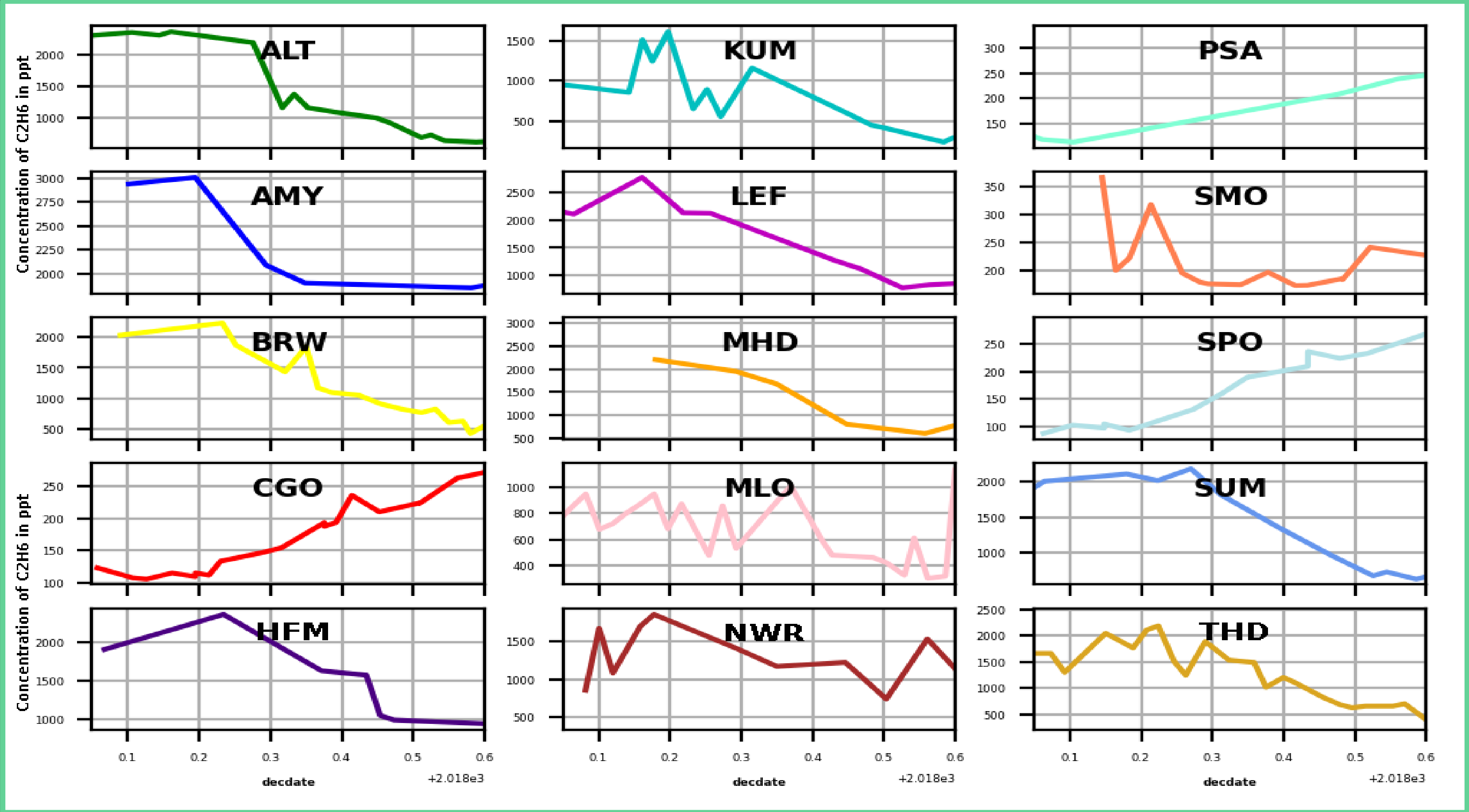
Analysis of Emission Scenarios vs. Observations at Key Observation Sites:

- The analysis of both NOAA's C_2H_6 concentration observations and GCHP's baseline C_2H_6 simulated concentration outputs took place within the python environment. (**Using Python Modules: os, numpy, netCDF4, pandas, xarray and matplotlib**)
- Each of site-dependent NOAA C_2H_6 observation file, and GCHP six global-monthly average species concentrations of C_2H_6 output, were read into python and were subsequently plotted in a set of subplots corresponding to each site from 20180101 to 20180601.

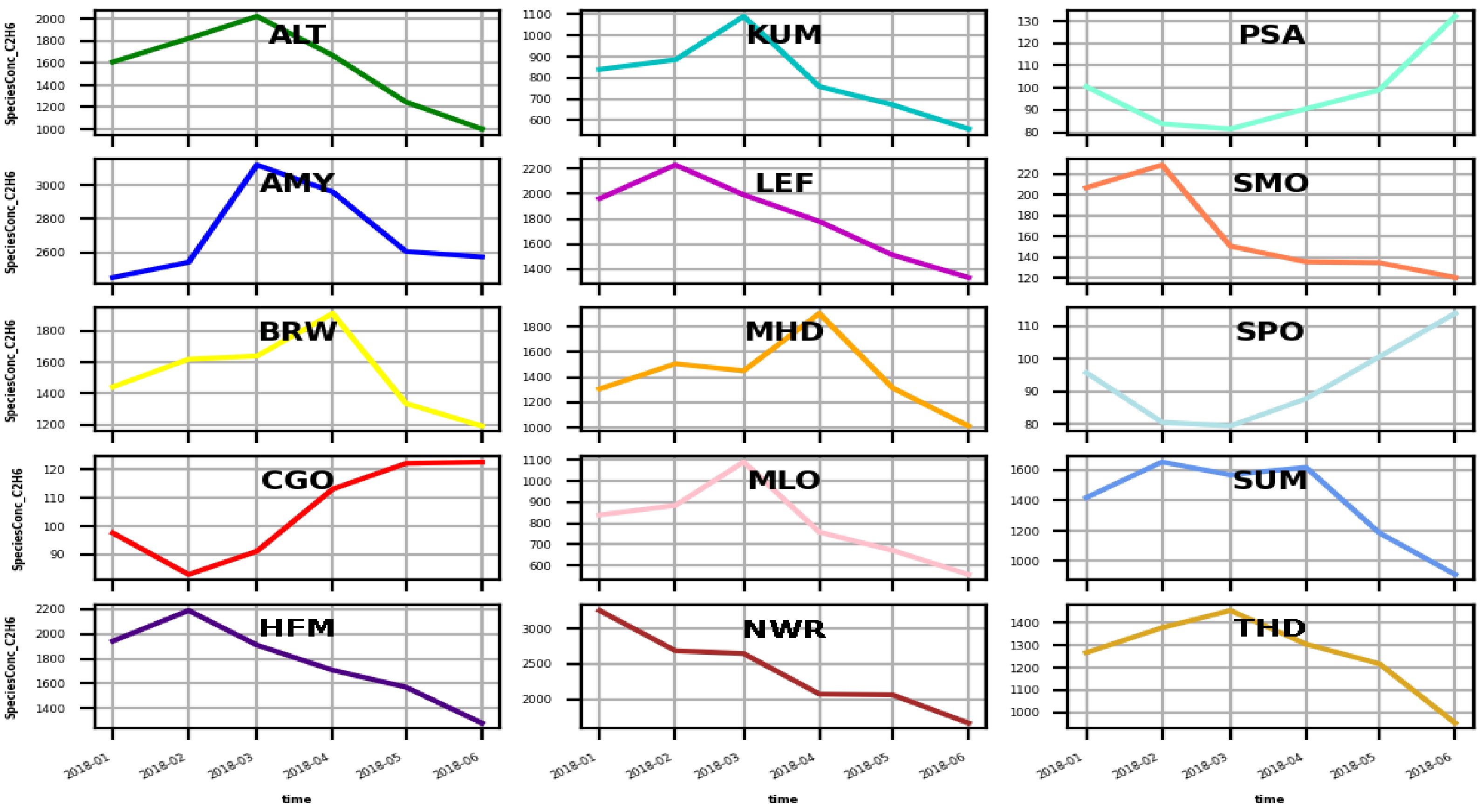
Emission Scenario Compositions		
Baseline Emission Scenario:		
Source Emission Categories	**Emission Inventory**	**Additional Notes**
Anthropogenic Fossil Fuel	Tzompa-Sosa: C_2H_6 (2010)	Baseline – N/A
Biofuel	Tzompa-Sosa: C_2H_6 (2010)	Baseline – N/A
Biomass Burning	GFEDv4 (2018)	Baseline – N/A
*Optimized Fossil Fuel Emission Scenario (**OFF**):*		
Source Emission Categories	**Emission Inventory**	**Additional Notes**
Anthropogenic Fossil Fuel	Tzompa-Sosa: C_2H_6 (2010)	Incremental scaling: starting at x1.4
Biofuel	Tzompa-Sosa: C_2H_6 (2010)	Not Optimized – N/A
Biomass Burning	GFEDv4 (2018)	Not Optimized – N/A
Biogenic	MEGAN-MACC (2010)	Additional emission inventory
Geologic	Etiope: GEOCH_4 (2018)	Additional emission inventory
Oceanic	RETRO (2000)	Additional emission inventory
*Optimized Biomass Burning Emission Scenario (**OBB**):*		
Source Emission Categories	**Emission Inventory**	**Additional Notes**
Anthropogenic Fossil Fuel	Tzompa-Sosa: C2H6 (2010)	Not Optimized – N/A
Biofuel	Tzompa-Sosa: C_2H_6 (2010)	Not Optimized – N/A
Biomass Burning	GFEDv4 (2018)	Incremental scaling: starting at x1.2
Biogenic	MEGAN-MACC (2010)	Additional emission inventory
Geologic	Etiope: GEOCH_4 (2018)	Additional emission inventory
Oceanic	RETRO (2000)	Additional emission inventory

Results

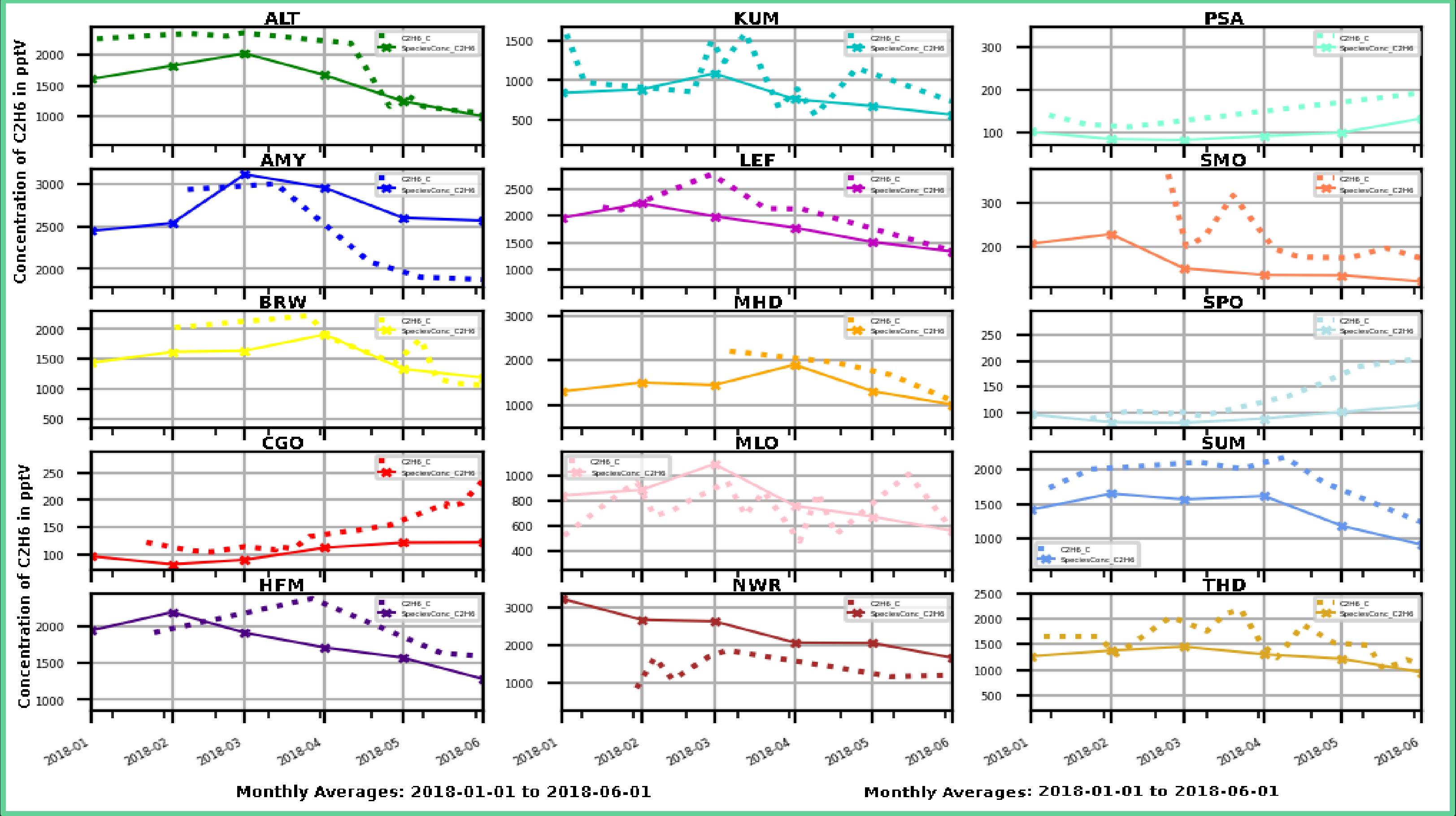
Series of Subplots: NOAA's C_2H_6 concentration observations:



Series of Subplots: GCHP's C_2H_6 Baseline Emission Scenario:



Series of Subplots: Comparison of NOAA Data & GCHP Data:



Analysis of Results: Statistics & Trends:

C_2H_6 Hemispheric & Zonal Gradient Statistics	
NOAA: C_2H_6 Observational Data (2018):	
Northern Hemispheric Gradient	**Southern Hemispheric Gradient**
~750pptv to ~2100pptv	~110pptv to ~230pptv
GCHP: C_2H_6 Simulated Data (2018):	
Northern Hemispheric Gradient	**Southern Hemispheric Gradient**
~1255pptv to ~1928pptv	~93pptv to ~145pptv

NOAA: C_2H_6 Observational Data (2018):		
Zonal Range	**Weighed Observation Sites**	**Average Zonal Concentration Gradient**
90°N—50°N	ALT, BRW, MHD, SUM	~750pptv to ~2250pptv
20°N—50°N	AMY, HFM, LEF, NWR, THD	~1000pptv to ~2300pptv
0°N—20°N	KUM, MLO	~450pptv to ~1250pptv
0°S—20°S	SMO	~200pptv to ~350pptv
20°S—50°S	CGO	~100pptv to ~250pptv
50°S—90°S	PSA, SPO	~125pptv to ~275pptv
GCHP: C_2H_6 Simulated Data (2018):		
Zonal Range	**Weighed Observation Sites**	**Average Zonal Concentration Gradient**
90°N—50°N	ALT, BRW, MHD, SUM	~1050pptv to ~1800pptv
20°N—50°N	AMY, HFM, LEF, NWR, THD	~1680pptv to ~2360pptv
0°N—20°N	KUM, MLO	~600pptv to ~1100pptv
0°S—20°S	SMO	~120pptv to ~220pptv
20°S—50°S	CGO	~90pptv to ~120pptv
50°S—90°S	PSA, SPO	~80pptv to ~120pptv

Discrepancies exist between the NOAA observational and GCHP simulated datasets, as the baseline emission scenario consistently lacks correspondence with the observational concentrations of atmospheric C2H6 at each of the key sites (*Except AMY & NWR*).

The following metric will be utilized in determining the correspondence between the sets of data:

- **Significant** under/over-estimation corresponding to an average ± ~500pptv to ~1000pptv (Northern Hemisphere) or ~50pptv to ~100pptv (Southern Hemisphere) discrepancy.
- **Moderate** under/over-estimation corresponding to an average ± ~250pptv to ~500pptv (Northern Hemisphere) or ~25pptv to ~50pptv (Southern Hemisphere) discrepancy
- **Marginal** under/over-estimation corresponding to an average ± ~125pptv to ~250pptv (Northern Hemisphere) or ~12.5pptv to ~25pptv (Southern Hemisphere) discrepancy.

The average scale magnitude of atmospheric C_2H_6 concentration at each site within each zone (*90°-50°; 20°-50°; 20°-0°*) corresponds to the relative zonal concentration gradient. This determination was made for both the observational data and the baseline emission scenario output.

Timeseries of GCHP C_2H_6 Baseline Emission Scenario (MP4):

Discussion of Ongoing Work

Timeline | 2021

August

Continue to work with HEMCO within GEOS-Chem GCHP to finalize the optimized emission scenarios. Running both optimized and baseline emission scenarios at a higher resolution (2x2.5).

September

Analyze yielded results from all three emission scenarios within the python environment and fine-tune emission inventory scales/variables of each scenario.

October

Continue fine-tuning simulation parameters, reanalyze output data, and prepare research deliverable for AGU: Fall Meeting, 2021.

November

Continue research analysis and finalize research deliverable for AGU: Fall Meeting, 2021.

December

Present concluded research at AGU: Fall Meeting, 2021

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Questions?