

Implementation of the RETRO Anthropogenic Emission Inventory into the GEOS-Chem Model

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1 Introduction

Anthropogenic VOC emissions in GEOS-Chem are currently derived from a combination of global (GEIA) and regional (EPA/NEI, EMEP, STREETS, among others) anthropogenic emission inventories. Datasets are converted to $2^\circ \times 2.5^\circ$ resolution for use in the model, but temporal resolution varies from monthly to annual between inventories. Aseasonal data (such as GEIA) are then scaled to simulate monthly resolution.

In addition to the lack of monthly resolution, global emissions in the model lack data for a number of NMVOC tracers in the ANTHSRCE diagnostic. As a result, simulated emissions are limited to select geographic regions, usually only the United States and Europe (EPA/NEI and EMEP are the most complete regional datasets).

This document describes the implementation of the RETRO emission inventory for anthropogenic VOCs into GEOS-Chem. RETRO has monthly temporal resolution and includes a wide suite of speciated VOC emissions, which offer advantages over the GEIA inventory currently employed in the model.

2 Description of RETRO emission inventory

2.1 Overview

The RETRO (REanalysis of the TROposhpheric chemical composition) emission inventory contains anthropogenic and biomass burning emissions for the years 1960-2000 at $0.5^\circ \times 0.5^\circ$ spatial resolution and monthly temporal resolution [1]. For this project, we are concerned with the anthropogenic emissions only. The RETRO team provides all emissions data on their ftp server:

<ftp://ftp.retro.enes.org/pub/emissions/>

Emissions are provided in both sectorized and aggregated formats. There is no differentiation between individual sectors in the GEOS-Chem simulation, so aggregated data was used. The most recent data was used (RETRO extends to the year 2000).

2.2 Conversion of RETRO species to GEOS-Chem tracers

The RETRO anthropogenic emission inventory contains gridded data for 24 chemical species. For use in the GEOS-Chem model, these chemical species had to be converted to match 13 tracers in the ANTHSRCE diagnostic (Table 1).

Table 1: RETRO species to GEOS-Chem tracers

ANTHSRCE tracer	applicable RETRO species	Comments
ALK4	Butanes Pentanes Hexanes and Higher Alkanes	ALK4 is alkanes ≥ 4 carbon atoms
ACET		Assume “Other Ketones” is all ketones other than acetone since a separate acetone category exists for biogenic data
MEK	Other Ketones	
ALD2	Other Alkanals	Assume all alkanals are acetaldehyde since no RCHO emissions are provided
RCHO		No anthropogenic emissions
PRPE	Propene	
C3H8	Propane	
CH2O	Methanal	
C2H6	Ethane	
BENZ	Benzene	
TOLU	Toluene	
XYLE	Xylene	
GLYX		No RETRO data
MGLY		No RETRO data
C2H4	Ethene	
C2H2	Ethyne	
HCOOH	Aggregated Acids	Assume HCOOH accounts for 25% of total acids based on Chebbi et al. (1996)
ACTA		

2.3 RETRO methodology

The RETRO anthropogenic emission inventory was based largely off of previous work by the Netherlands Organisation for Applied Scientific Research (TNO) [1]. TNO developed a model for estimating emissions, called TNO Emissions Assessment Model (TEAM), which was based in turn off of an earlier project, Tropospheric Ozone and Precursors, Trends, Budgets, and Policy (TROTREP) [2].

The TROTREP team developed emissions and technology factors as well as rates of emissions for specific activities. TEAM was created to use these data to produce a gridded emission inventory by compiling a database of technologies and their emission factors for each timestep and country [2]. The equation is as follows [1]:

$$E_{pollutant}(t) = \sum_{activities} \left(\sum_{tec/mologies} (AR_{activity}(t) \times P_{activity,tec/mology}(t) \times EF_{tec/mology,pollutant}) \right)$$

In the equation above, AR is the Activity Rate of the process which produces emissions and is based on economic data. P is the Penetration, the fraction of the activity performed using a specific technology. Penetration can be found by correlating activities with the technologies that they employ. EF is the Emission Factor, an attribute of the technology selected determining the linear relation between the activity rate and the resulting emission of a certain pollutant, using a specific technology. Emission Factors can be calculated using technological data for each region [2].

The RETRO team combined these factors with data from the International Energy Agency and an inventory for solvent use and biomass burning intended for input into modeling software [1]. These data were used with TEAM to produce a gridded global anthropogenic emissions dataset. The RETRO team then distributed national totals based on gridded population data from the Center for International Earth Science Information Network (CIESIN) to provide global gridded data [1]. NMVOCs were speciated based on country specific profiles developed in TROTREP. The resulting annual data was then divided into monthly data by LOTOS groups. To improve continuity, the data was smoothed before distribution.

3 Comparison of RETRO to existing GEOS-Chem inventories

3.1 Comparison to GEOS-Chem base inventory (GEIA)

To compare RETRO with the existing inventories, a GEOS-Chem simulation was run as follows:

- Version 8-02-01 dicarbonyls simulation
- Anthropogenic emissions and aerosols enabled
- Regional inventories disabled
- Timeframe Jan 01, 2000 to Jan 01, 2001
- ANTHSRCE diagnostic output with 13 tracers included in RETRO:

– ALK4	– CH ₂ O	– TOLU
– ALD2	– C ₂ H ₆	– XYLE
– PRPE	– MEK	– C ₂ H ₄
– C ₃ H ₈	– BENZ	– C ₂ H ₂

The following figures compare output from two GEOS-Chem simulations: one with GEIA anthropogenic emissions and the other with RETRO anthropogenic emissions added in the update.

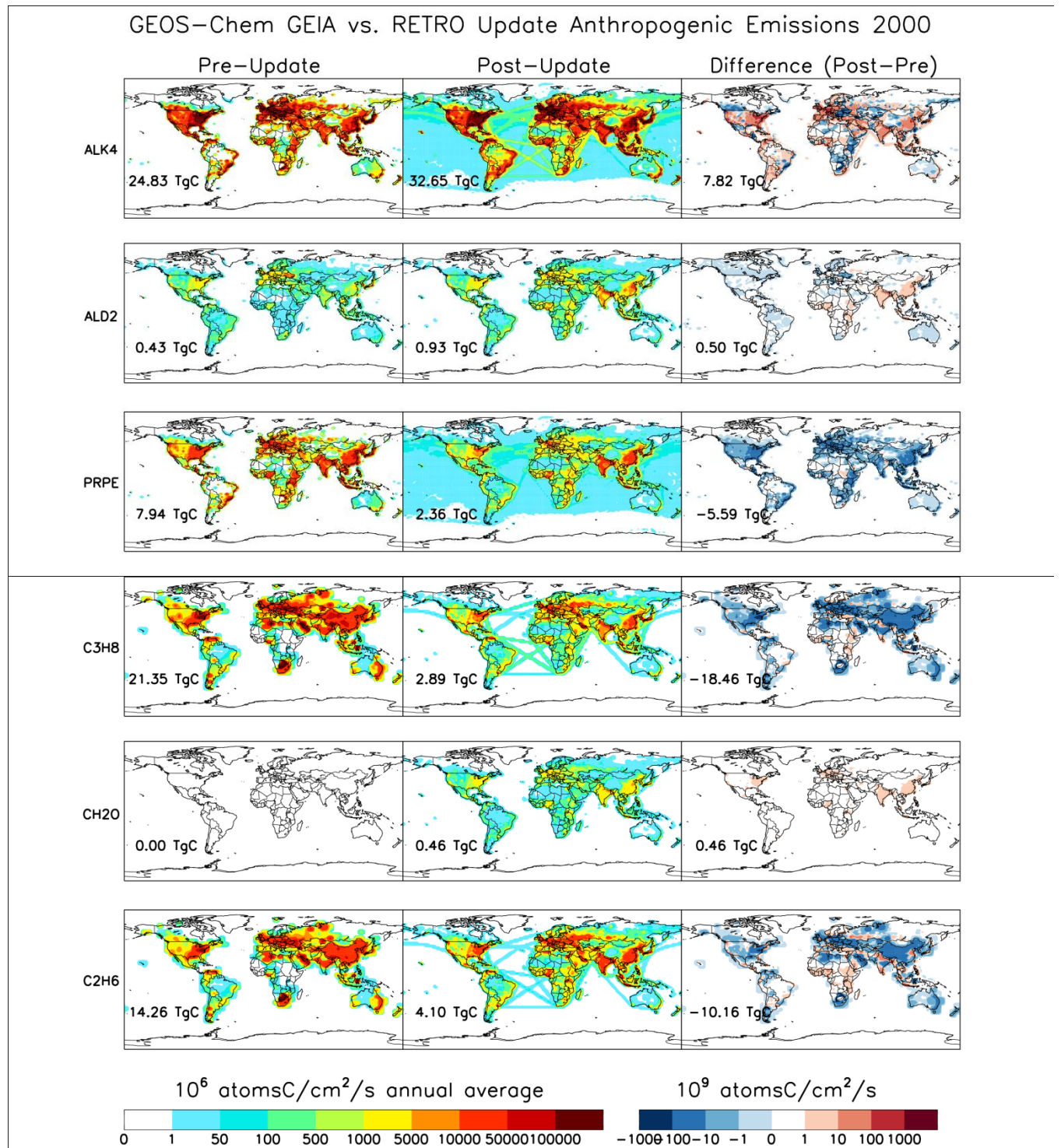


Figure 1: GEIA vs. RETRO anthropogenic emissions simulation output for the year 2000

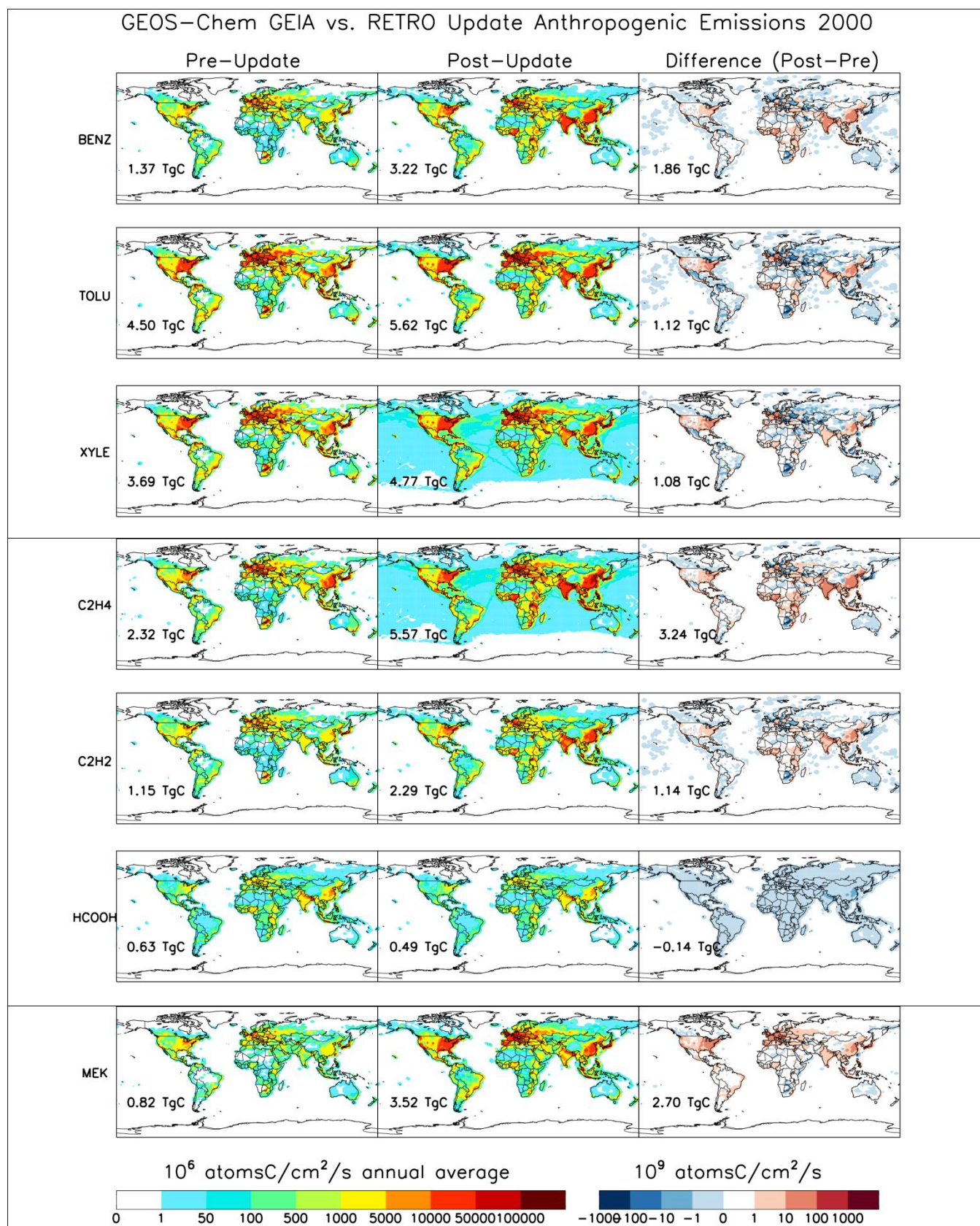


Figure 1 (ctd): GEIA vs. RETRO anthropogenic emissions for the year 2000

3.2 Comparison to GEOS-Chem regional inventories

GEOS-Chem allows for regional inventories to overwrite the base global inventory, GEIA, within defined geographic regions. These regional inventories often have finer spatial and temporal resolution than the base inventory. The RETRO inventory underwent comparison to these regional inventories as follows:

- Version 8-03-01 dicarbonyls simulation
- Anthropogenic emissions and aerosols enabled
- Optional/regional inventories enabled:
 - EMEP
 - BRAVO
 - STREETS
 - CAC
 - EPA/NEI99
- Timeframe Jan 01, 2006 to Jan 01, 2007
- ND36 output with 12 of the 13 tracers included in RETRO:

- ALK4	- CH2O	- TOLU
- ALD2	- C2H6	- XYLE
- PRPE	- MEK	- C2H4
- C3H8	- BENZ	- C2H2

The following figures compare output from two GEOS-Chem simulations: one with GEIA anthropogenic emissions and the other with RETRO anthropogenic emissions added in the update.

GEOS-Chem Regional vs. RETRO Update Anthropogenic Emissions 2006

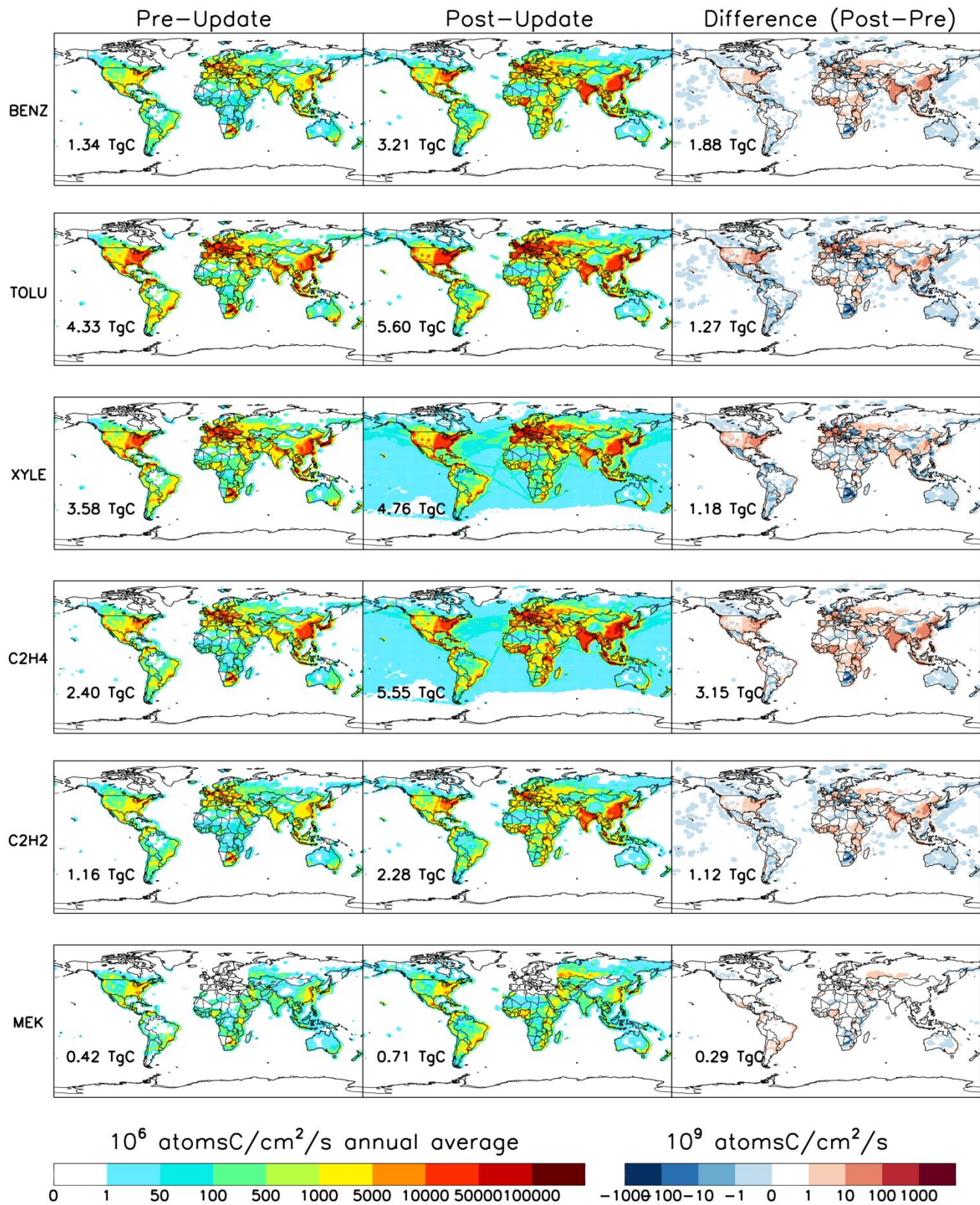
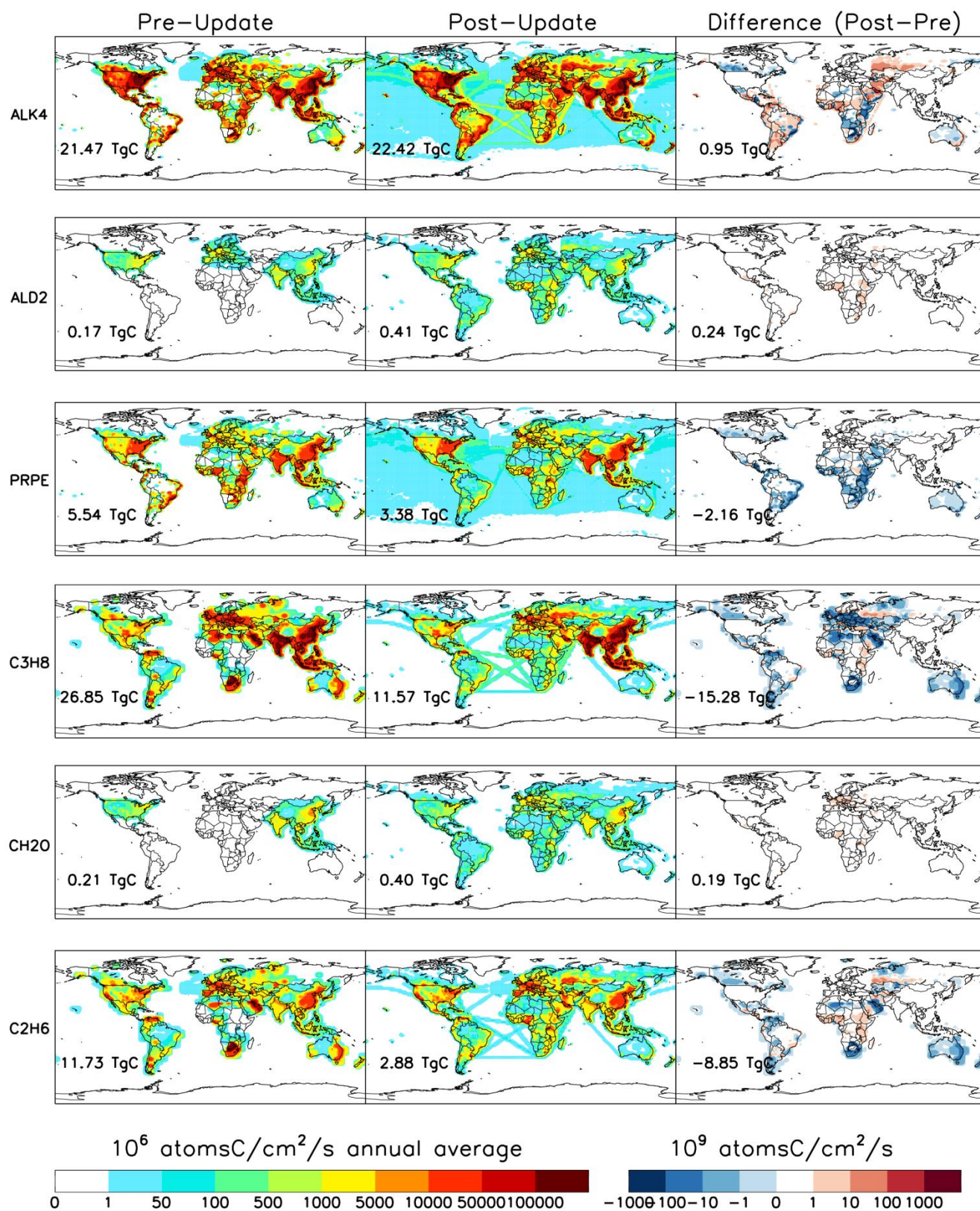


Figure 2: Regional GEOS-Chem inventories vs. RETRO anthropogenic emissions simulation output for the year 2000

GEOS-Chem Regional vs. RETRO Update Anthropogenic Emissions 2006

**Figure 2 (ctd):** Regional GEOS-Chem inventories vs. RETRO anthropogenic emissions for the year 2000

3.3 Comparison of Chemical Impacts

Sections 3.1 and 3.2 compared anthropogenic emissions with chemistry turned off. A set of full chemistry simulations were also performed to compare chemical impacts of RETRO versus non-RETRO emissions. The following settings were used for these simulations:

- Version 8-03-01 dicarbonyls simulation
- Anthropogenic emissions, aerosols, deposition, chemistry enabled
- Optional/regional inventories enabled per Section 3.2
- Timeframe Jan 01, 2006 to Jan 01, 2007
- ND45 Tracer Concentration CO and O₃ output
- ND43 24-hour averaged OH output

The following figures are monthly difference plots which highlight key characteristics of the full-chemistry comparisons. An annual comparison was conducted, but only selected months are presented for brevity.

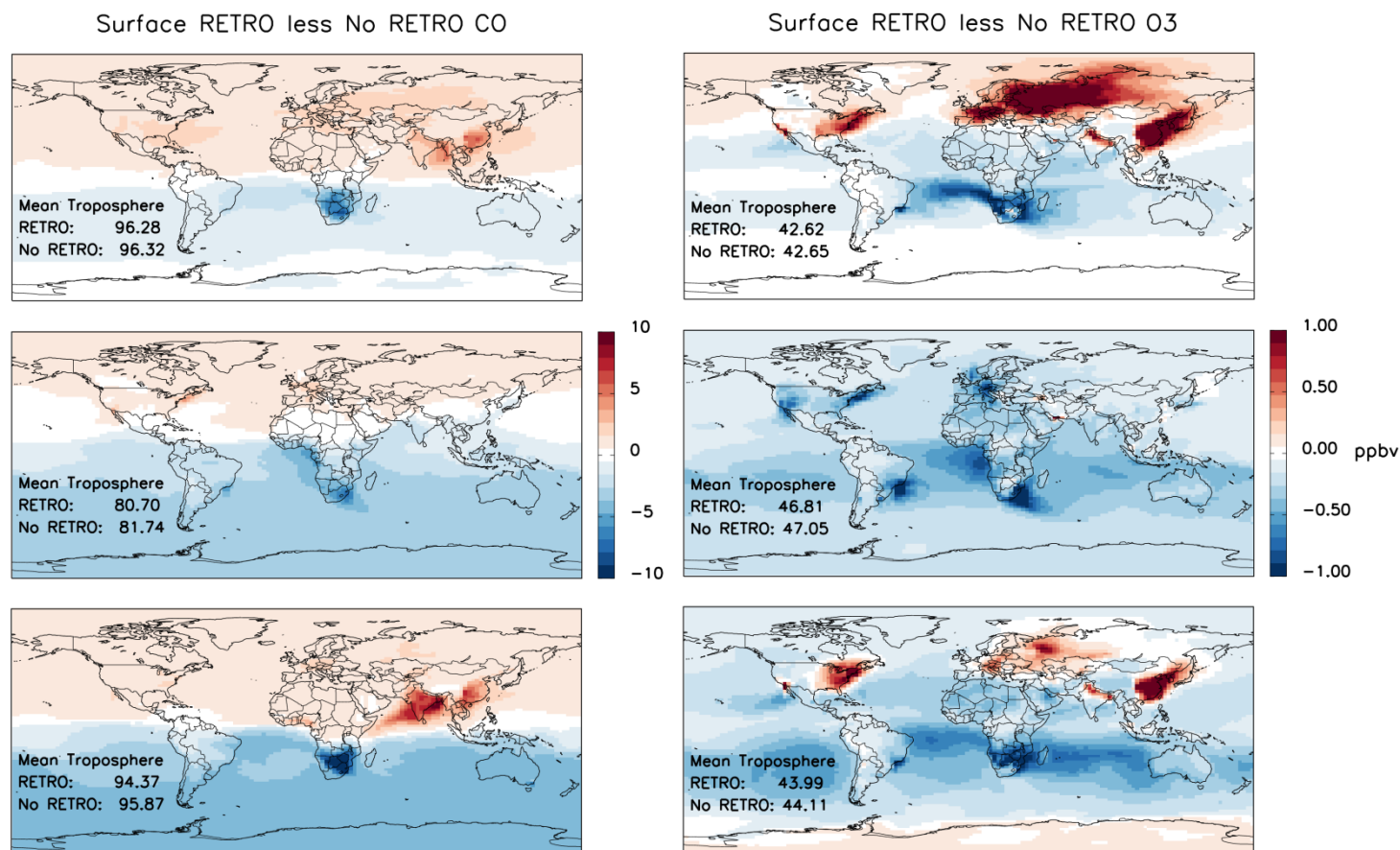


Figure 3: Surface CO difference plots for March, July, and December 2006

Figure 4: Surface O₃ difference plots for February, July, and December 2006

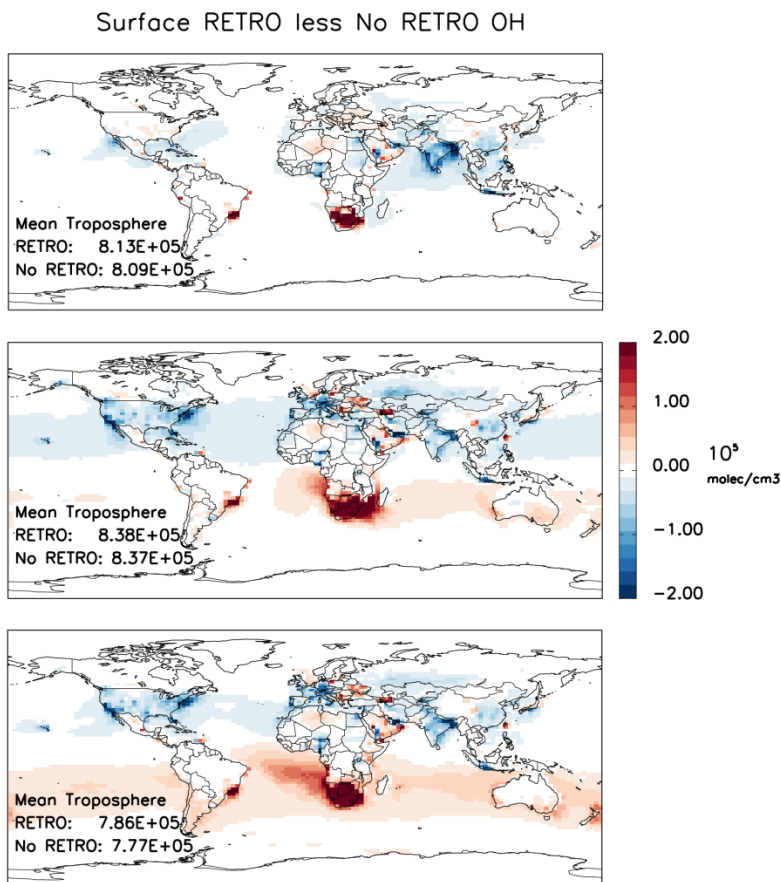


Figure 5: Surface OH difference plots for January, May, and September 2006

3.4 Key points from comparison of RETRO to existing GEOS-Chem inventories

3.4.1 GEIA comparison (v-8-02-01)

There is a significant change in emissions for many tracers, but especially for C₃H₈ and C₂H₆. For these compounds the GEIA flux is similar to RETRO in unpopulated areas, but is several orders of magnitude larger in densely populated areas. We also see this effect for the PRPE tracer. ALK₄, however, is the reverse: RETRO emissions are higher than GEIA in populated areas and lower in unpopulated ones. No CH₂O data are available in GEIA.

3.4.2 Regional comparison (v-8-03-01)

In general the regional inventories seem to be in closer agreement with RETRO. C₃H₈ and C₂H₆ still have significant differences, but ALK₄ is very similar. CH₂O emissions are available for only some of the regional inventories. RETRO CH₂O emissions are generally similar to the regional inventories. Though global MEK emissions are similar, MEK emissions from the EMEP inventory appeared erroneously low – on the order of 10^{-5} Tg annually. This was outside the scope of the update and therefore was not investigated. Note that this anomaly persisted upon updating to version 8-03-01. The much higher emissions in South Africa for some tracers are related to a scaling bug with the GEIA emissions.

3.4.3 Full chemistry Comparison (v-8-03-01)

A full chemistry simulation of CO, OH, and O₃ showed generally small changes with the RETRO update. Simulated CO increases in the northern hemisphere and decreases in the southern hemisphere. South Africa and Asia are areas of peak differences, though differences in South Africa are mainly due to a scaling bug in GEIA. Simulated O₃ has significant regional changes. Peak differences occur over highly populated areas as with anthropogenic emissions comparisons. Tropospheric mean OH experiences many local changes with the RETRO update, though the global mean differs little. The largest regional difference is over southern Africa related to the GEIA scaling bug.

4 Modification of GEOS-Chem

GEOS-Chem version 8-02-01 was modified to read in RETRO anthropogenic emissions as a base for global NMVOC emissions. The use of the RETRO inventory can be toggled with a switch in the emissions menu of /run_directory/input.geos. The RETRO emissions are overwritten by any regional inventories that are enabled from within input.geos. The following programs were modified to allow RETRO data to be read in:

Table 2: List of modified programs

directory	program(s)
/code_directory/	cleanup.f emfossil.f emissions_mod.f input_mod.f logical_mod.f Makefile
/run_directory/	input.geos

In addition to the modification of the programs above, the program retro_mod.f was created, using epa_nei_mod.f as a framework. The EPA/NEI routines were used because of the shared monthly temporal resolution and the number of common tracers between the EPA/NEI inventory and RETRO.

In March 2011, the RETRO code was ported to version 8-03-01 from 8-02-01 with very minor changes. Similar results were observed and the code is believed to be stable. The fix previously included to deal with CH₂O from EPA/NEI was removed, as version 8-03-01 included this update. Also note that HCOOH was unique to our version of v8-02-01 and was removed when the code was updated.

Acknowledgements

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References

1. Bolshcer, M, et al., *RETRO Deliverable D1-6*, RETRO Documentation, 2007.
2. Pulles, T, et al., *Assessment of Global Emissions from Fuel Combustion in the Final Decades of the 20th Century*, TNO report A-R0132/B, 2007.