

Simulation of current and future tropospheric chemistry with the Earth System Model EMAC

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Motivation

The global climate change and the increase in methane (CH_4) and nitrous oxide (N_2O) are leading to a different future tropospheric chemistry as today.

In this study, we are showing the first results of the simulated (future) changes in tropospheric chemistry with focus on hydroxyl radical (OH), acetone (CH_3COCH_3), ethane (C_2H_6), formic acid (HCOOH) and peroxy acetyl nitrate (PAN).

We use two different simulations from the project [ESCiMo](#) (Earth System Chemistry Integrated Modelling, [Jöckel et al., 2016](#)) performed with the Earth System Model ECHAM/MESSy Atmospheric Chemistry ([EMAC](#), [Jöckel et al., 2010](#)).



Comparison of results of EMAC with GLORIA

In different studies we could show that EMAC has the ability to simulate selected tropospheric substances in comparison to results of the GLORIA (Gimballed Limb Observer for Radiance Imaging of the Atmosphere) instrument, used on board of the research aircrafts Geophysica and HALO during the STRATOCLIM (July/August 2017) and WISE (August to October 2017) campaigns.

In the following EGU contributions these comparisons are shown:

Johansson et al.: Pollution trace gas distributions in the Asian monsoon UTLS derived from measurements of the airborne imaging limb sounder GLORIA during the StratoClim campaign, [EGU2020-6606](#), AS1.17

and

Wetzel et al.: GLORIA observations of pollution tracers C₂H₆, C₂H₂, HCOOH, and PAN in the North Atlantic UTLS region, [EGU2020-6931](#), AS3.5

Simulations

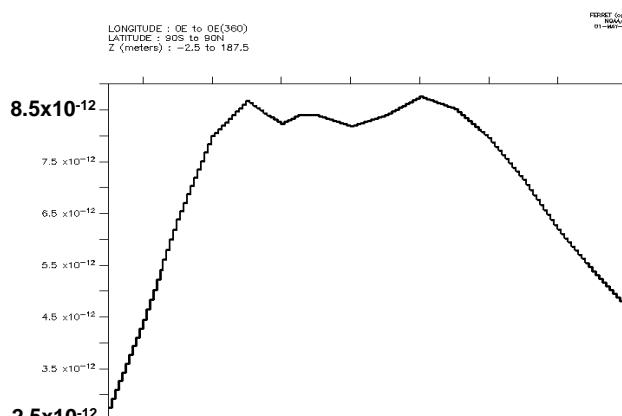
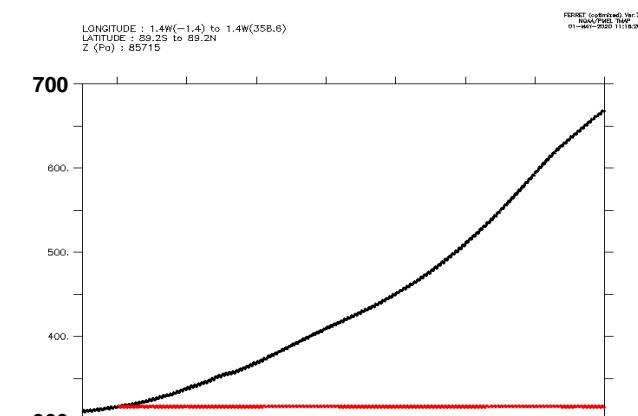
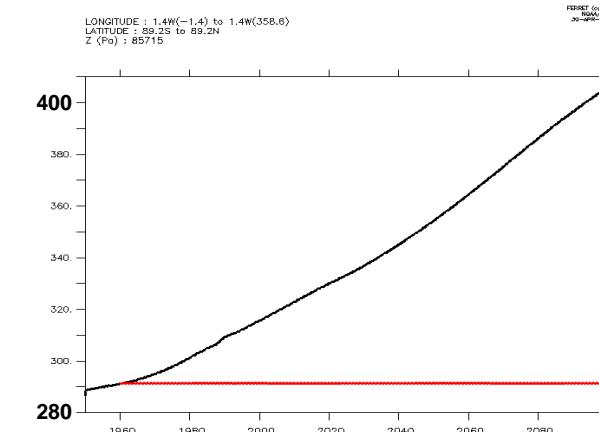
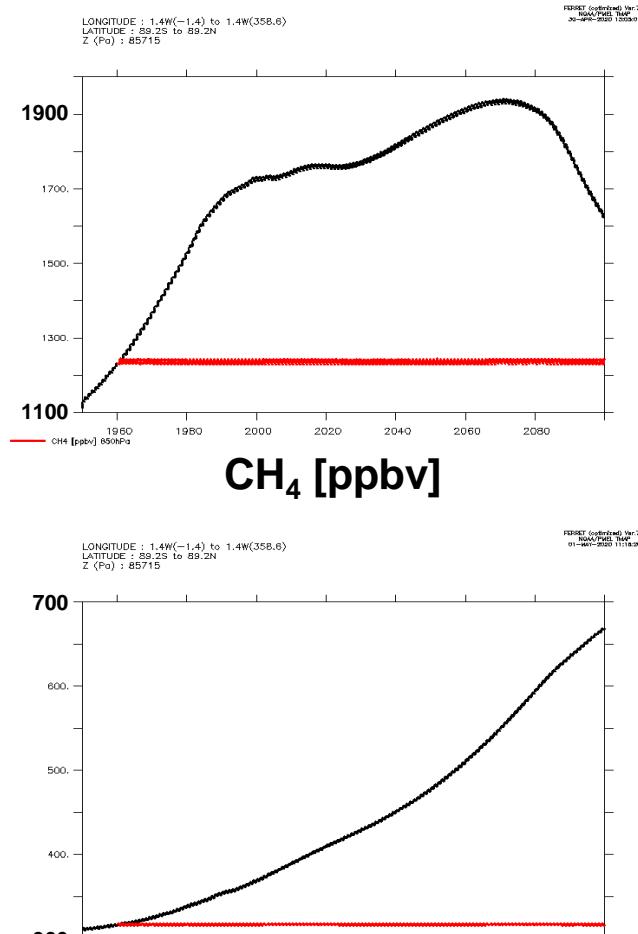
Within the [ESCiMo](#) project various chemistry-climate-simulations were performed for the [CCMI project](#) and the [WMO ozone assessment report](#).

For the current study we use the transient EMAC simulations RC2-base-04 (details in [Jöckel et al., 2016](#)) and SC2-fGHG-01.

RC2-base-04 is a free-running hindcast and future simulation from 1950 to 2100 (REF-C2) performed in the resolution T42L90 (approx. $2.8 \times 2.8^\circ$, from ground up to 0.01 hPa/80 km). The boundary conditions are defined from CCMI (described in [SPARC Newsletter 40](#)), and includes the RCP6.0 scenario for greenhouse gases (GHG), and the A1 scenario for CFCs. The used SSTs and SICs are taken from RCP6.0 simulations of the HadleyCentre Global Environment Model version 2 - Earth System (HadGEM2-ES). The simulation includes a detailed chemistry.

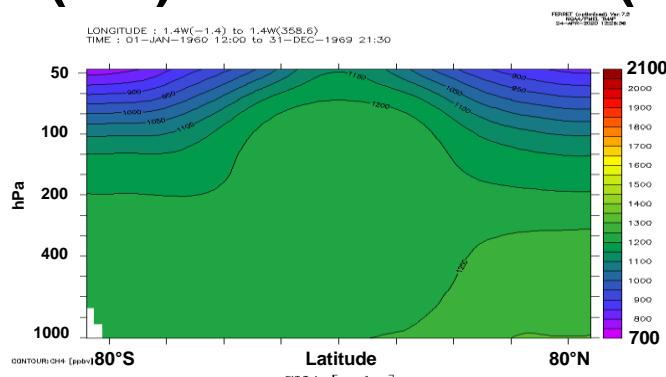
SC2-fGHG-01 were performed from 1960 to 2100 and initialized from a rerun file of RC2-base-04. The simulation has the same model setup as RC2-base-04, but fixes the GHG at 1960 levels and also repeats the SST and SICs of 1960 (climatological average of 1955 to 1964).

Exemplary boundary conditions of RC2-base-04 (black) and SC2-fGHG-01 (red)

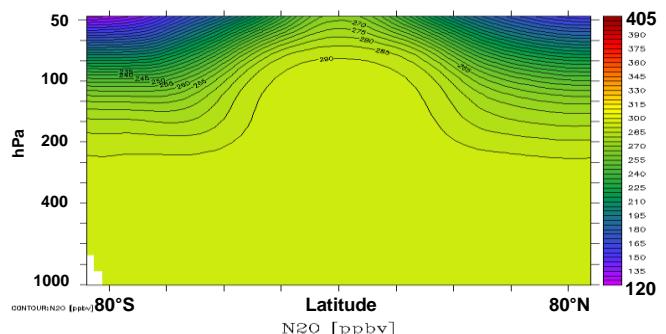


Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

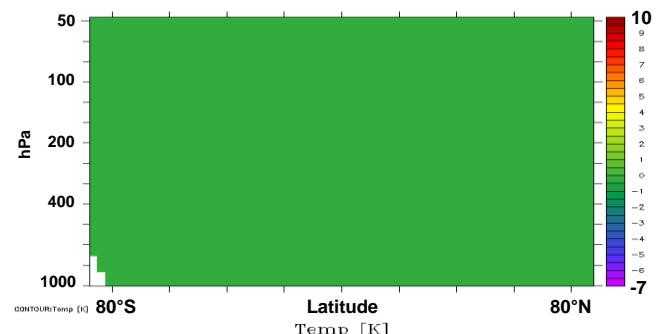
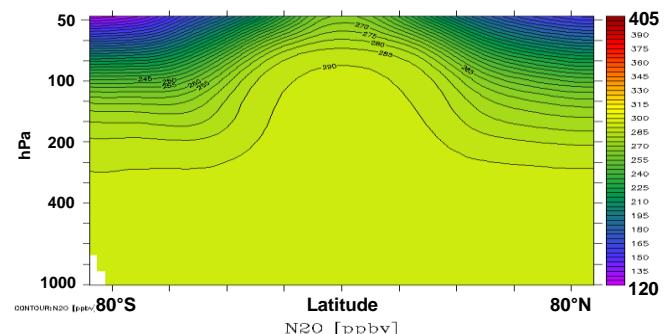
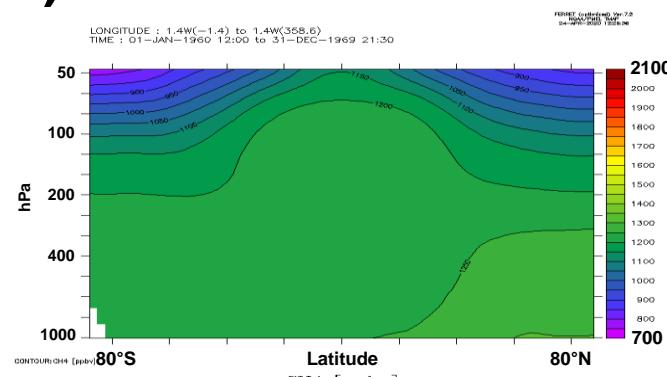
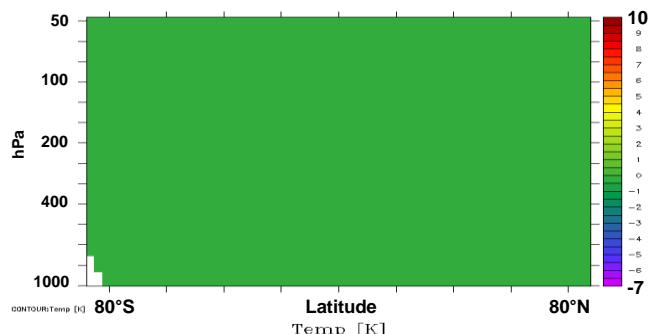
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



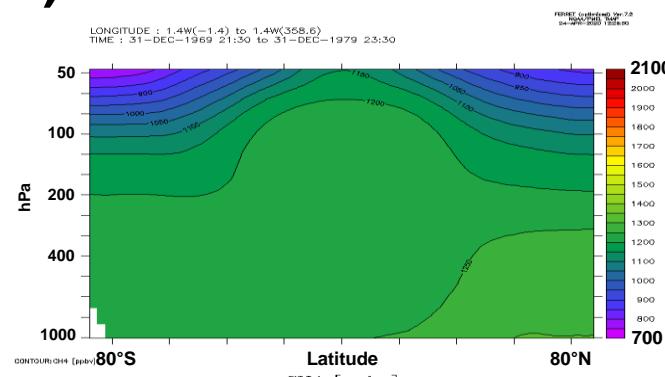
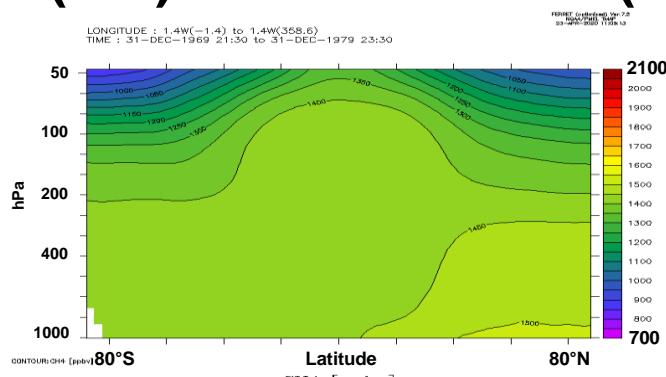
Temp. (K)
Difference to
1960-1969



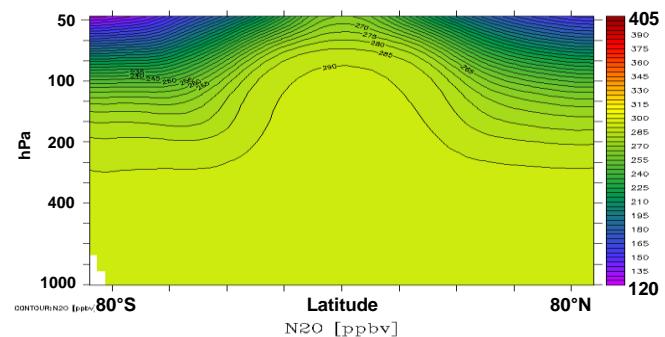
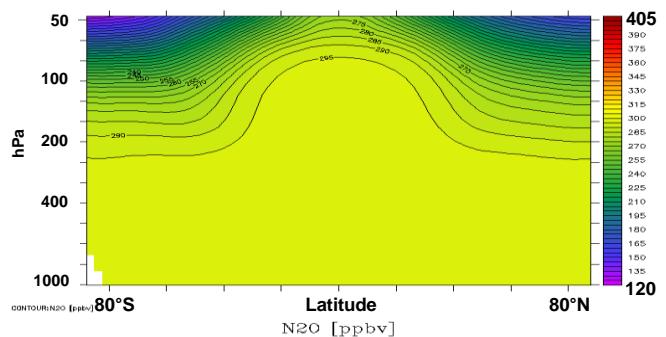
1960-69

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

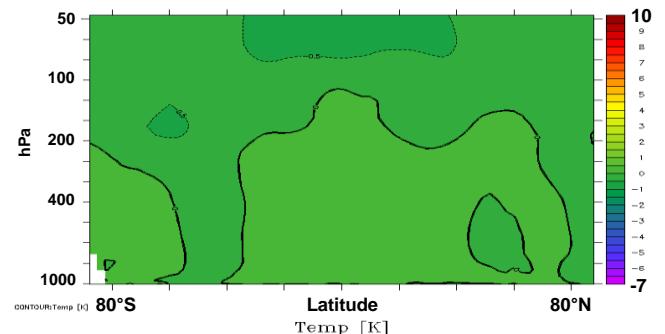
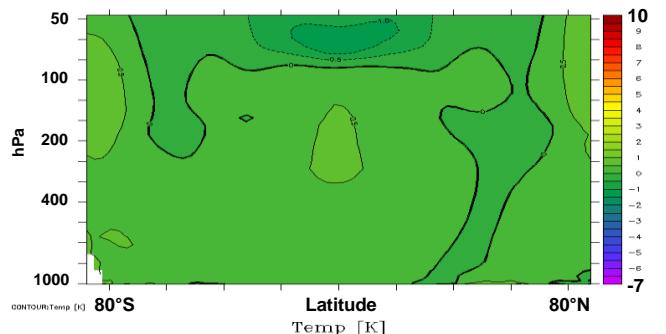
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



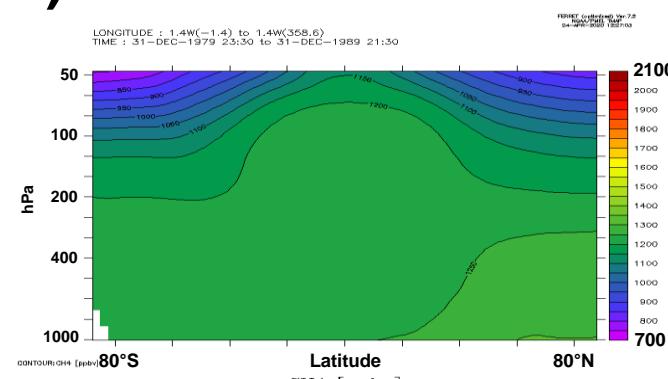
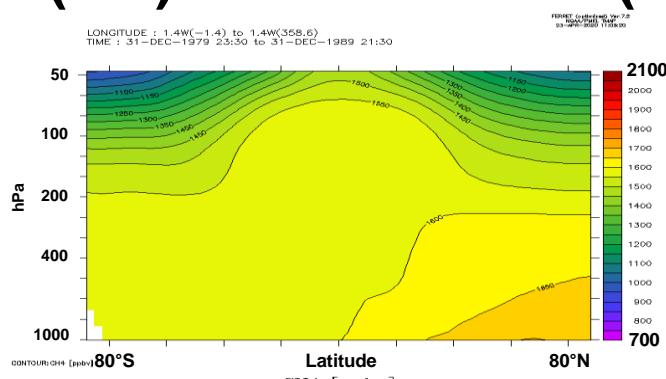
Temp. (K)
Difference to
1960-1969



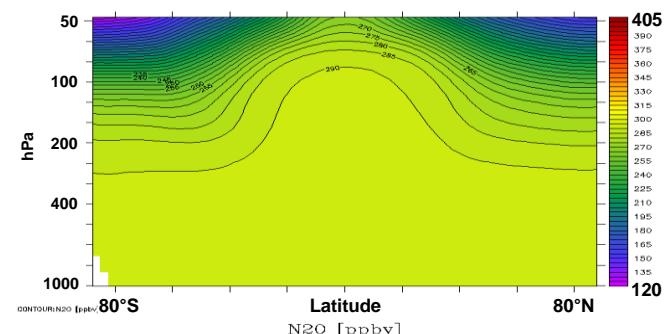
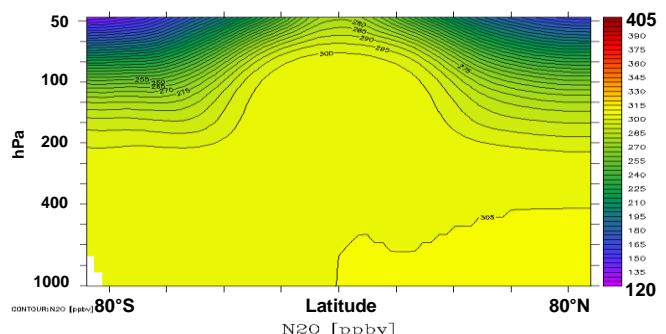
1970-79

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

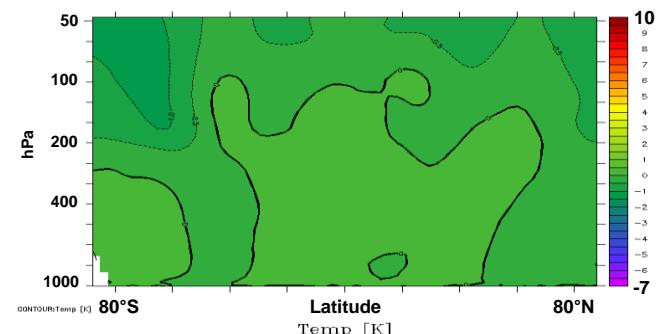
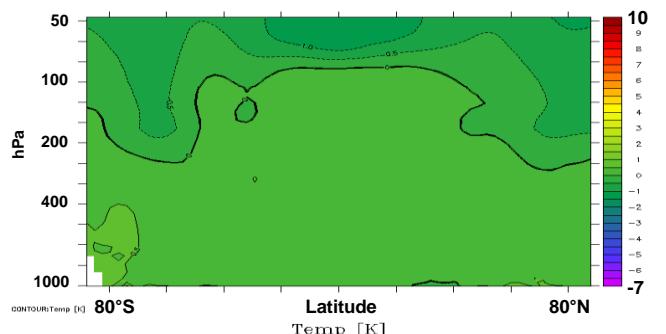
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



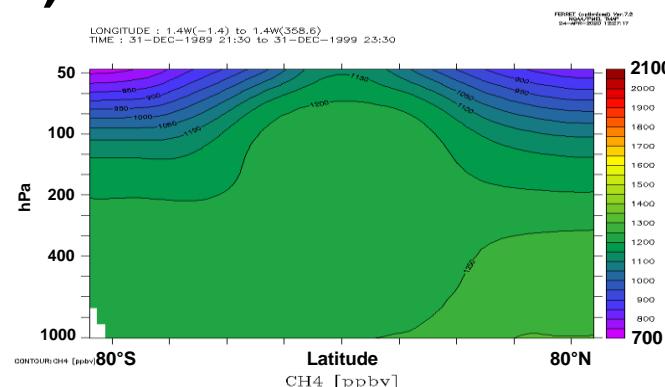
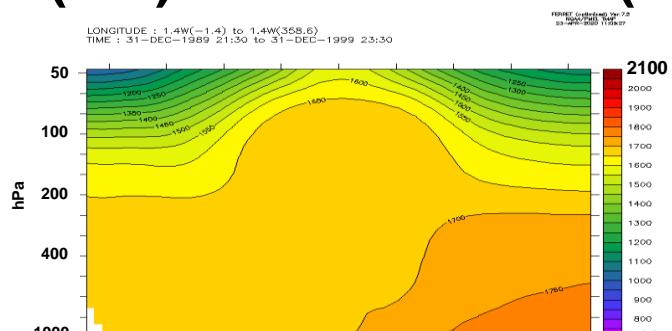
Temp. (K)
Difference to
1960-1969



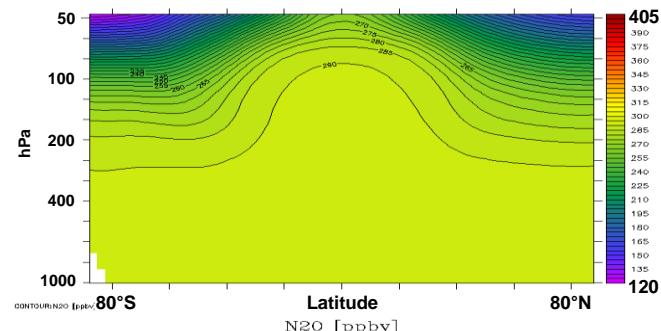
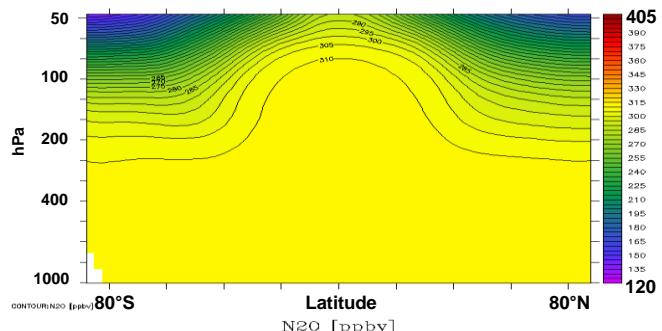
1980-89

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

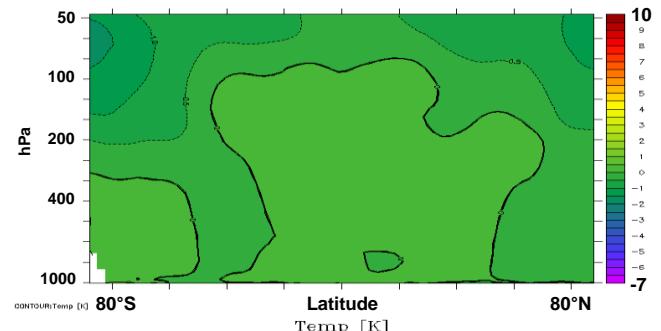
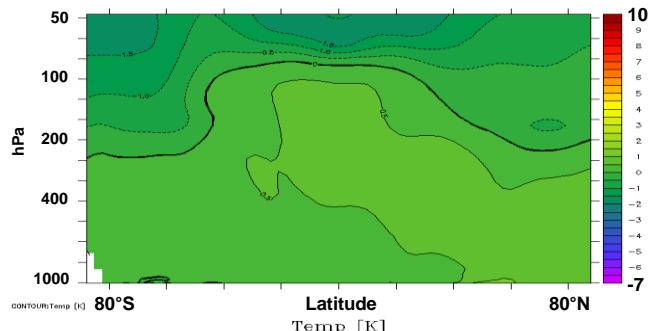
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



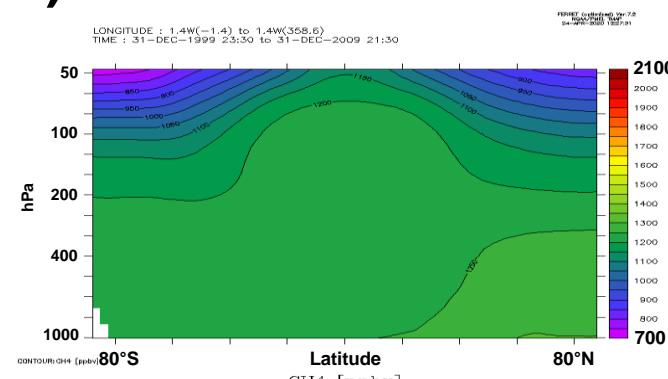
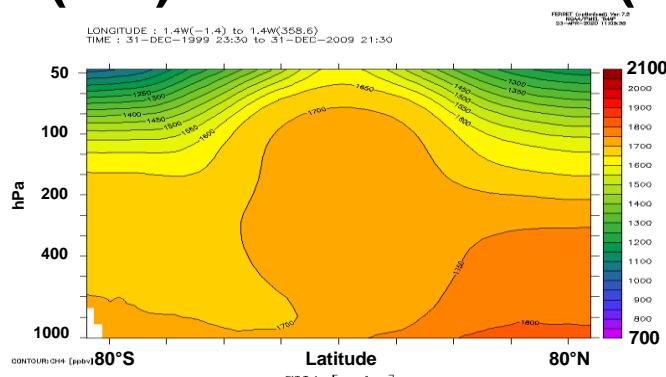
Temp. (K)
Difference to
1960-1969



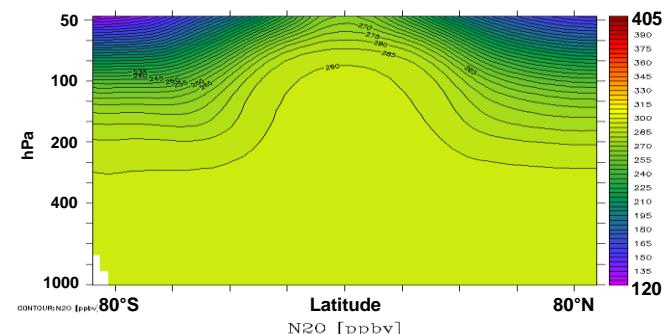
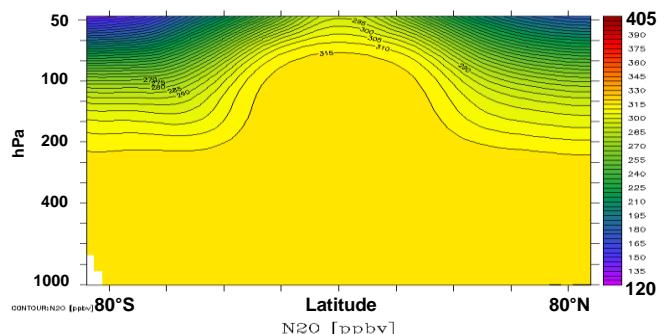
1990-99

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

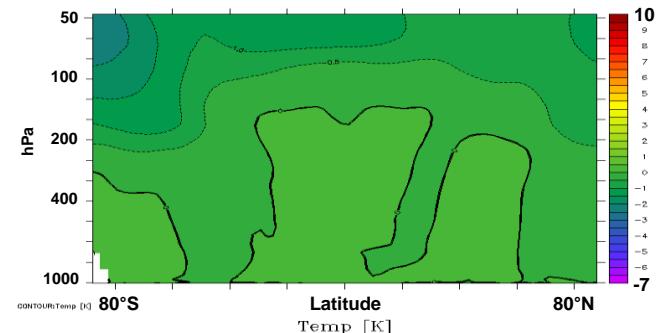
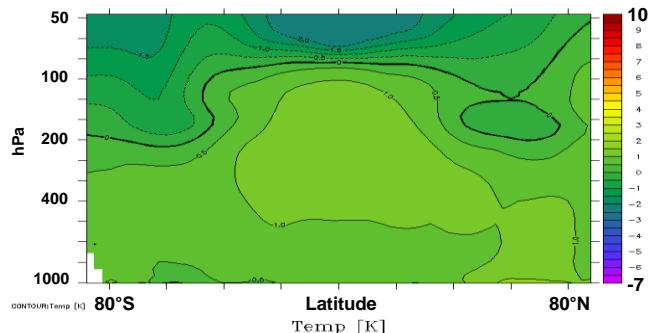
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



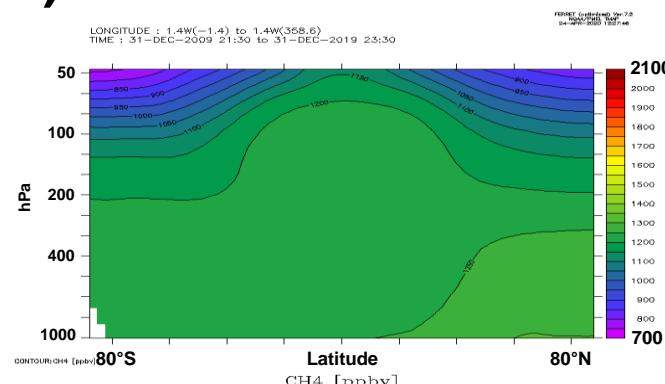
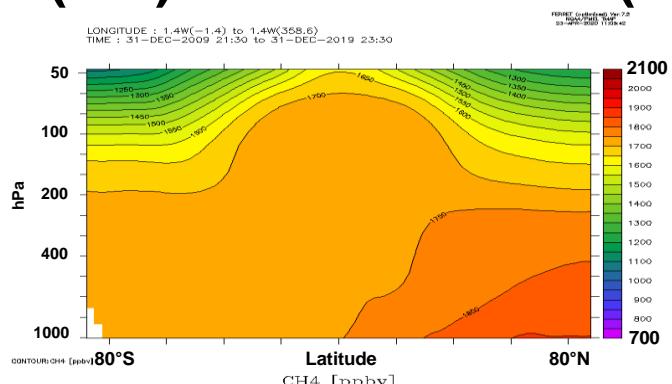
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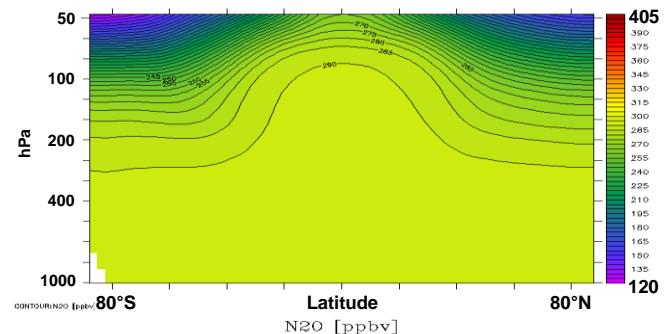
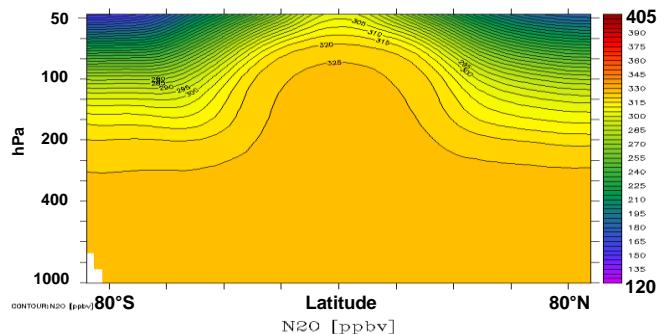
2000-09

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

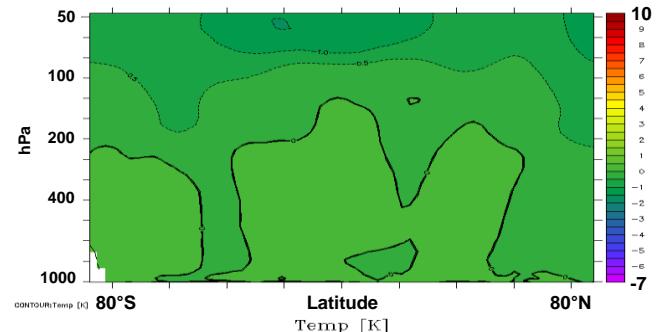
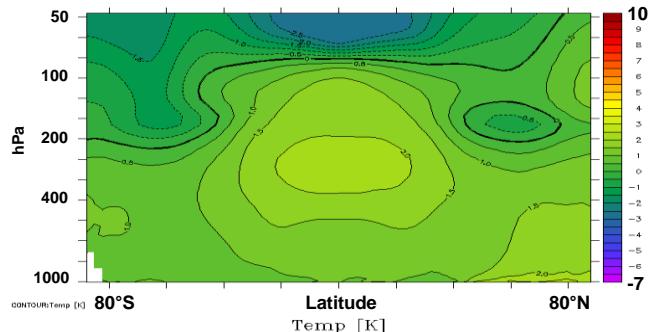
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



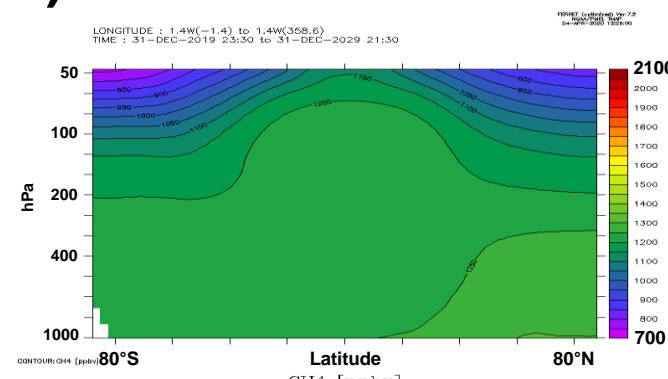
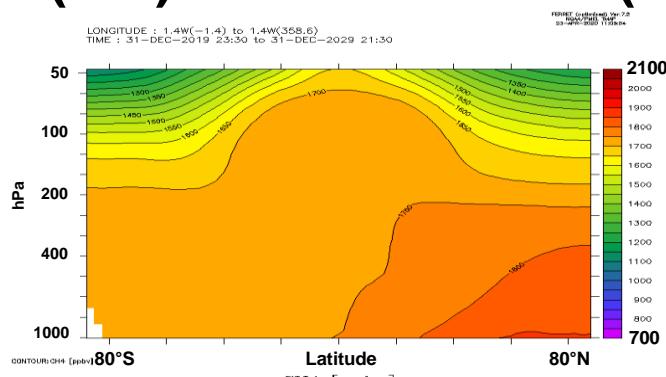
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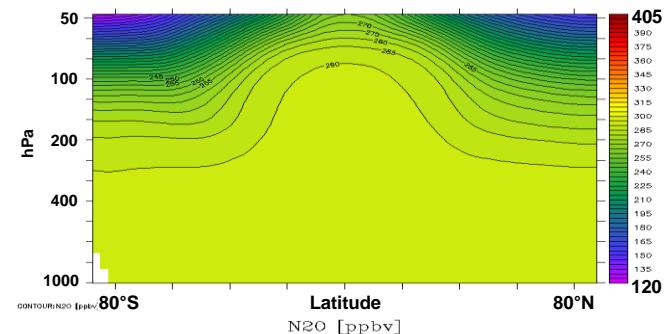
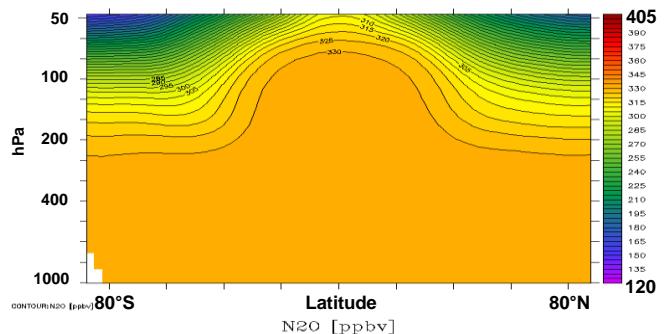
2010-19

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

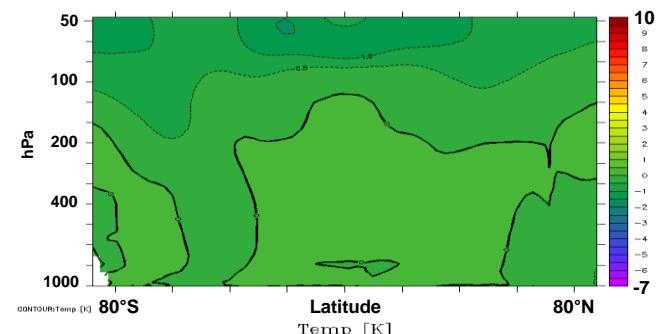
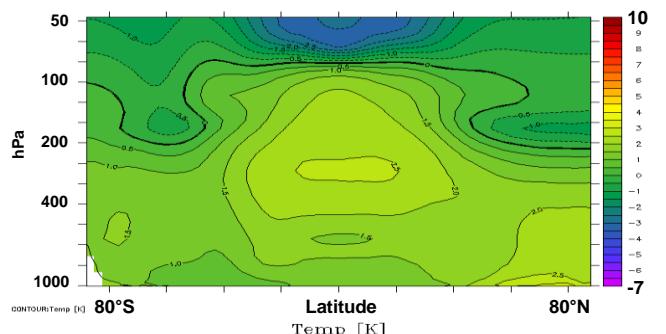
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
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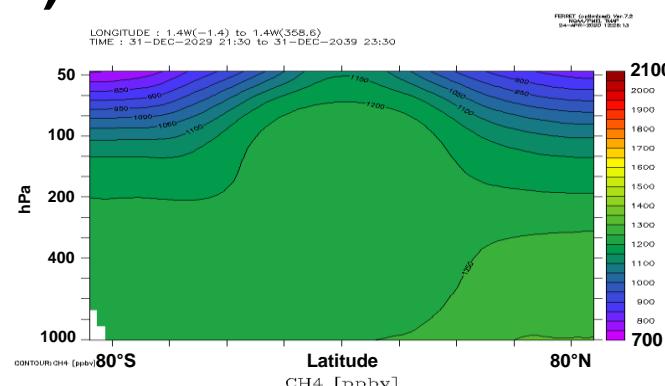
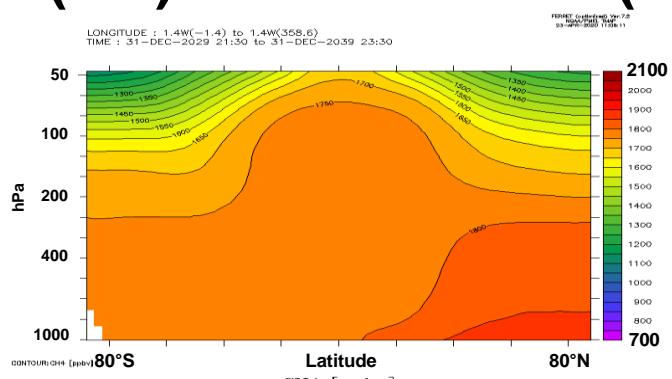
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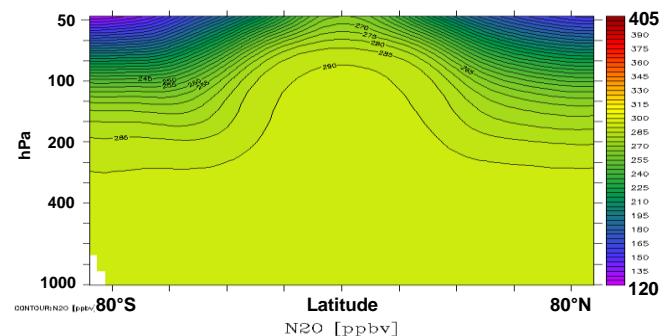
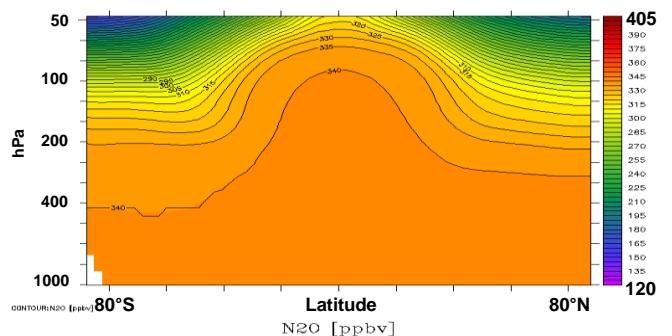
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Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

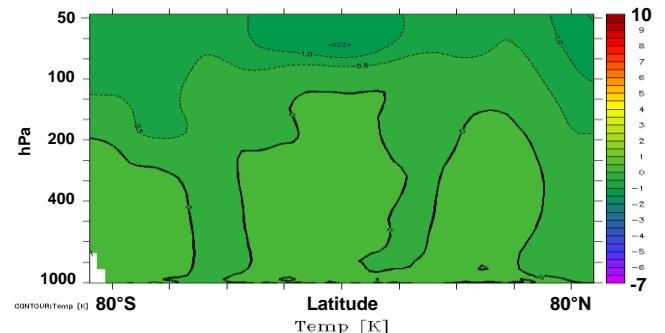
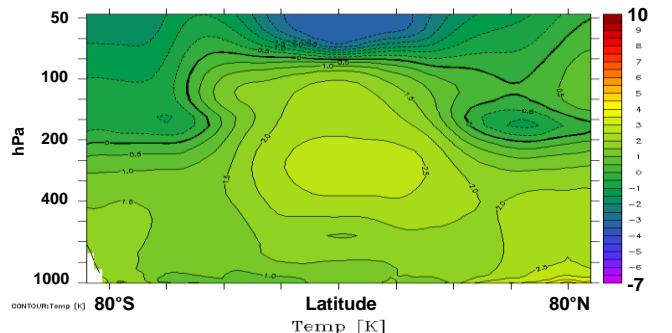
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



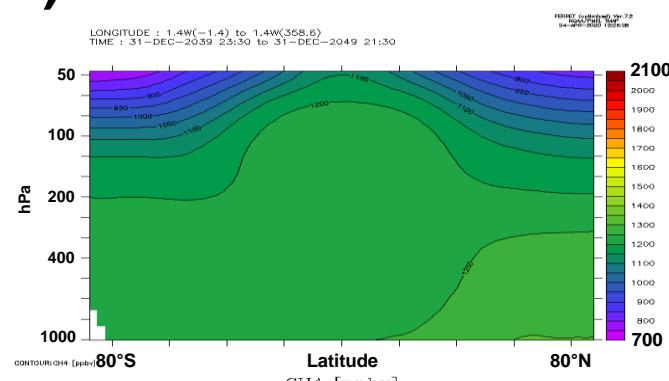
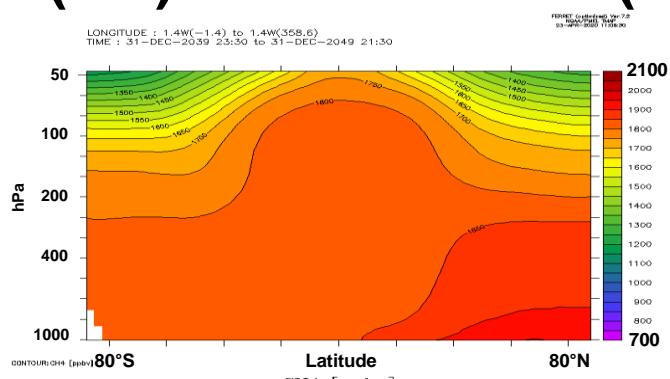
Temp. (K)
Difference to
1960-1969



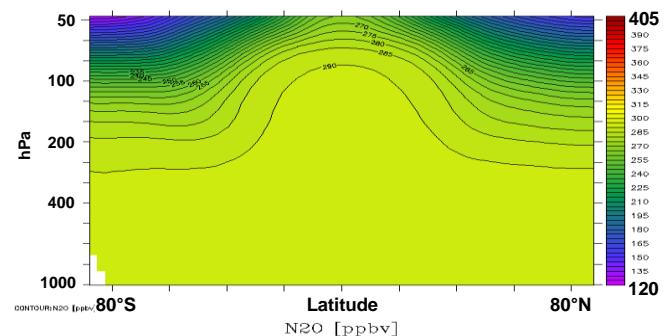
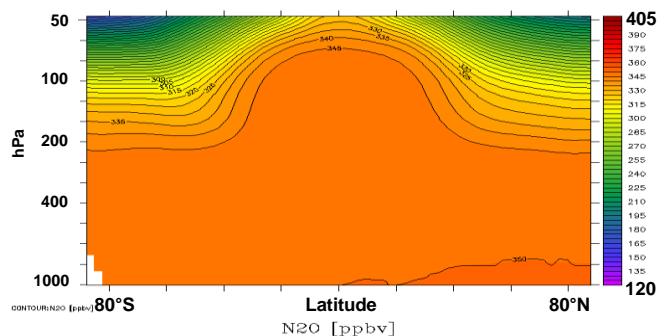
2030-39

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

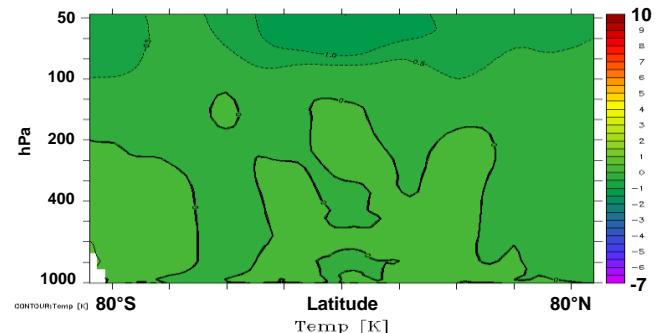
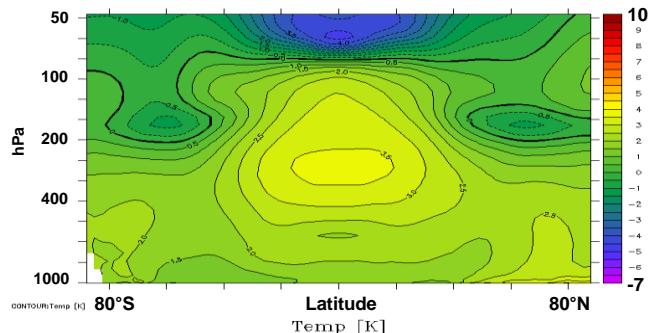
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



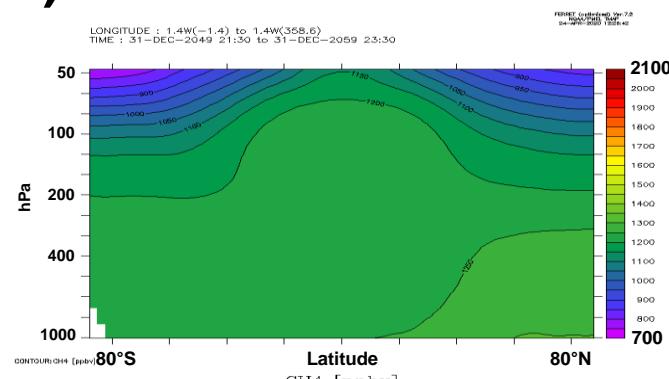
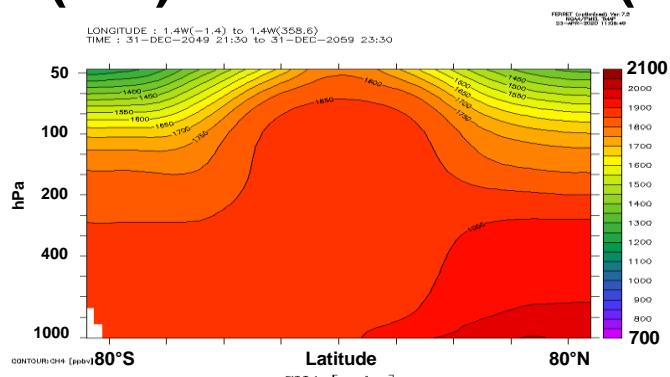
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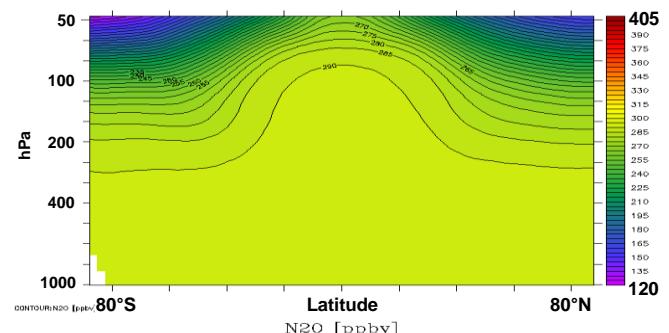
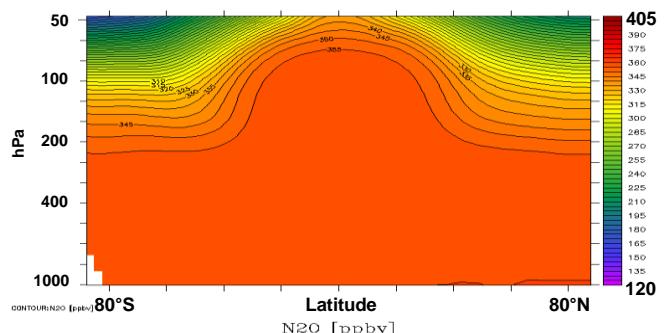
2040-49

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

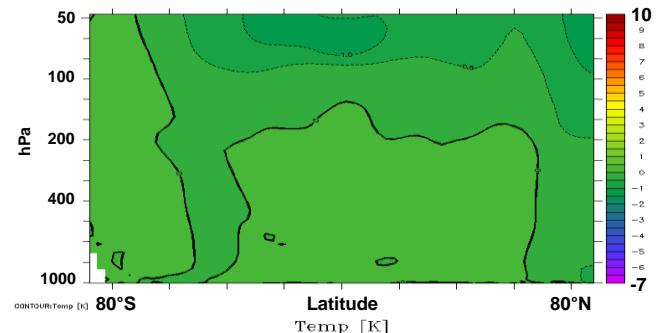
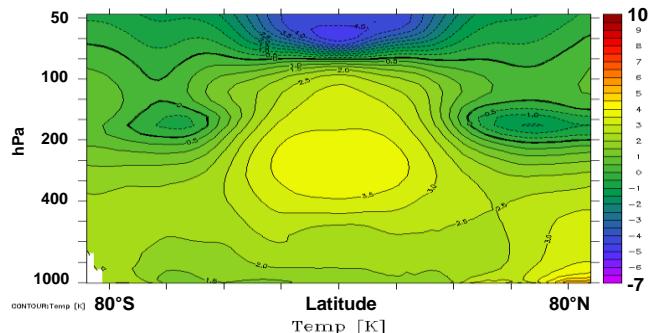
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



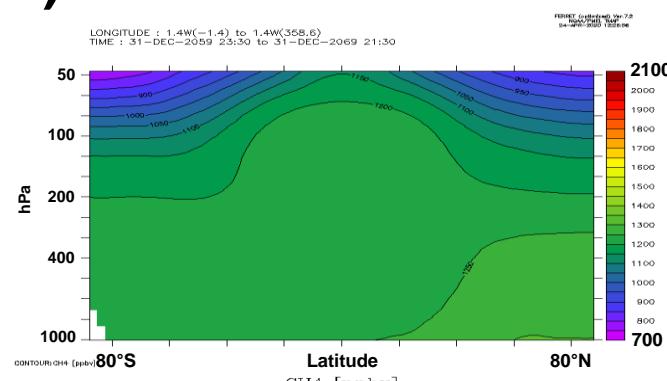
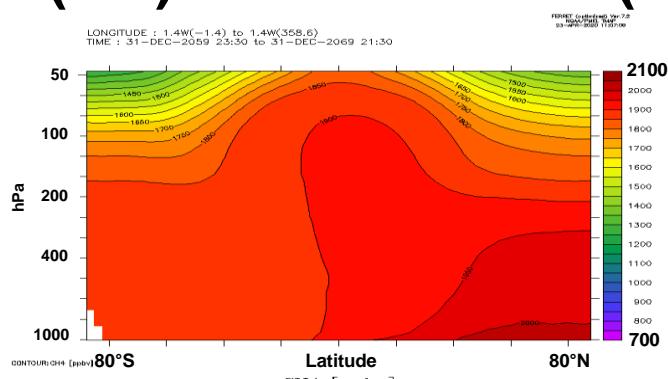
Temp. (K)
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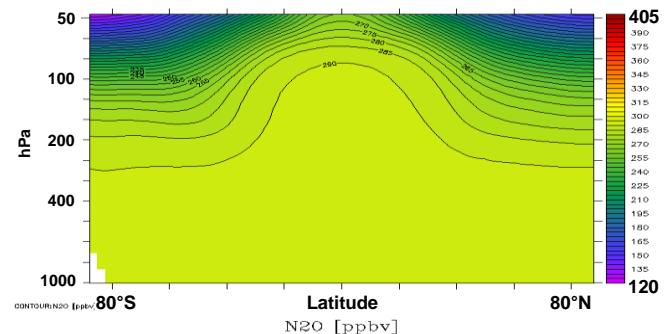
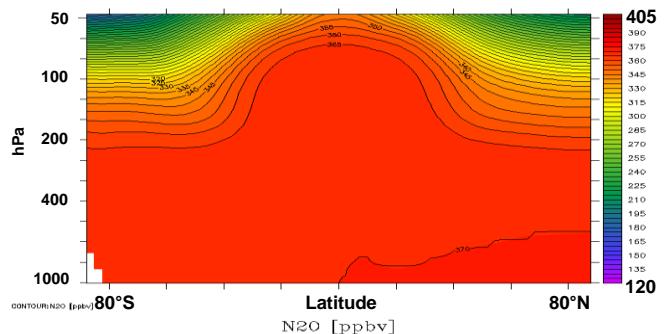
2050-59

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

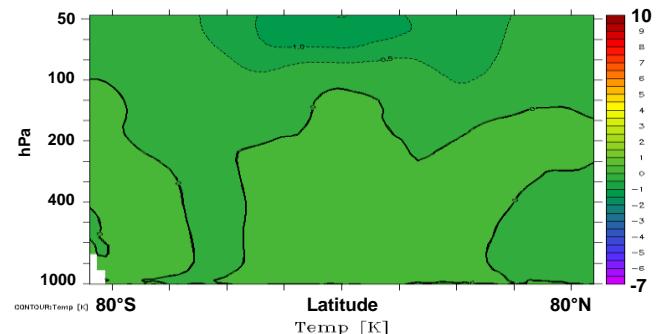
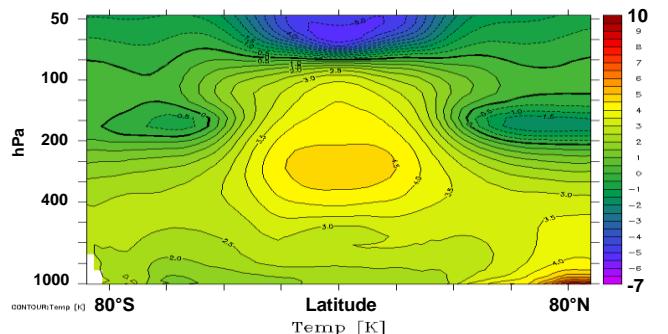
CH₄ (ppbv)
Ten year and
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N₂O (ppbv)
Ten year and
zonal mean



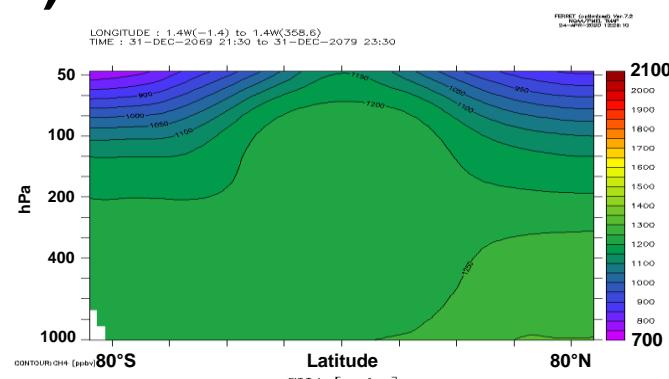
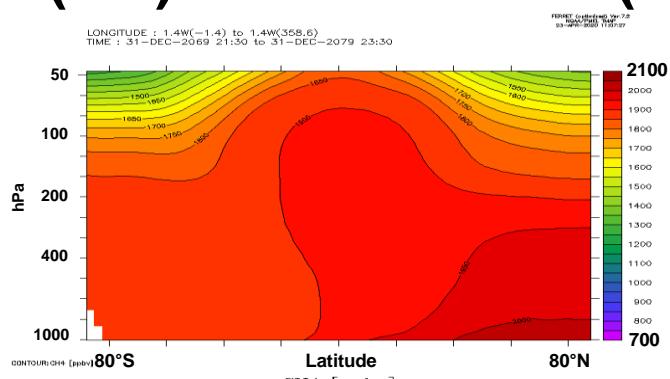
Temp. (K)
Difference to
1960-1969



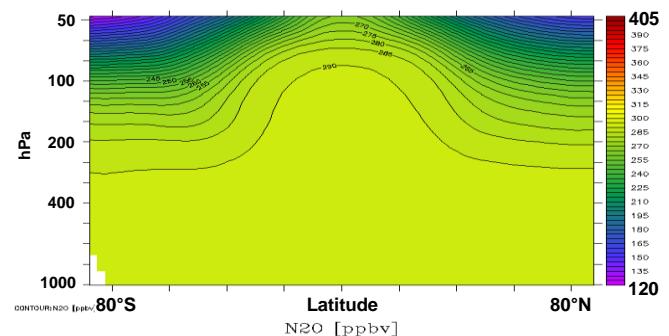
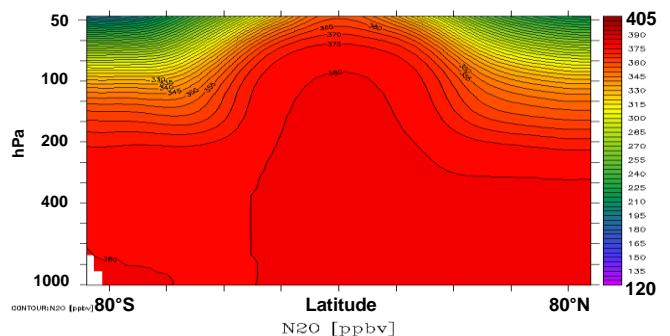
2060-69

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

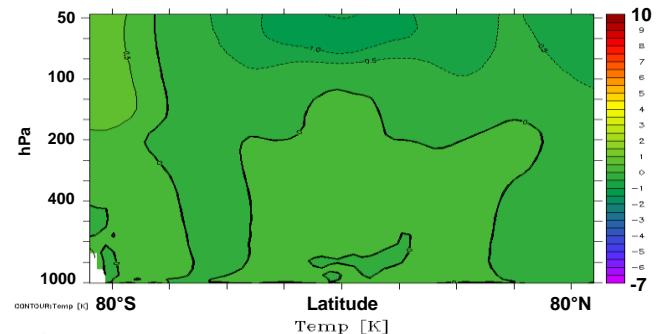
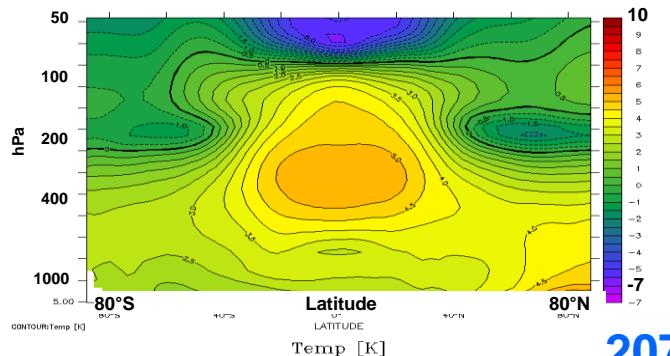
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



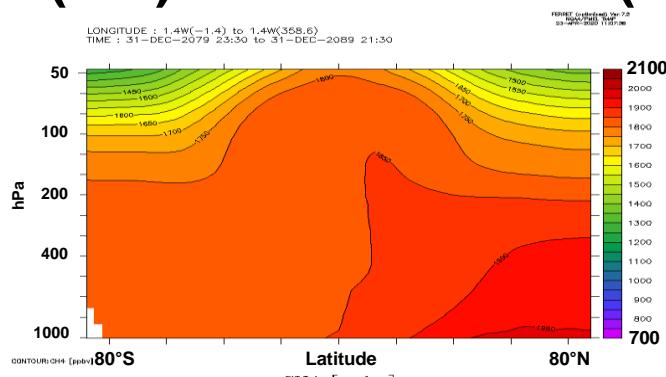
Temp. (K)
Difference to
1960-1969



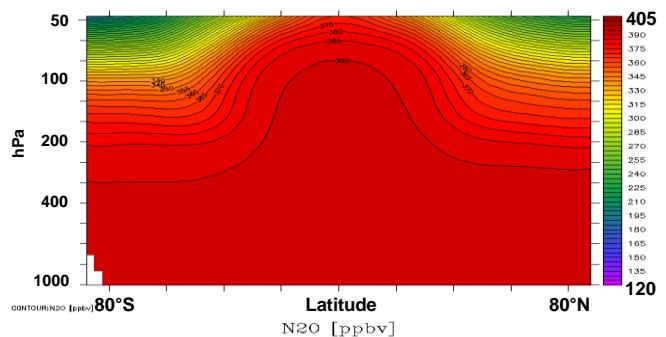
2070-79

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

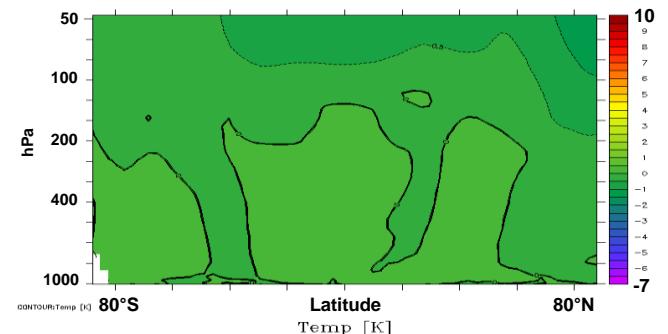
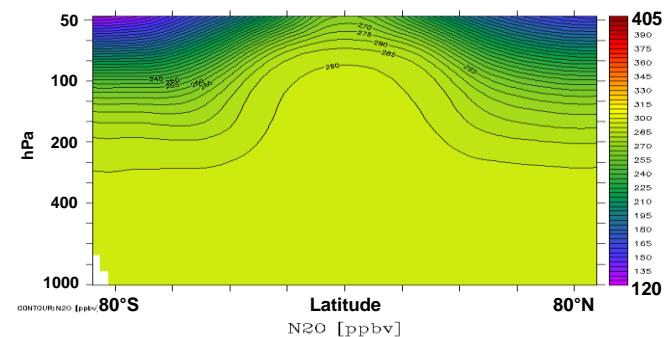
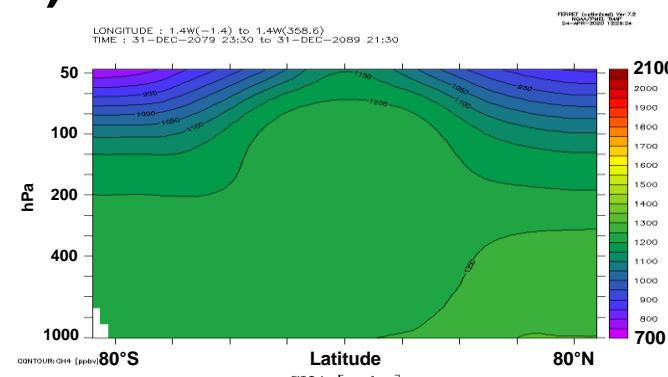
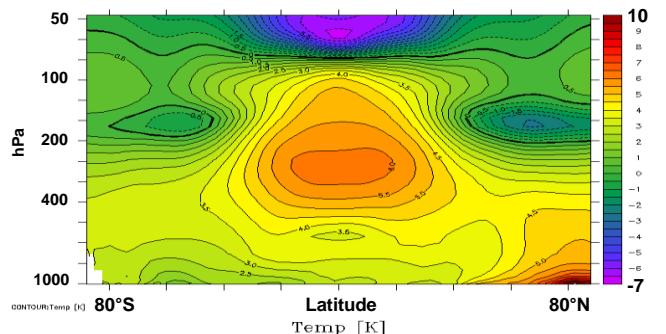
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



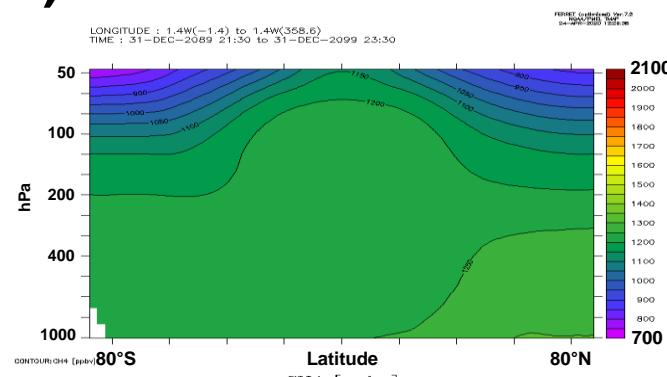
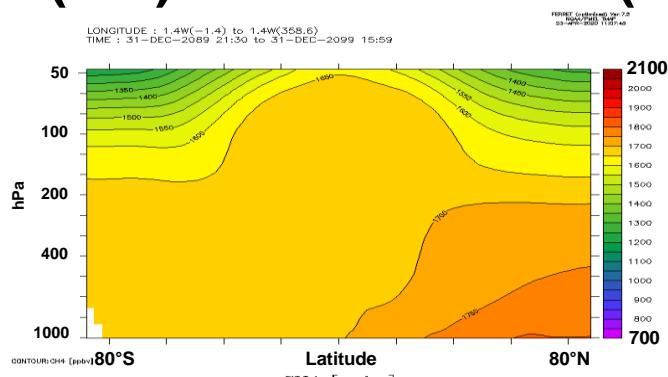
Temp. (K)
Difference to
1960-1969



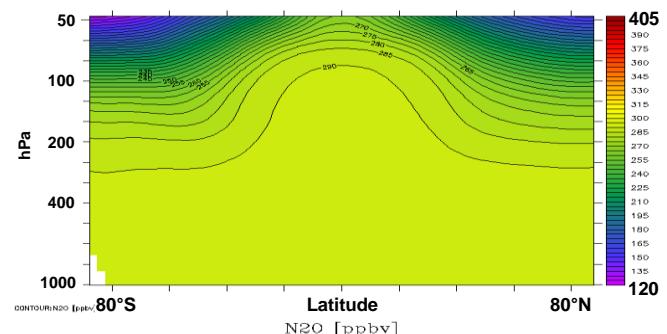
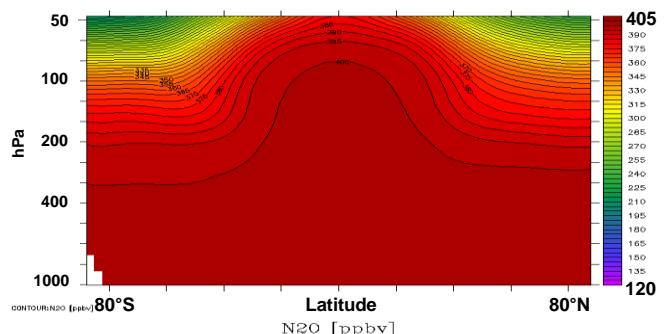
2080-89

Development of N₂O, CH₄ and temperature in RC2-base (left) and SC2-fGHG (right) from 1960-2099

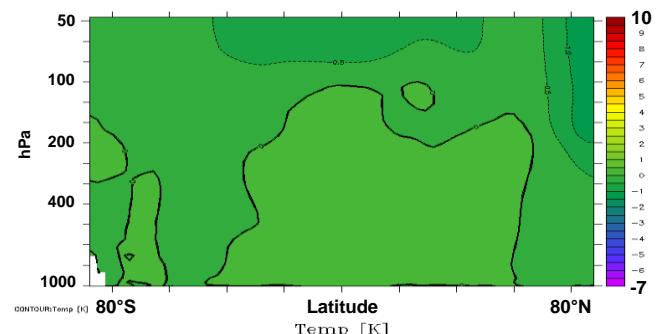
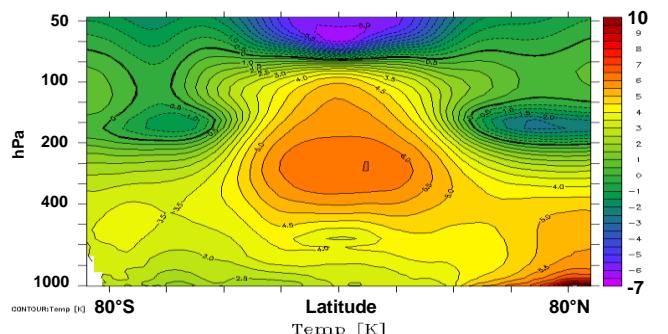
CH₄ (ppbv)
Ten year and
zonal mean



N₂O (ppbv)
Ten year and
zonal mean



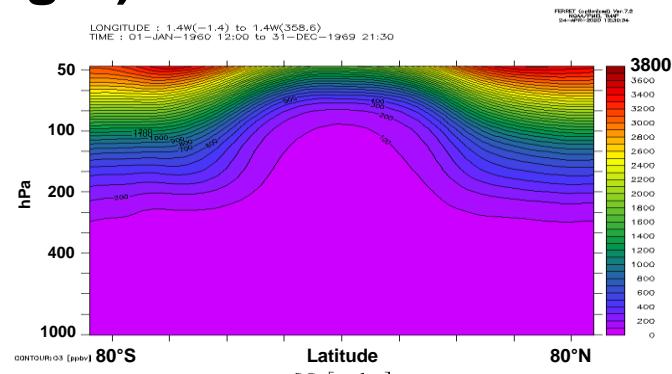
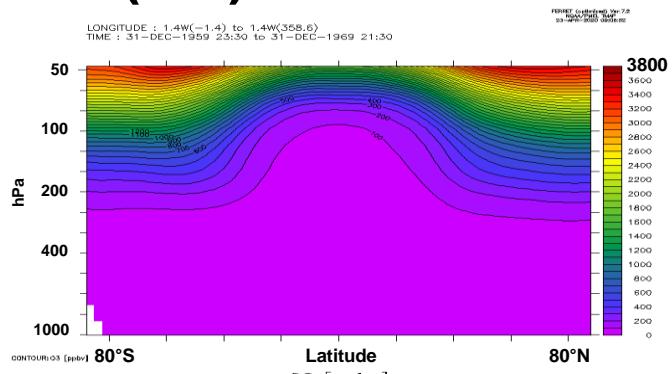
Temp. (K)
Difference to
1960-1969



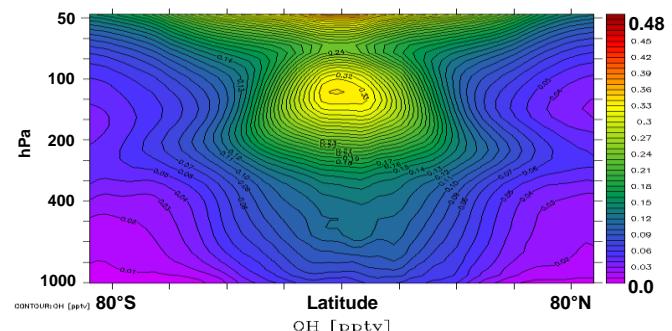
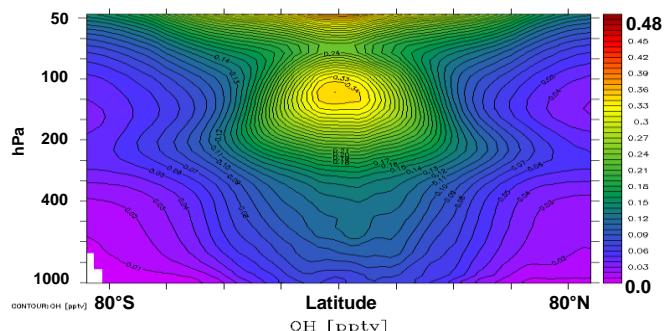
2090-99

Distribution of ozone (O_3), OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) 1960-1969

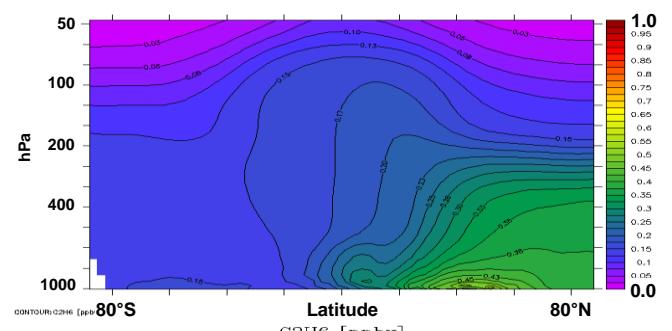
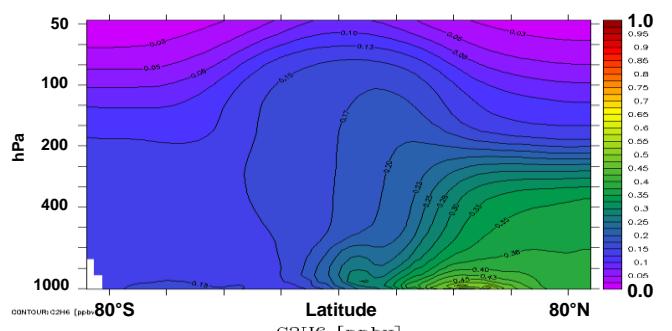
O_3 (ppbv)
Ten year and
zonal mean



OH (pptv)
Ten year and
zonal mean



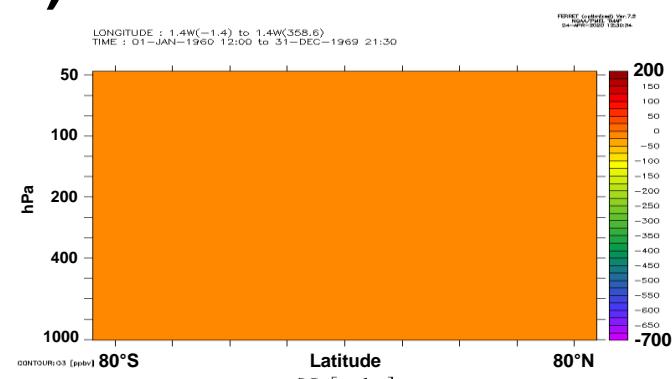
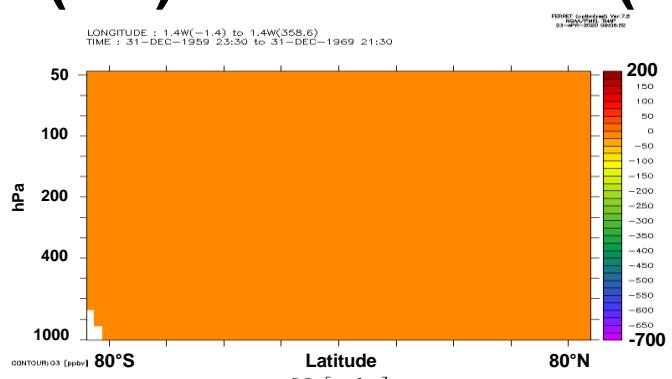
C_2H_6 (ppbv)
Ten year and
zonal mean



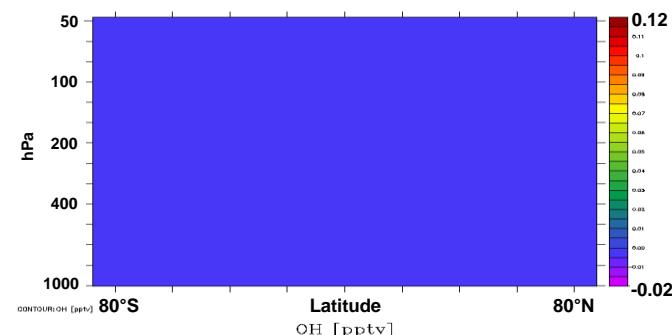
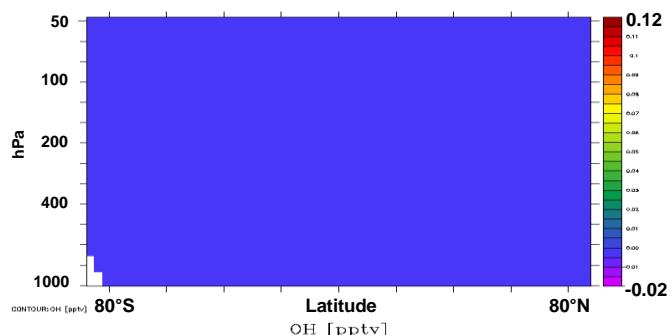
1960-69

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

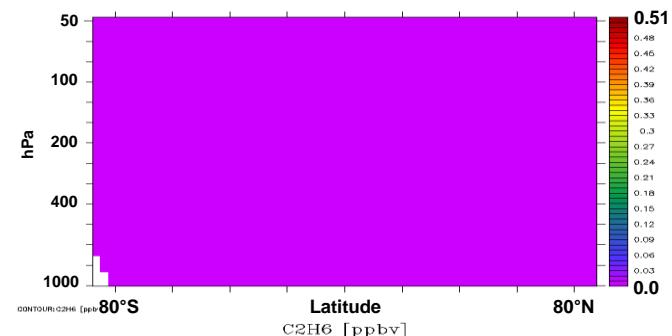
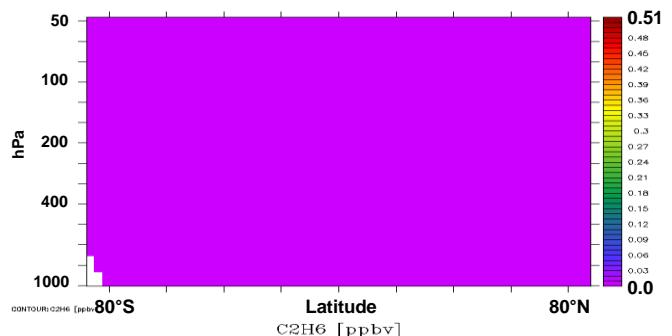
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



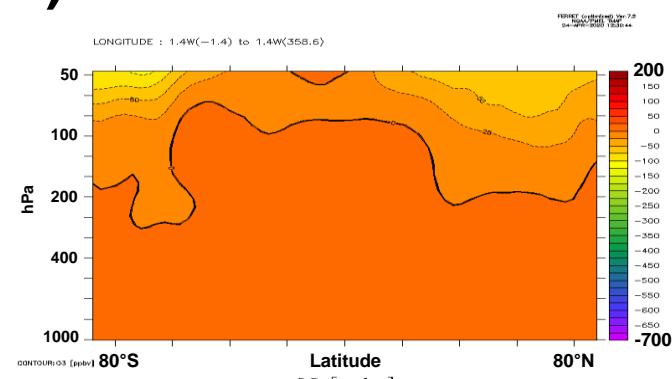
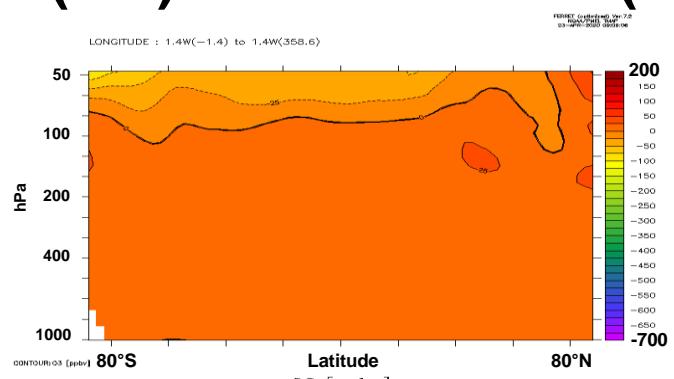
C₂H₆ (ppbv)
Difference to
1960-1969



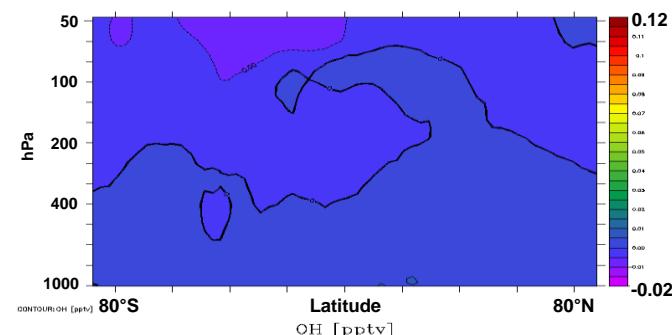
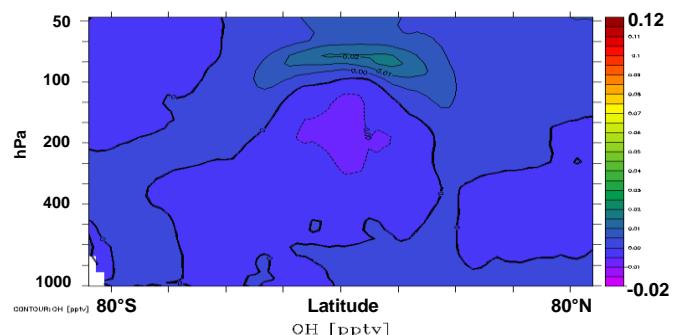
1960-69

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

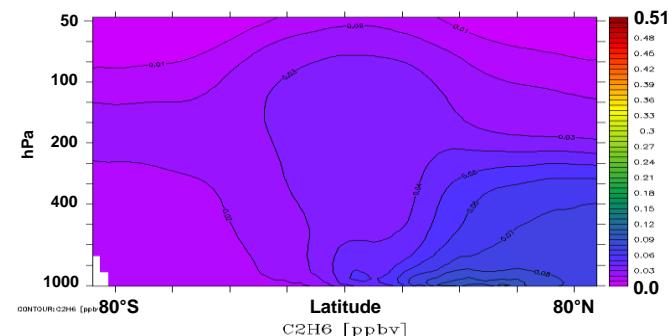
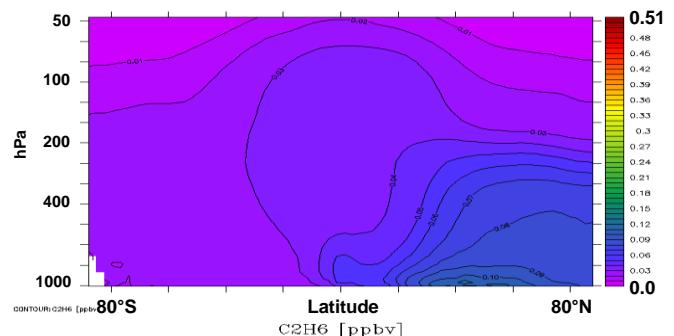
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



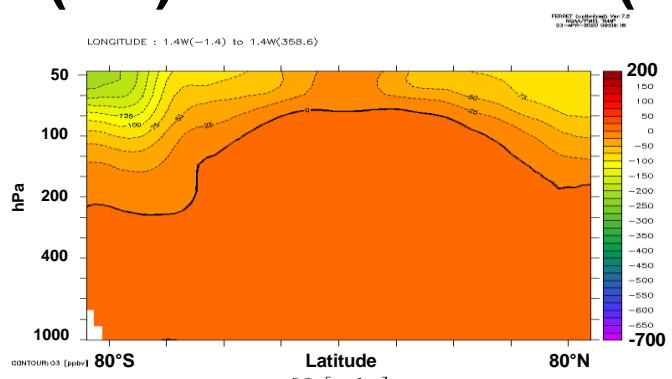
C_2H_6 (ppbv)
Difference to
1960-1969



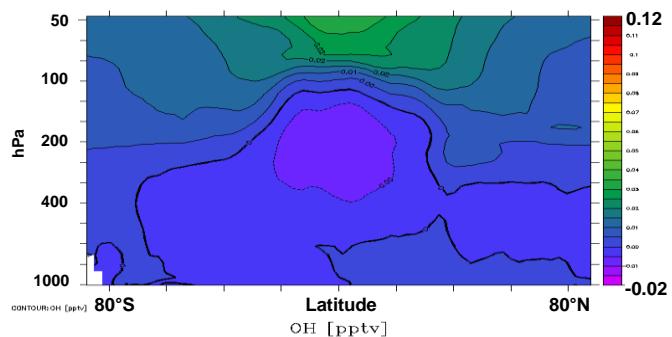
1970-79

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

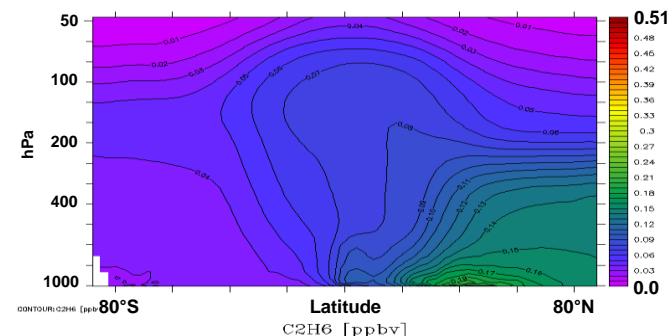
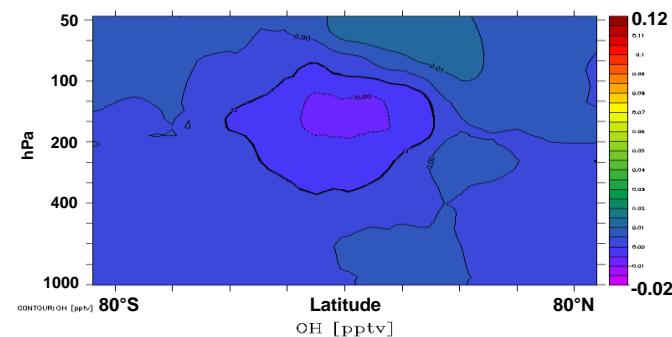
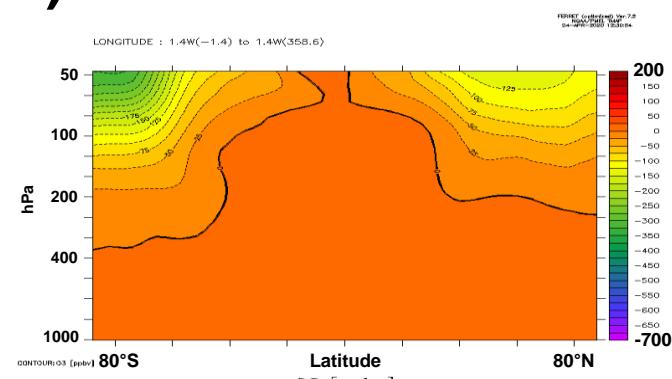
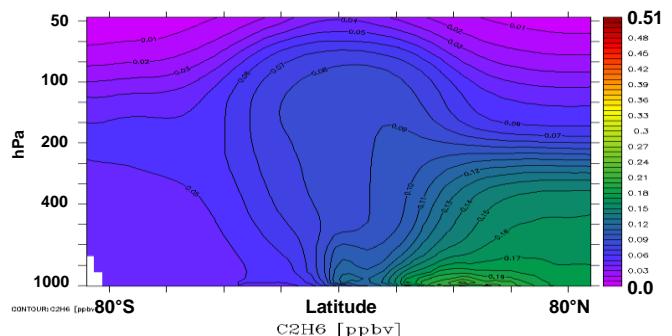
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



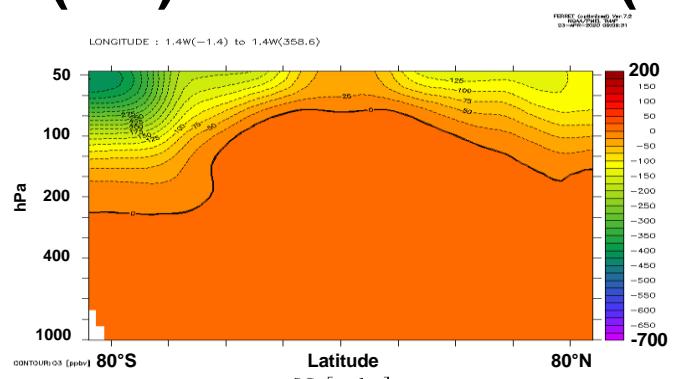
C₂H₆ (ppbv)
Difference to
1960-1969



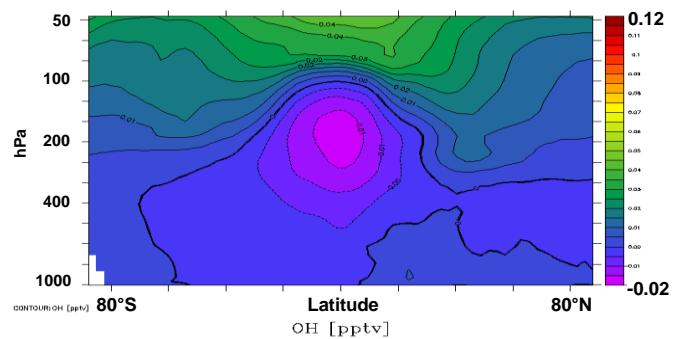
1980-89

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

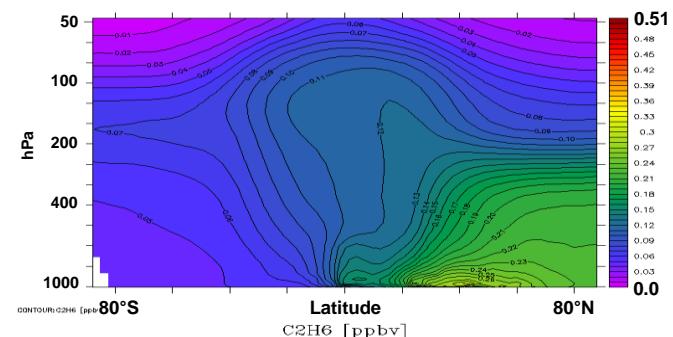
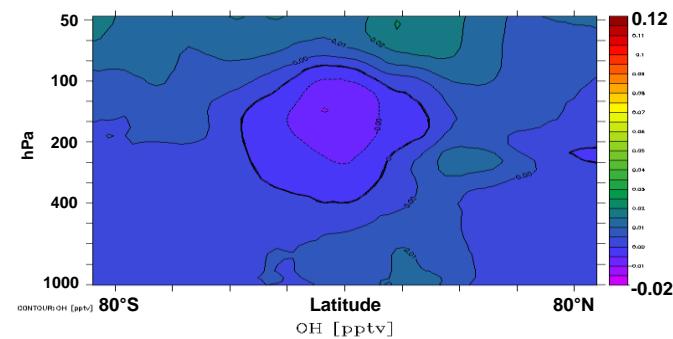
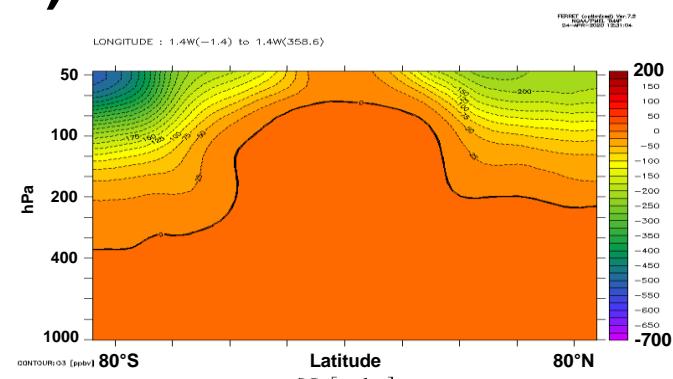
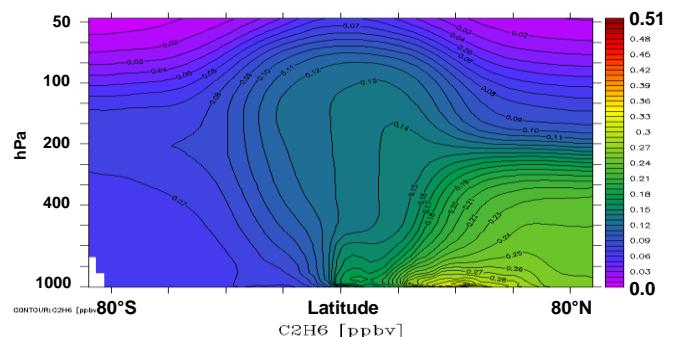
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



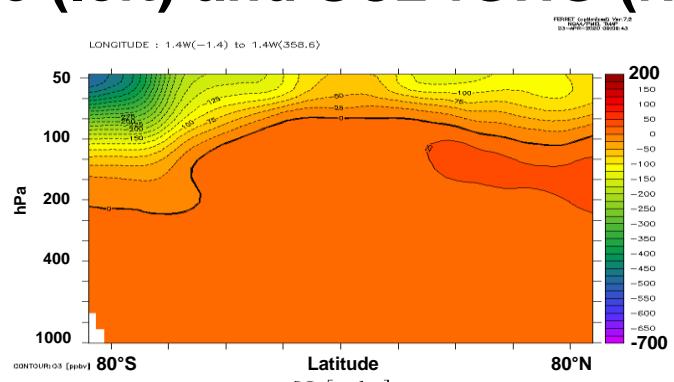
C_2H_6 (ppbv)
Difference to
1960-1969



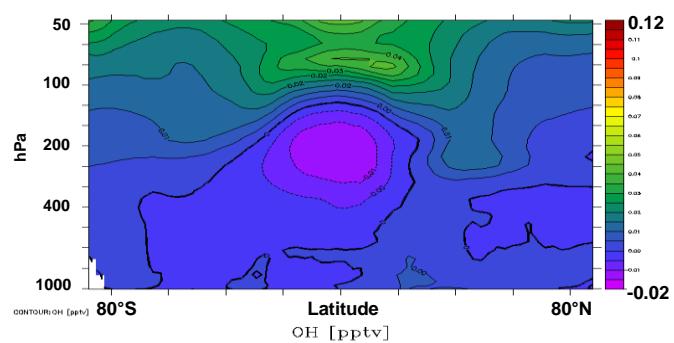
1990-99

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

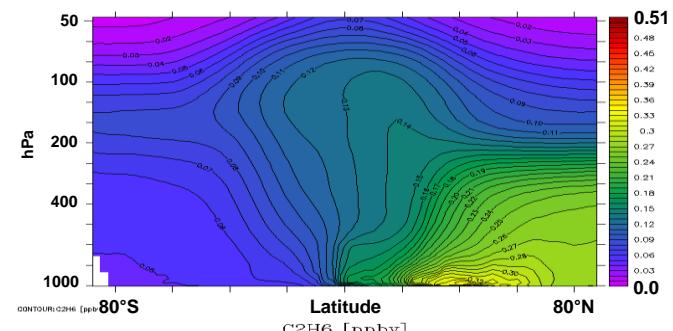
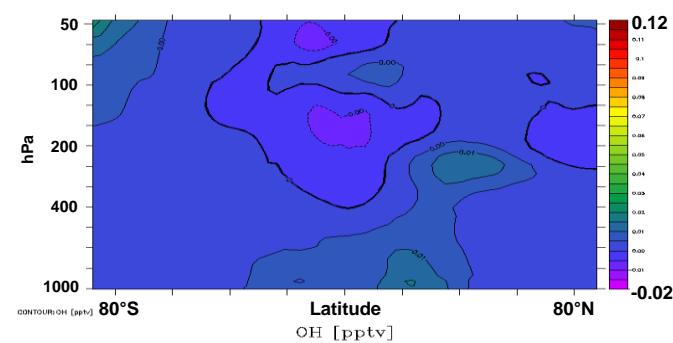
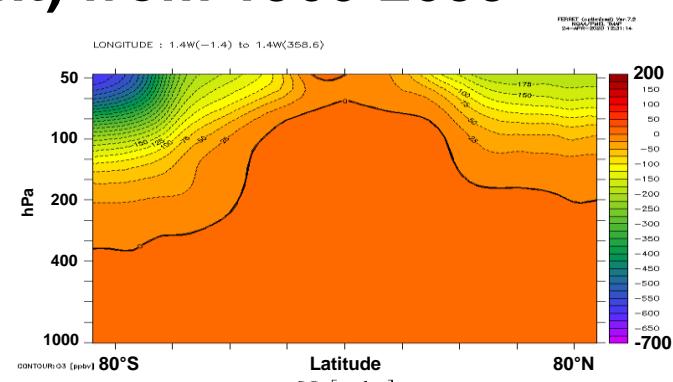
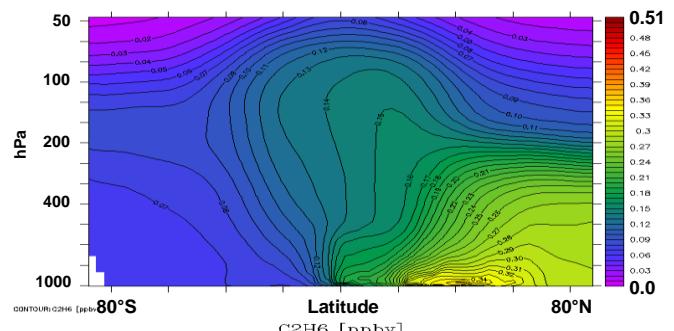
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



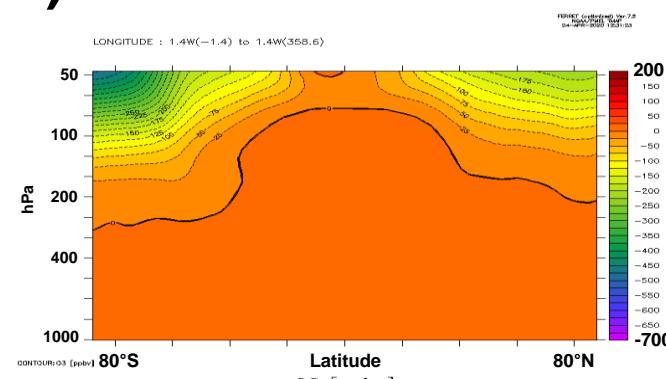
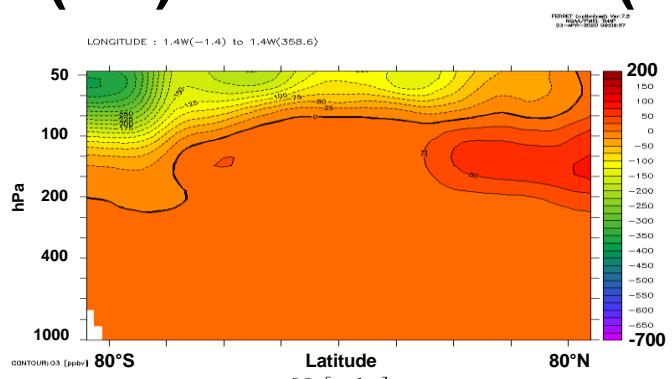
C_2H_6 (ppbv)
Difference to
1960-1969



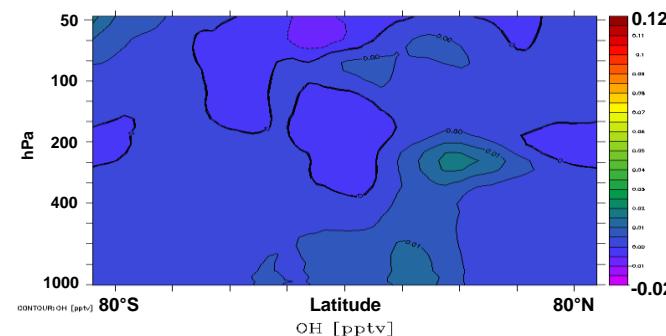
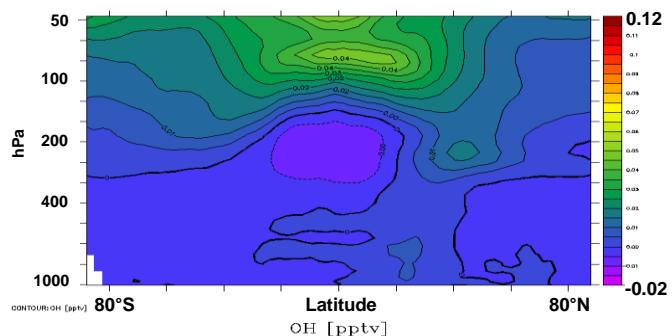
2000-09

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

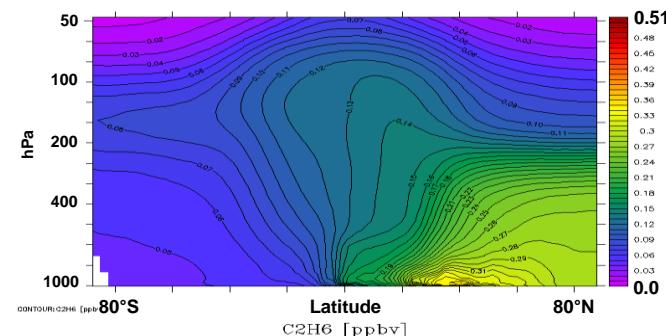
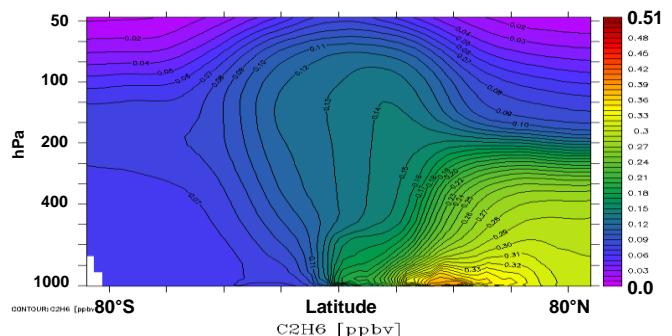
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



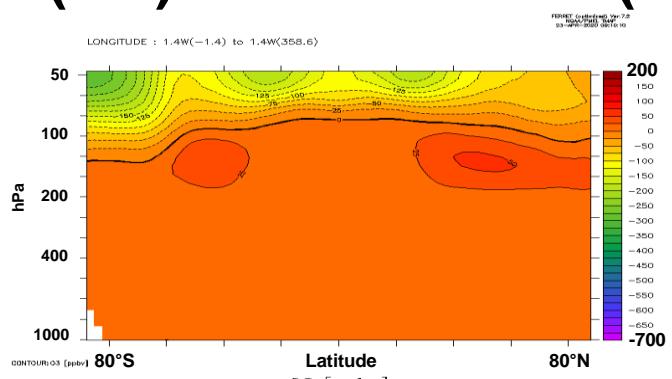
C₂H₆ (ppbv)
Difference to
1960-1969



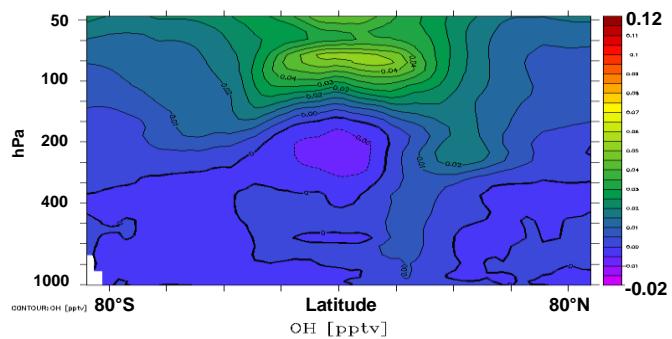
2010-19

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

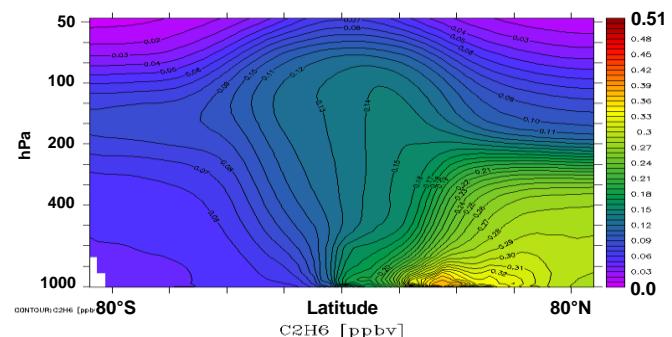
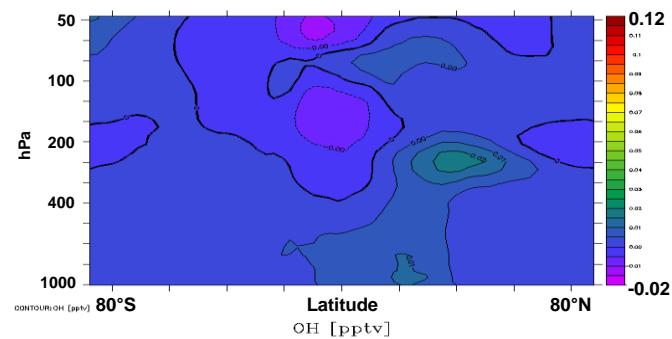
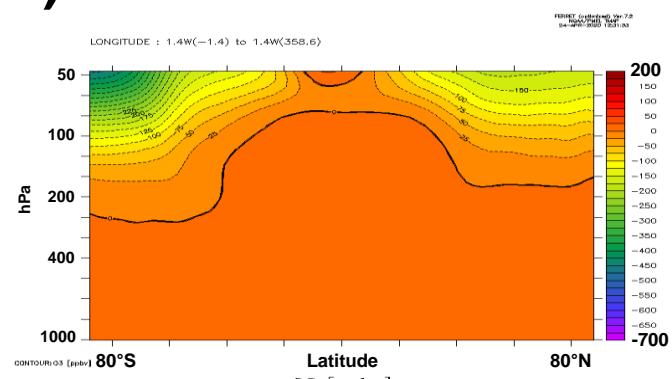
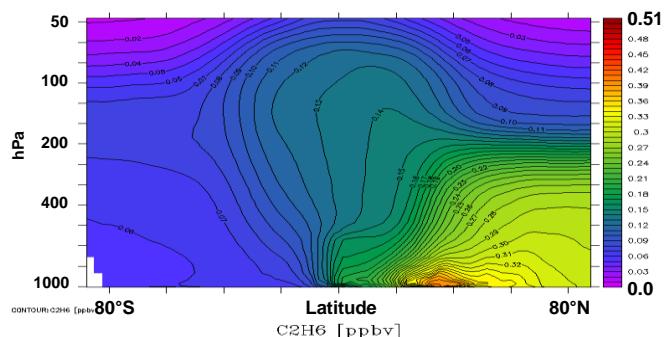
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



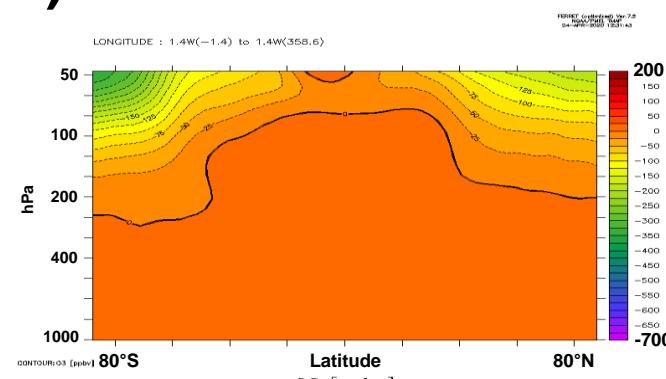
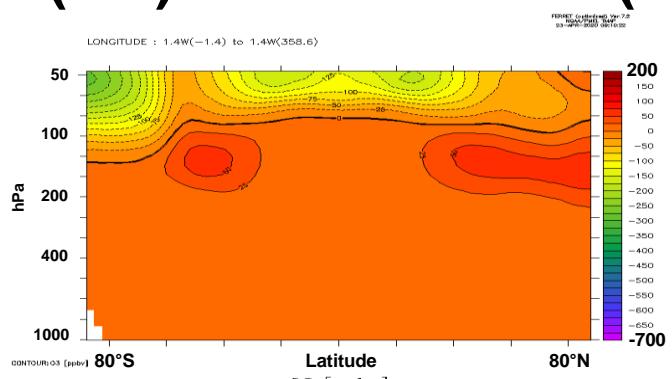
C_2H_6 (ppbv)
Difference to
1960-1969



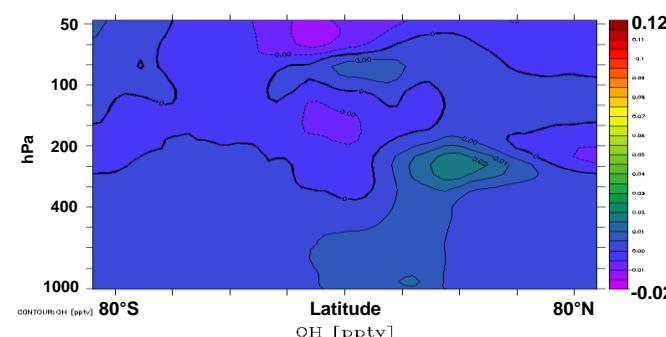
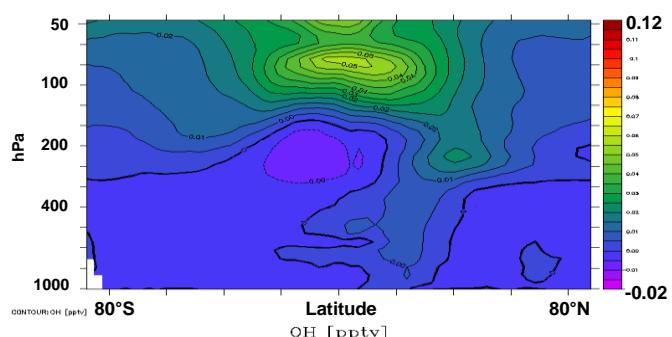
2020-29

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

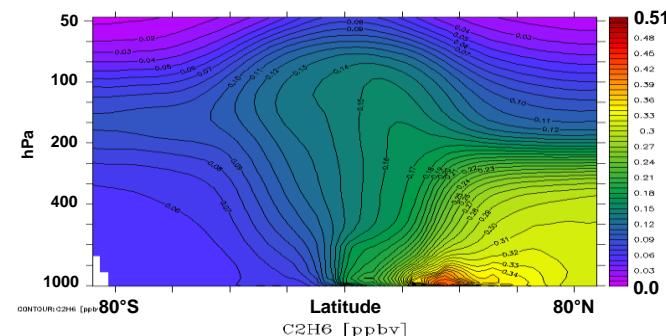
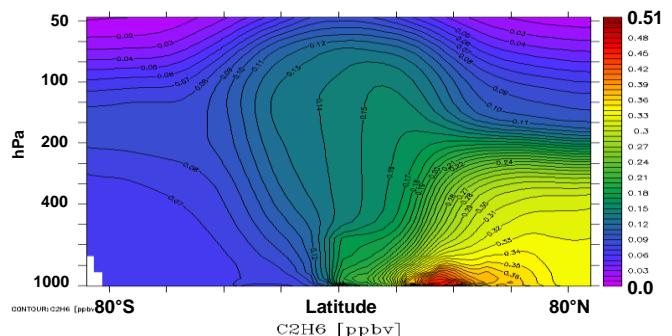
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



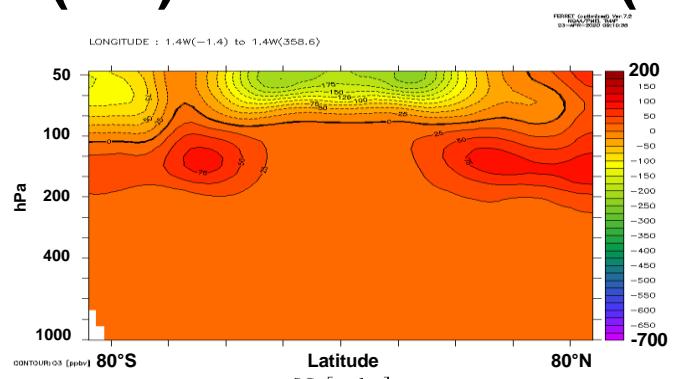
C_2H_6 (ppbv)
Difference to
1960-1969



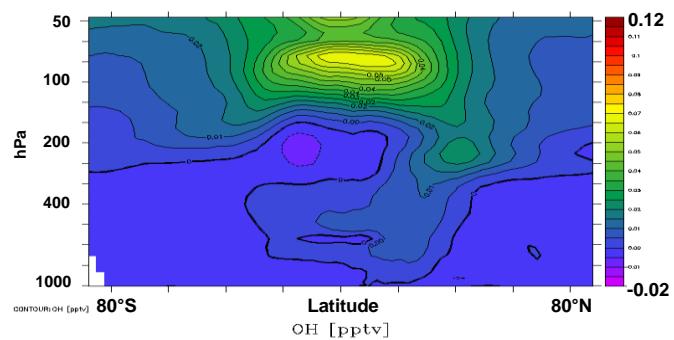
2030-39

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

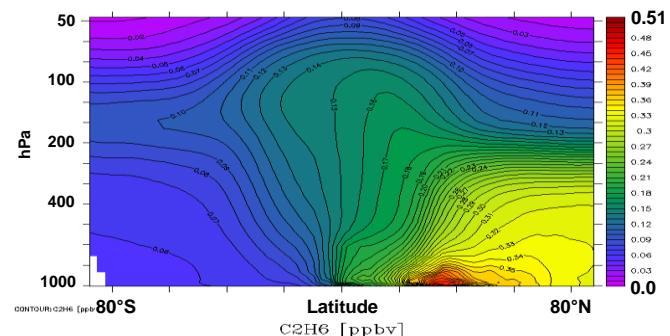
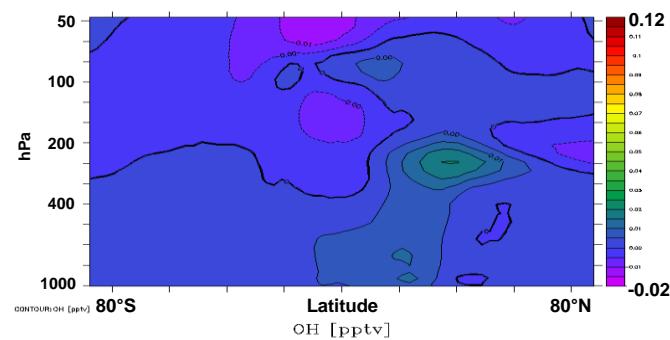
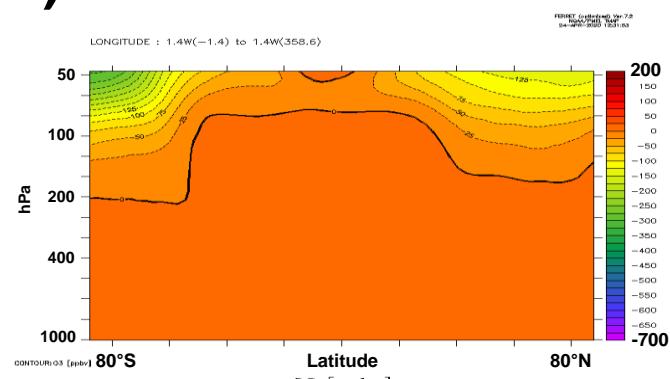
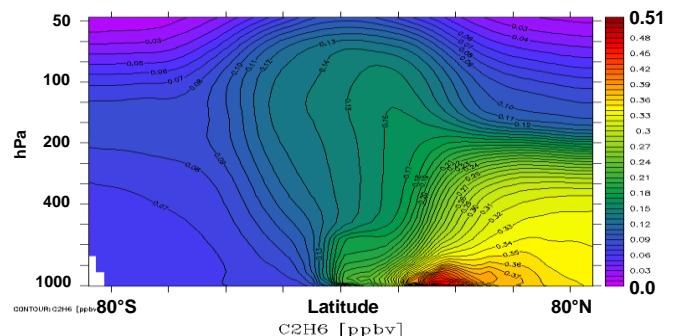
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



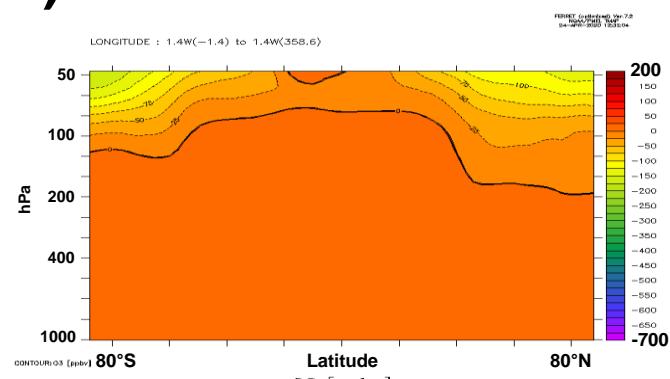
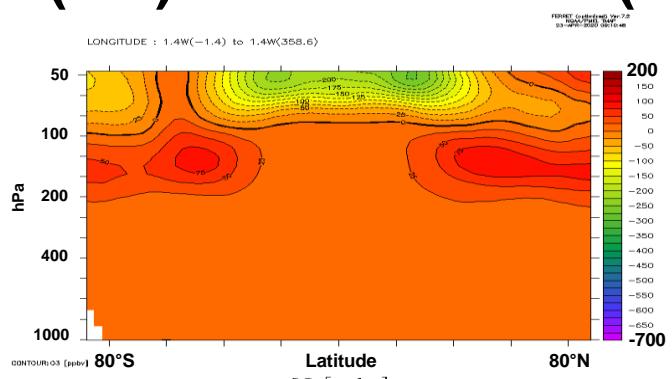
C_2H_6 (ppbv)
Difference to
1960-1969



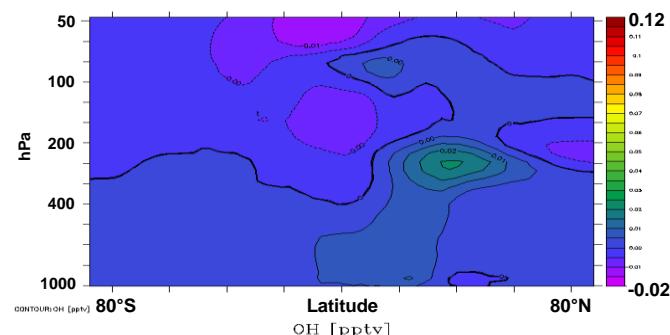
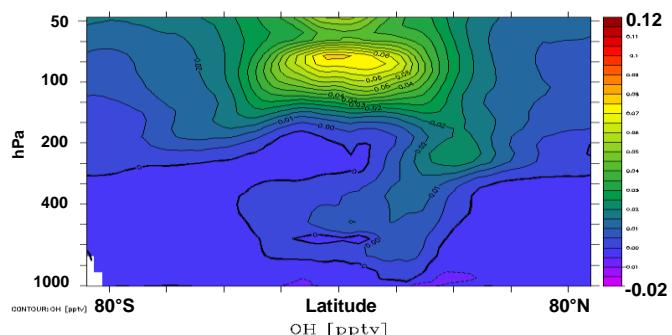
2040-49

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

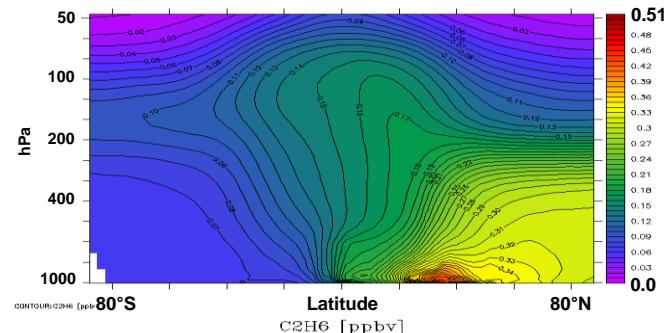
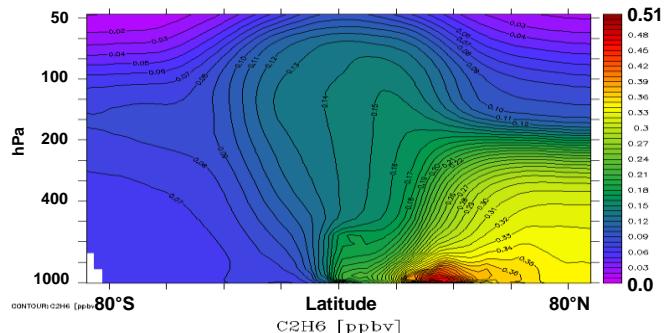
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



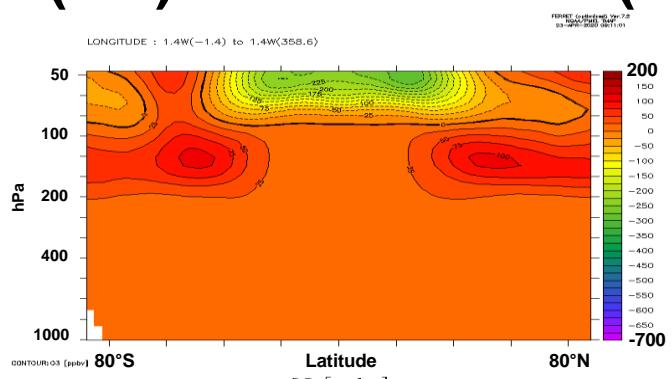
C₂H₆ (ppbv)
Difference to
1960-1969



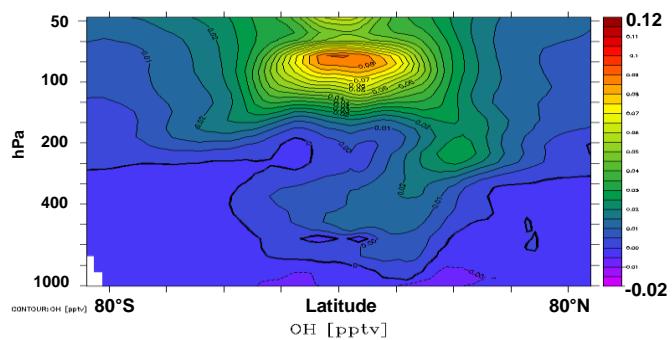
2050-59

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

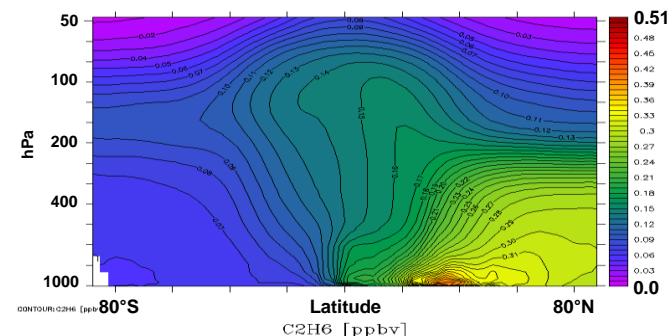
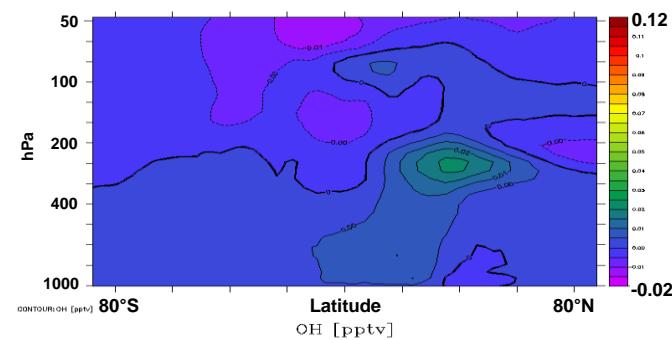
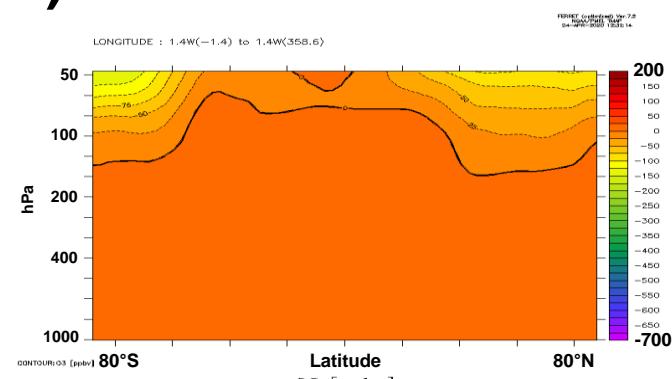
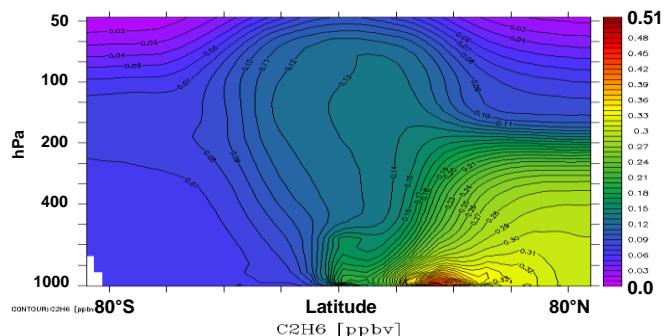
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



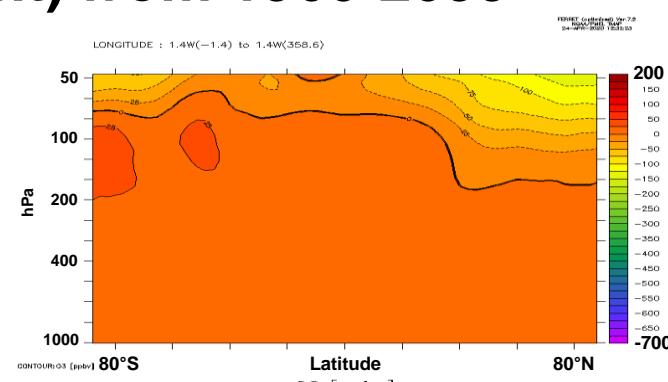
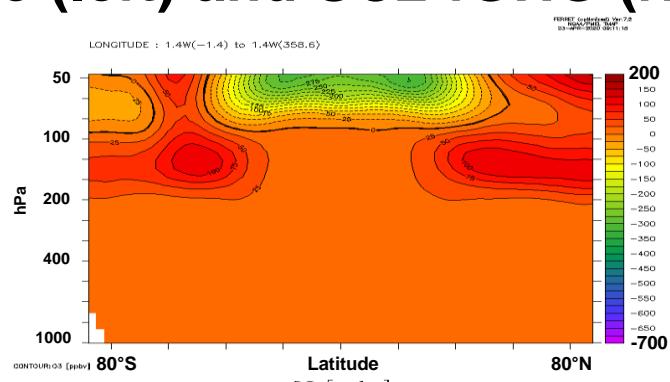
C_2H_6 (ppbv)
Difference to
1960-1969



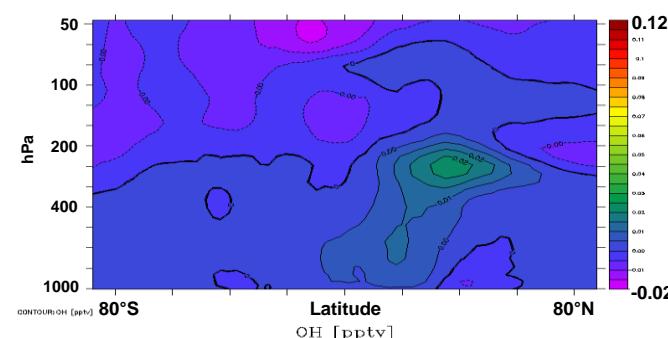
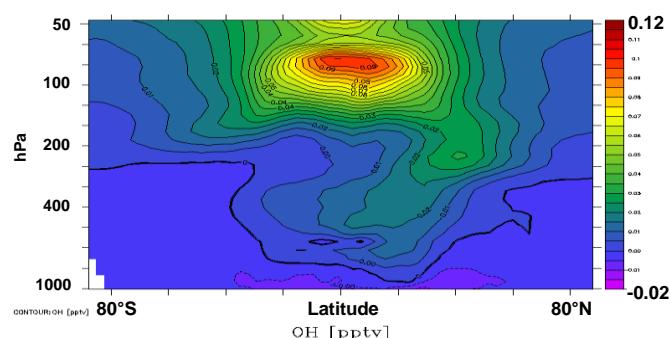
2060-69

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

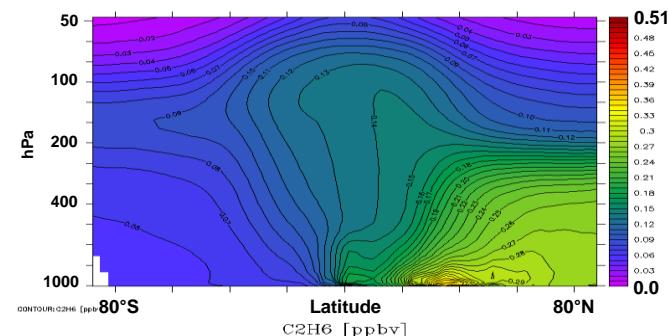
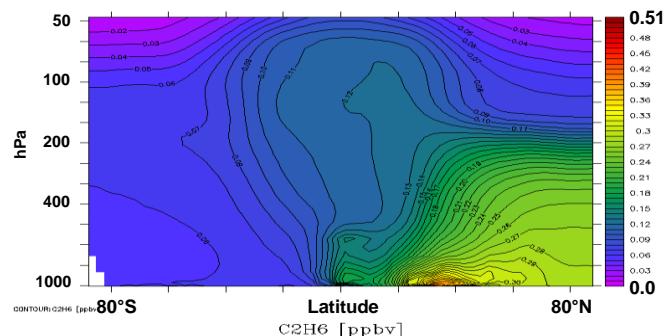
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



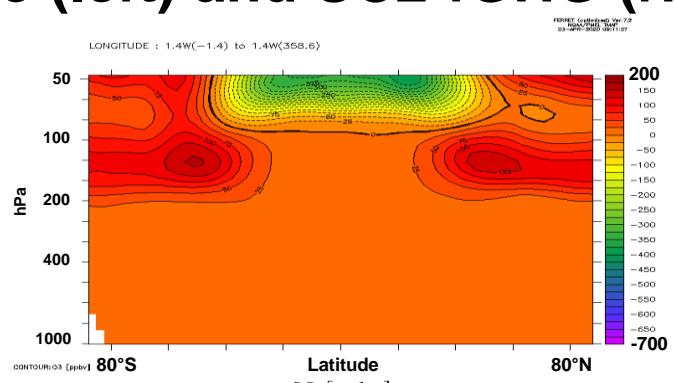
C₂H₆ (ppbv)
Difference to
1960-1969



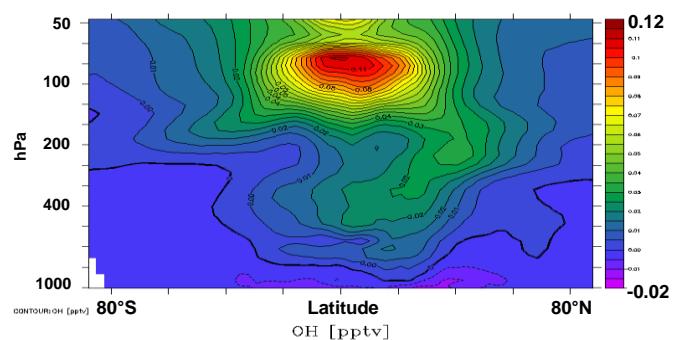
2070-79

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

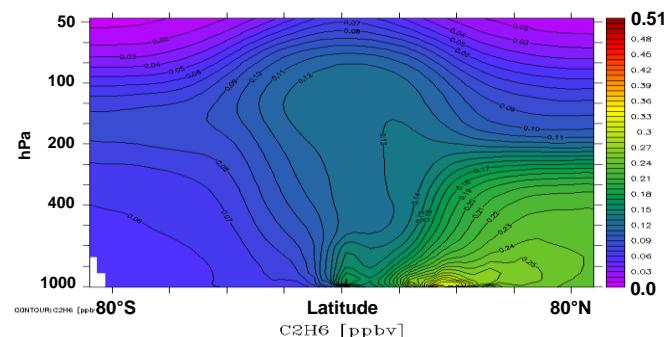
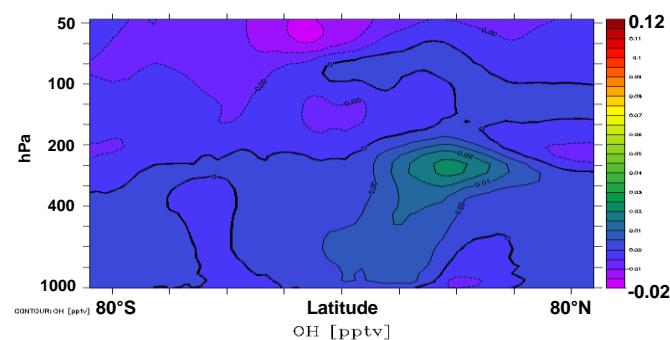
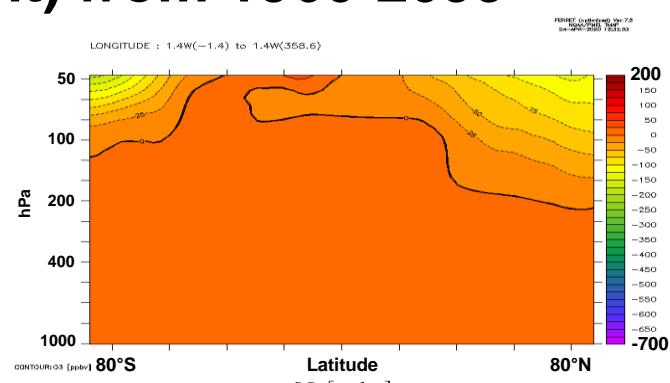
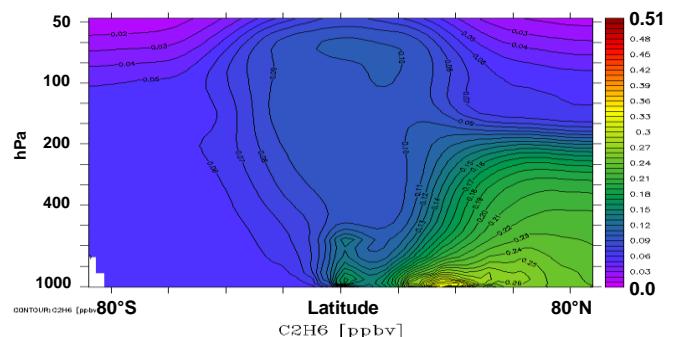
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



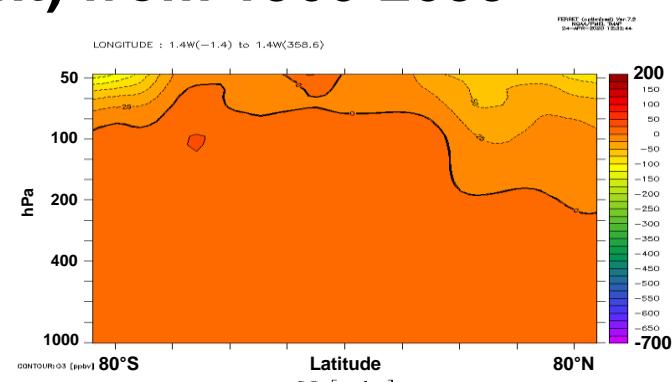
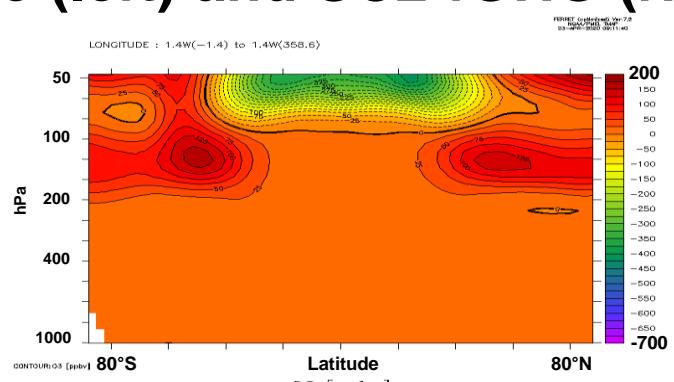
C_2H_6 (ppbv)
Difference to
1960-1969



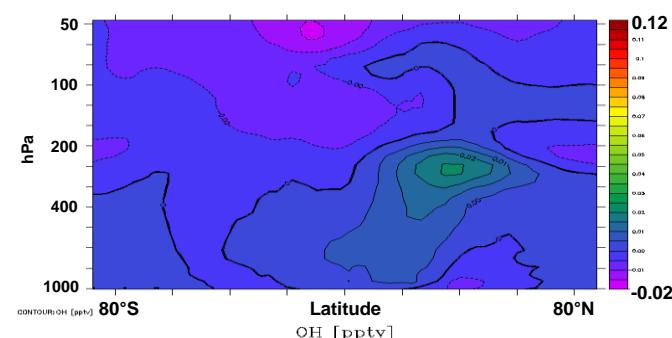
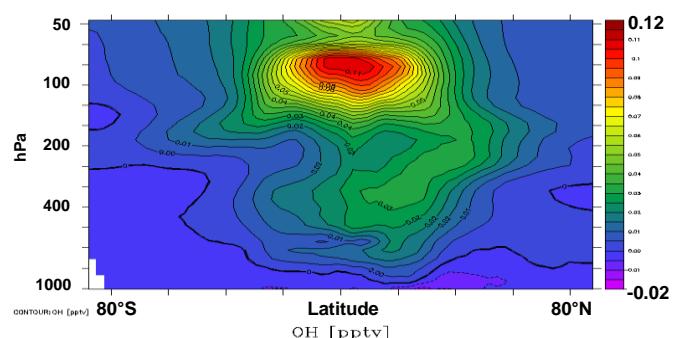
2080-89

Development of ozone, OH and ethane (C_2H_6) in RC2-base (left) and SC2-fGHG (right) from 1960-2099

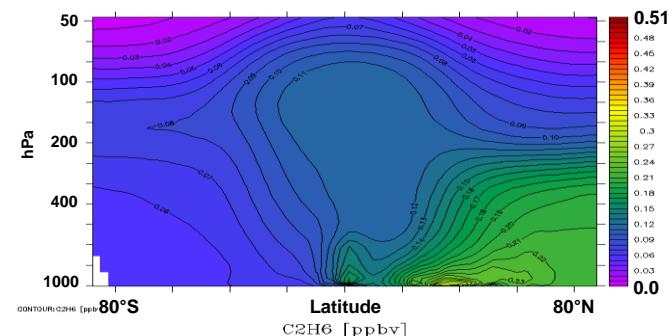
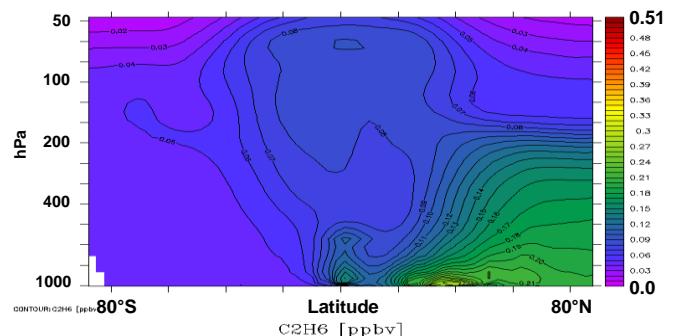
O₃ (ppbv)
Difference to
1960-1969



OH (pptv)
Difference to
1960-1969



C₂H₆ (ppbv)
Difference to
1960-1969

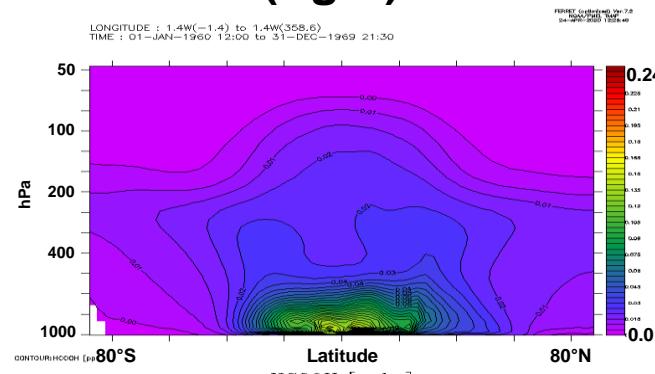
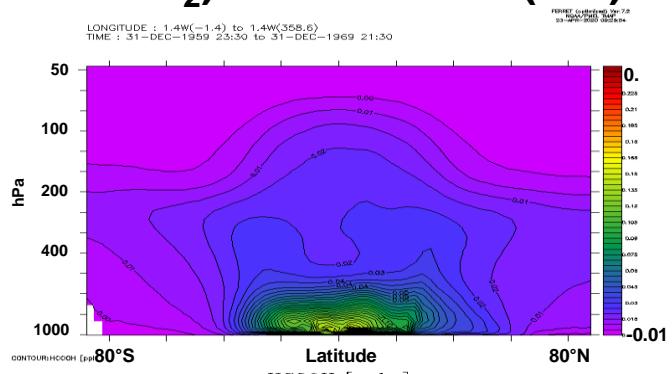


2090-99

Distribution of formic acid (HCOOH) , acetone (CH_3COCH_3) and PAN ($\text{CH}_3\text{COOONO}_2$) in RC2-base (left) and SC2-fGHG (right) 1960

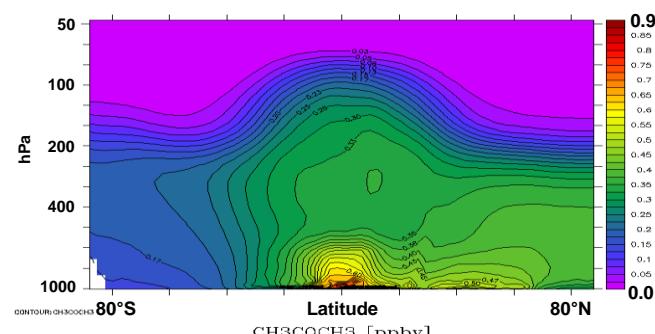
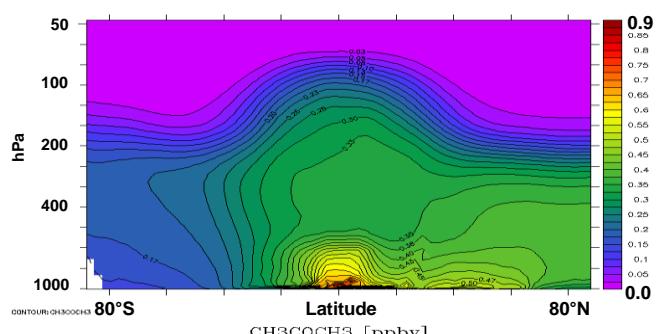
HCOOH (ppbv)

Ten year and
zonal mean



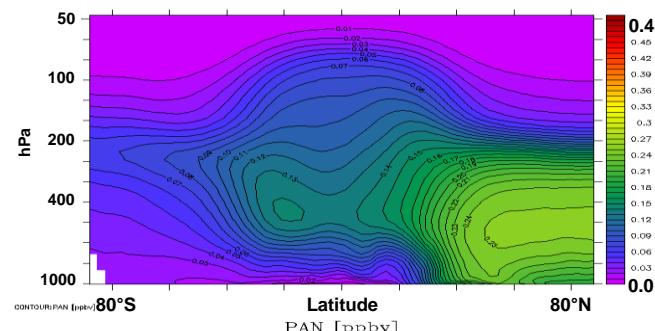
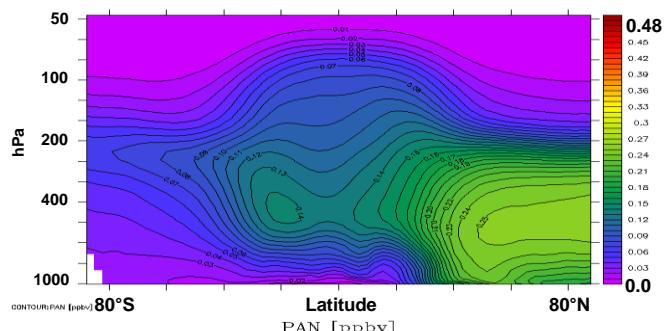
CH_3COCH_3 (ppbv)

Ten year and
zonal mean



PAN (ppbv)

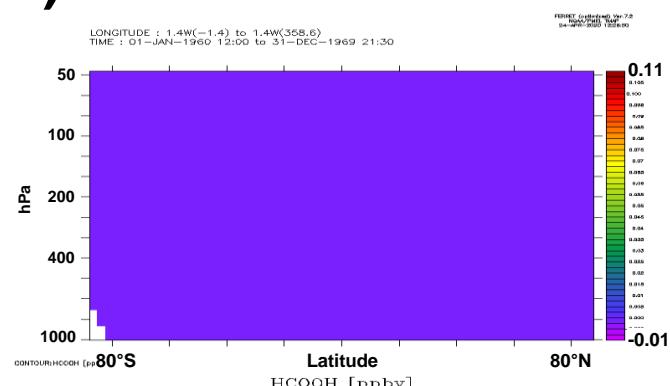
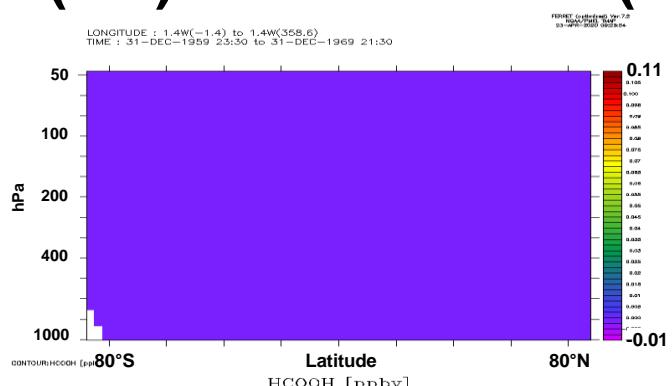
Ten year and
zonal mean



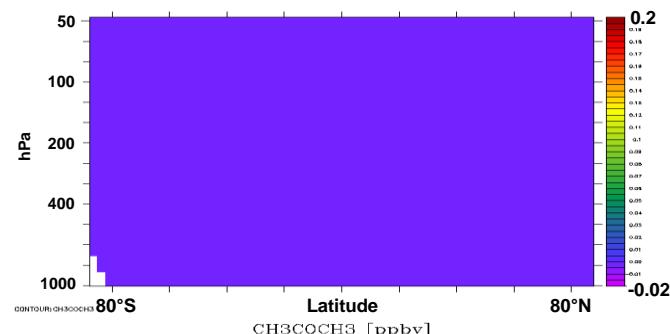
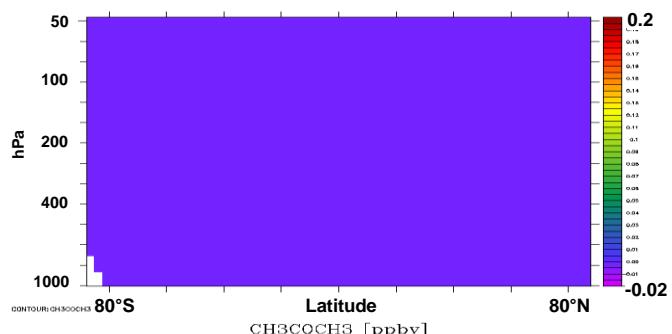
1960-69

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

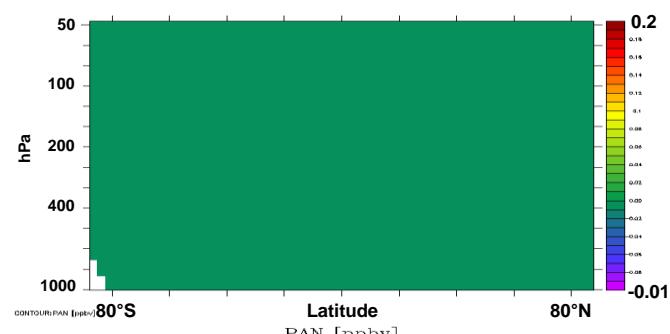
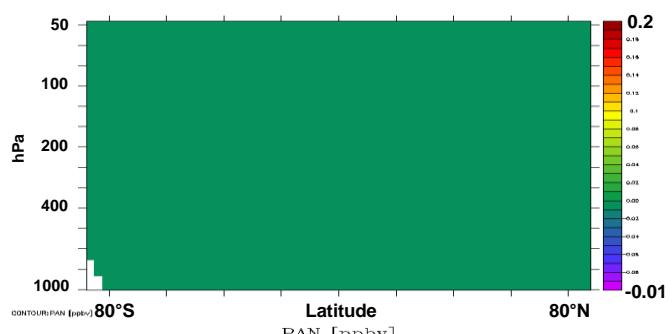
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



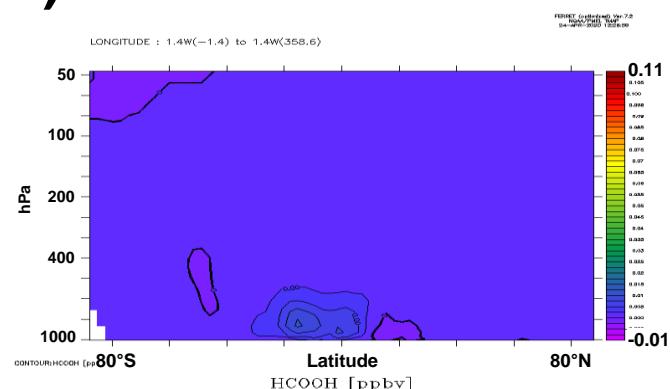
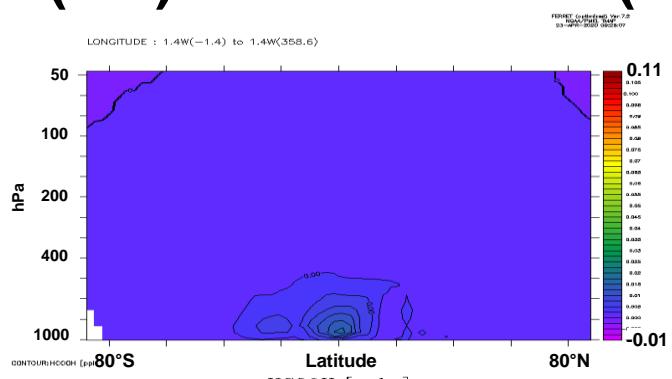
PAN (ppbv)
Difference to
1960-1969



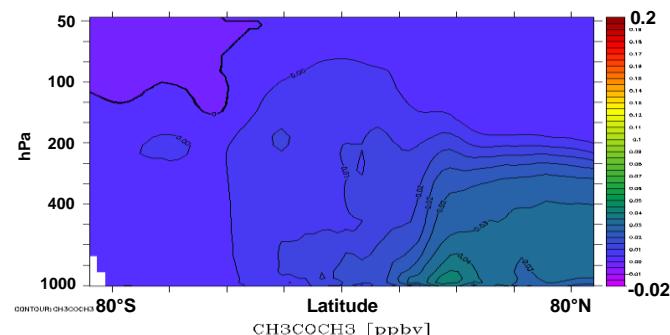
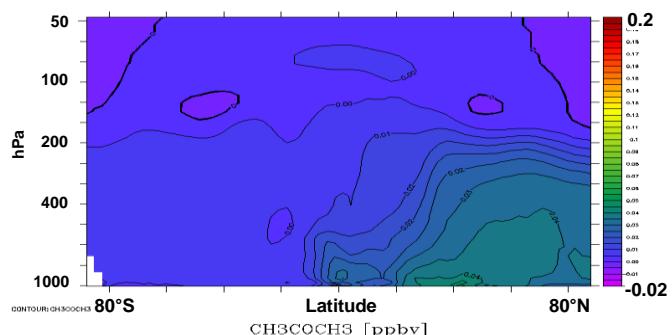
1960-69

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

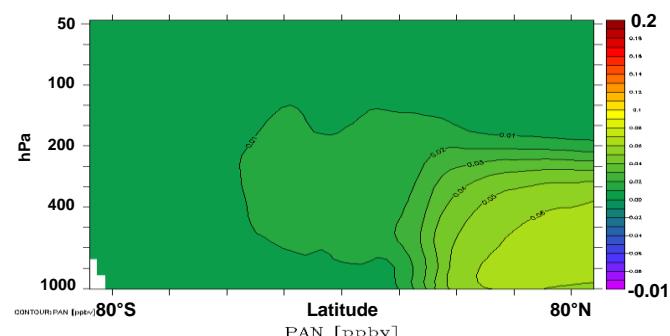
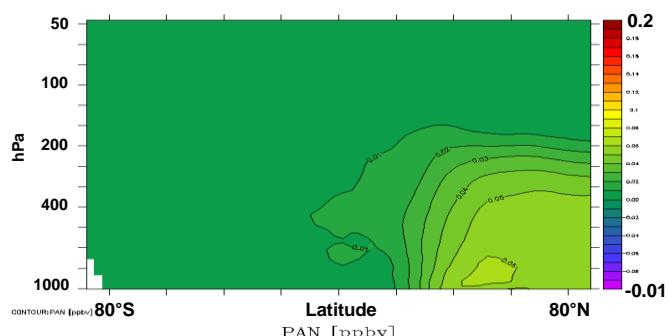
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



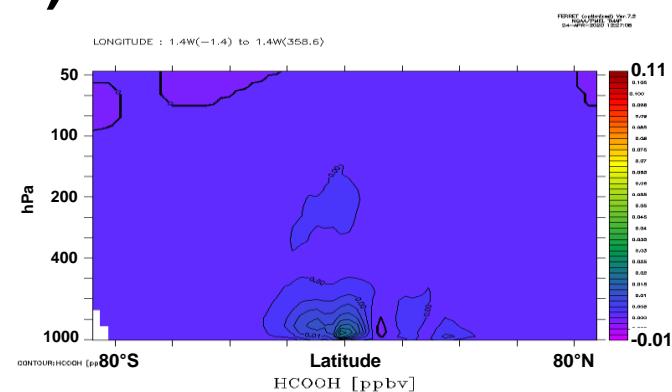
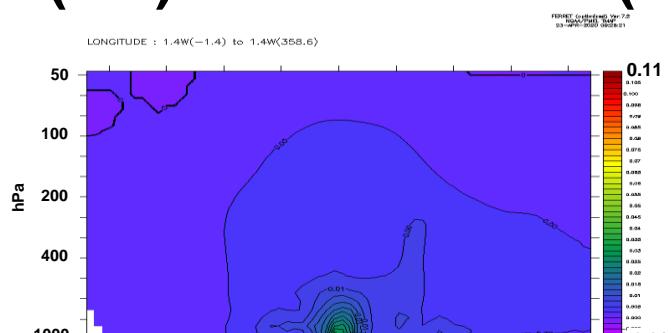
PAN (ppbv)
Difference to
1960-1969



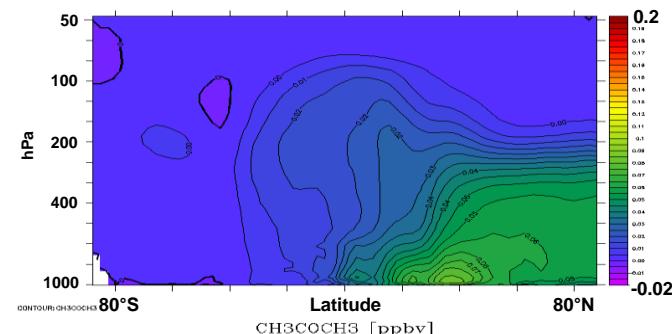
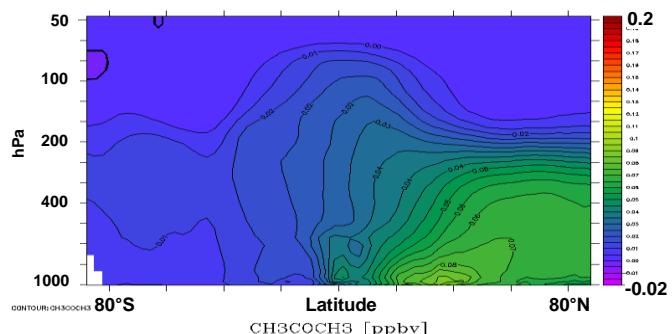
1970-79

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

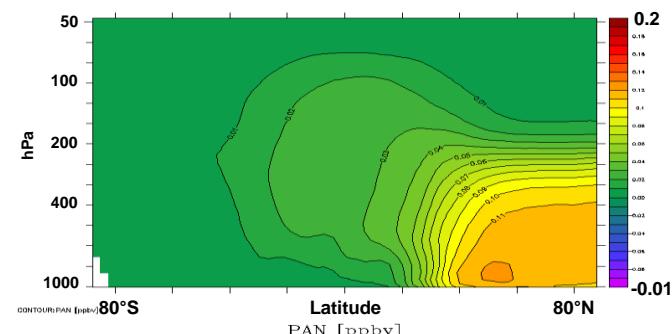
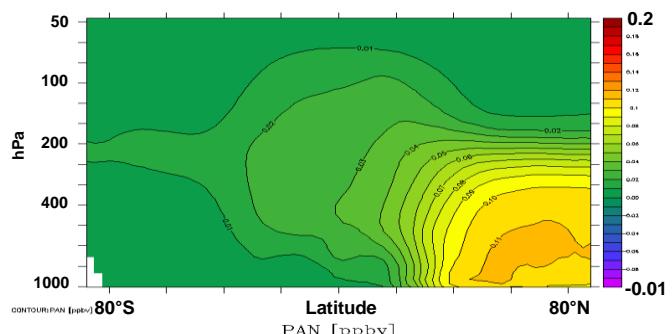
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



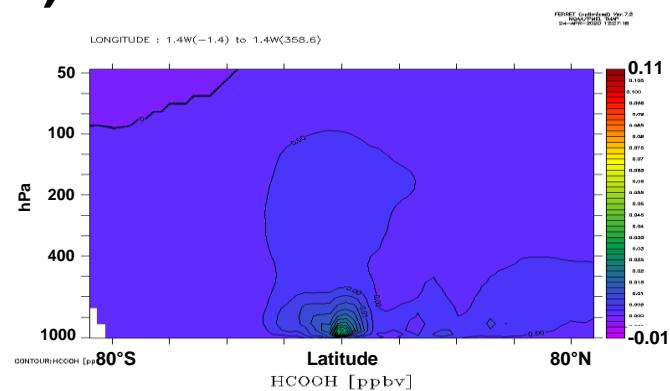
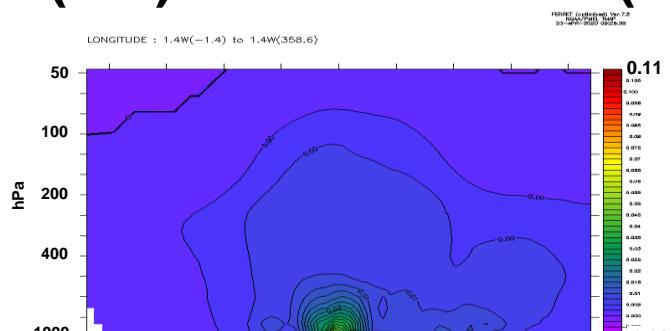
PAN (ppbv)
Difference to
1960-1969



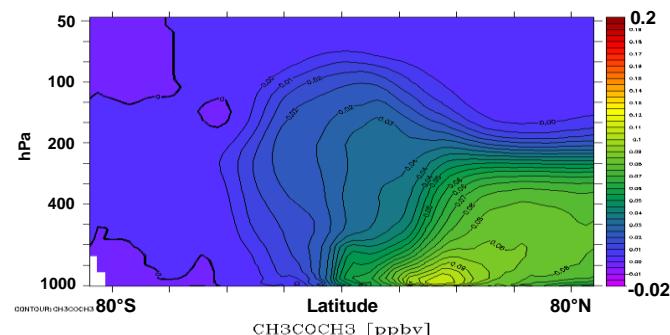
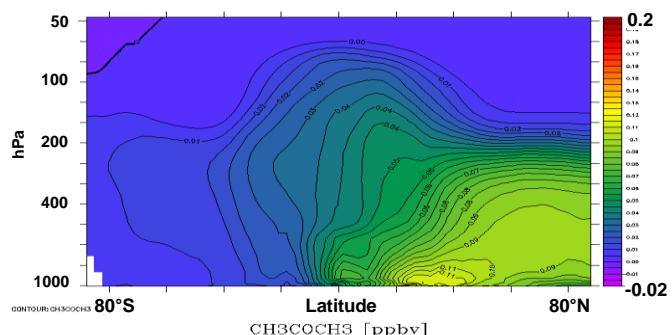
1980-89

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

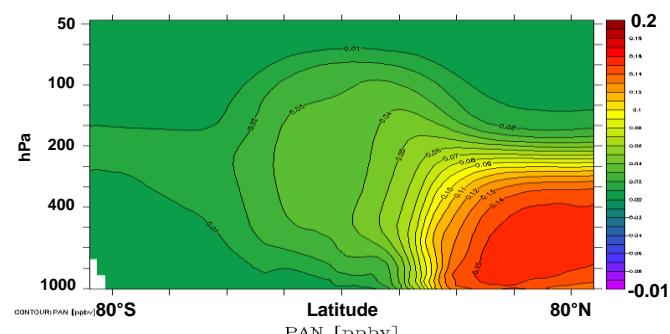
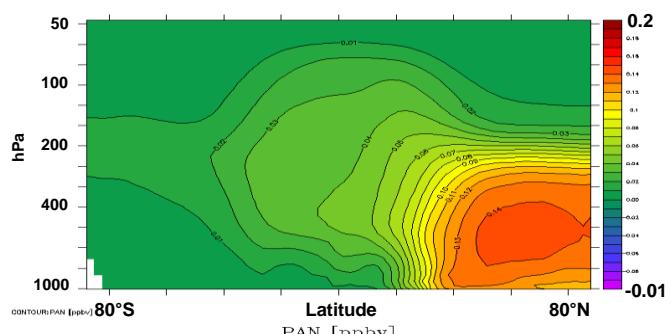
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



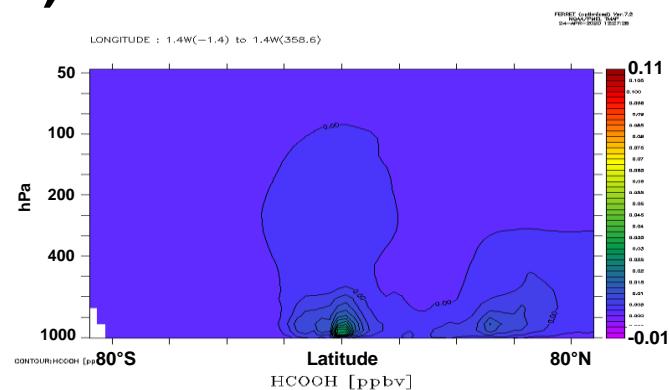
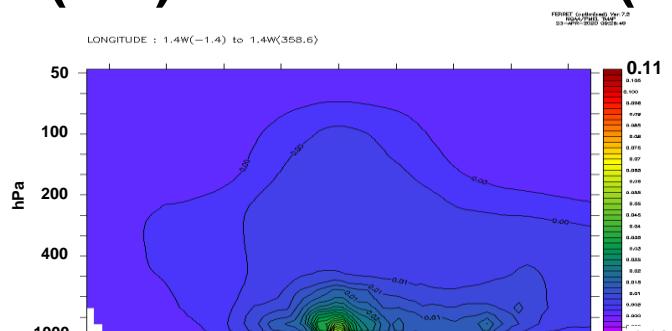
PAN (ppbv)
Difference to
1960-1969



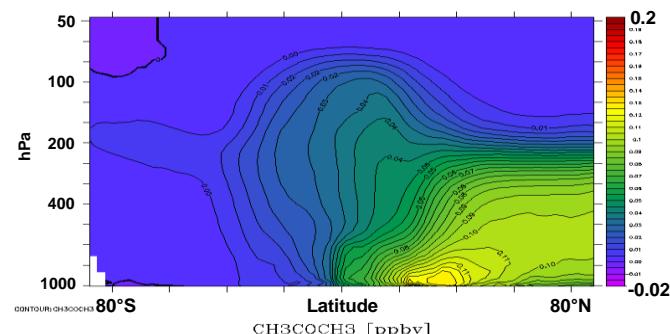
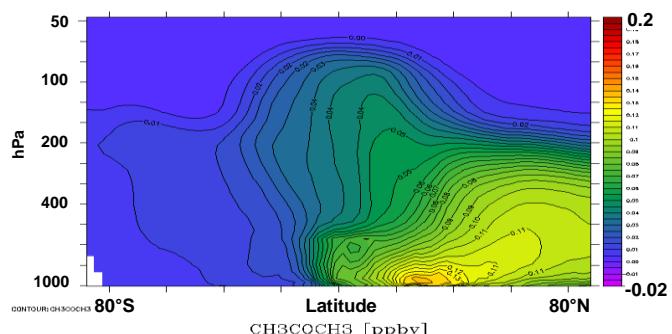
1990-99

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

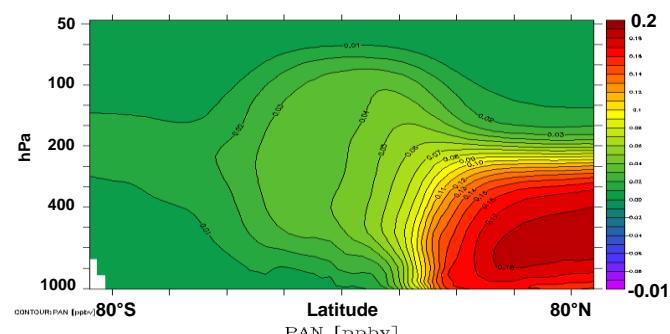
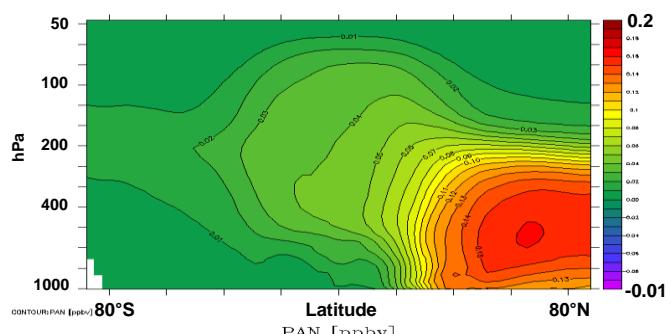
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



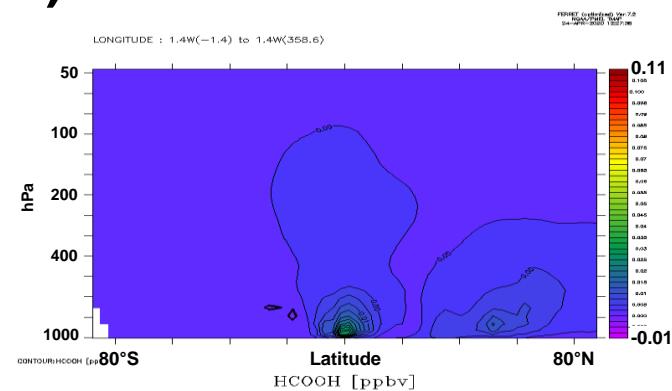
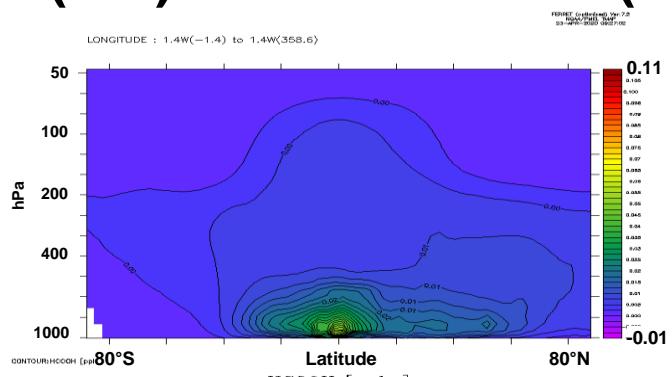
PAN (ppbv)
Difference to
1960-1969



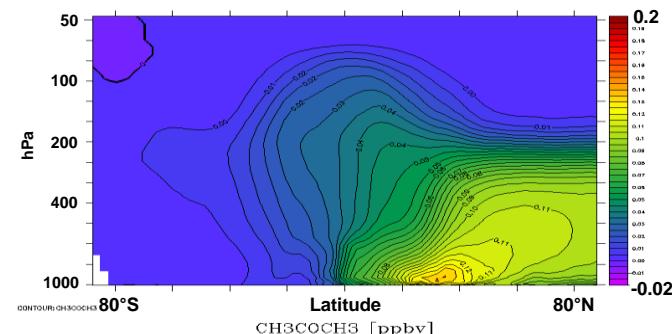
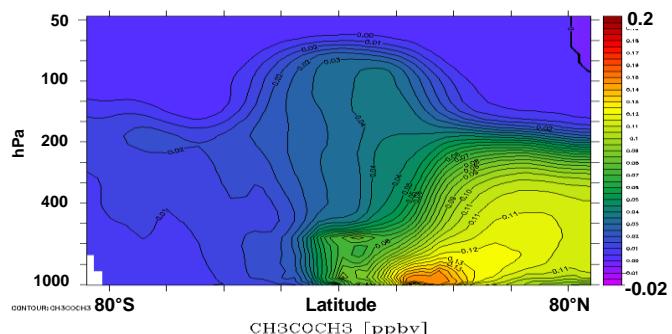
2000-09

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

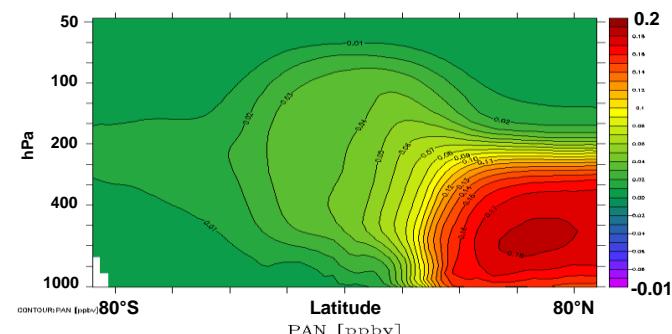
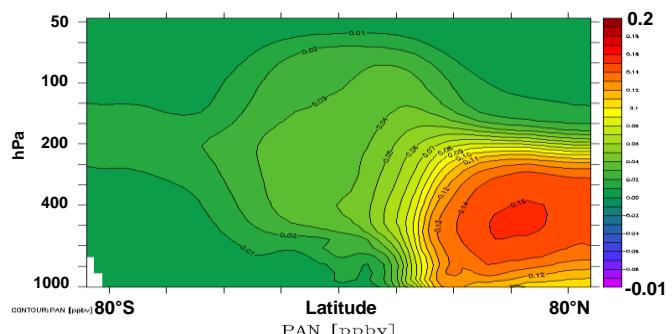
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



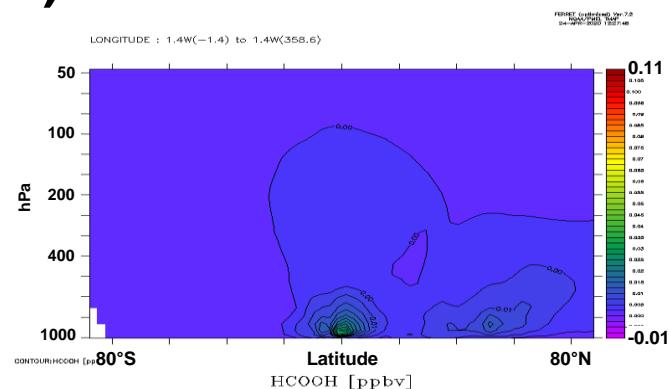
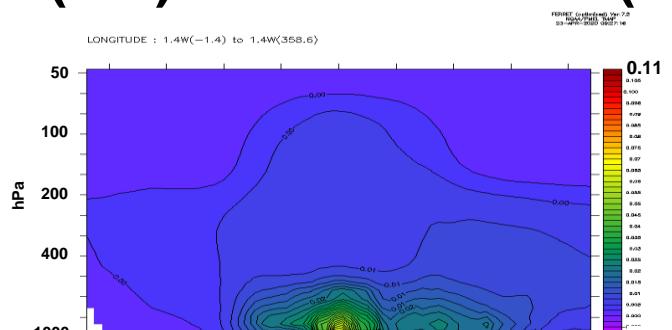
PAN (ppbv)
Difference to
1960-1969



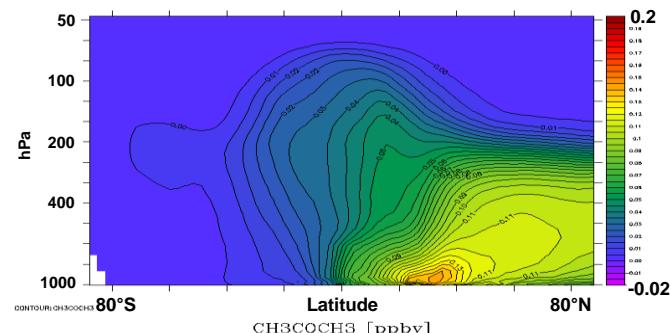
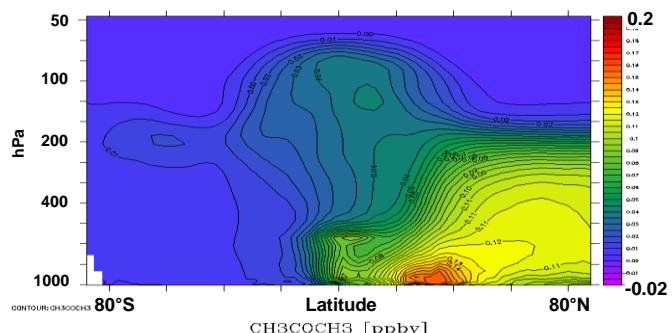
2010-19

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

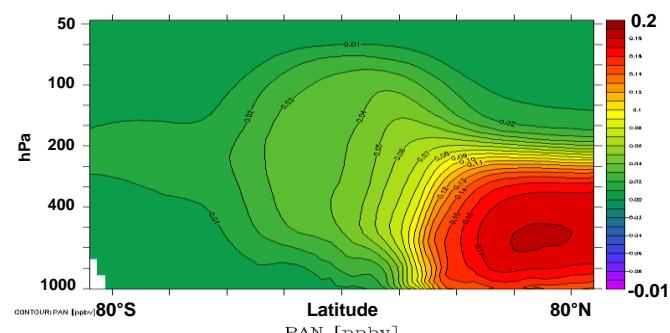
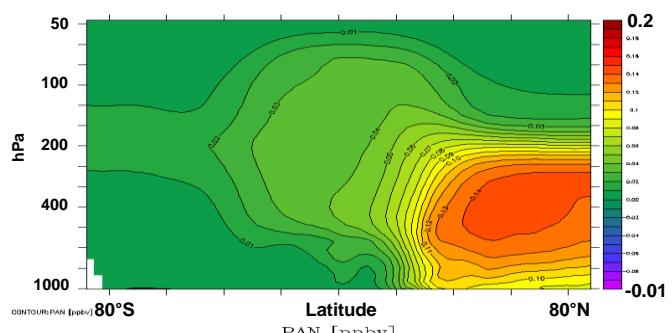
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



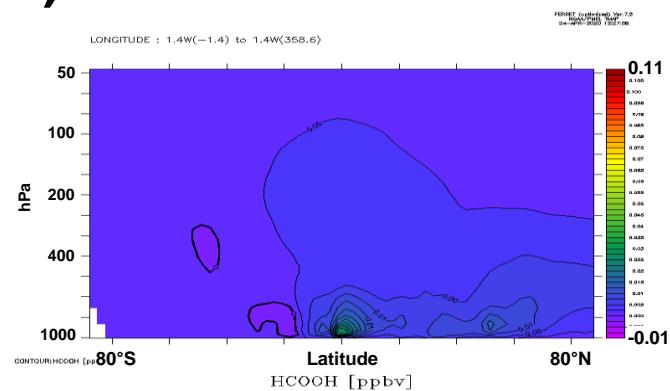
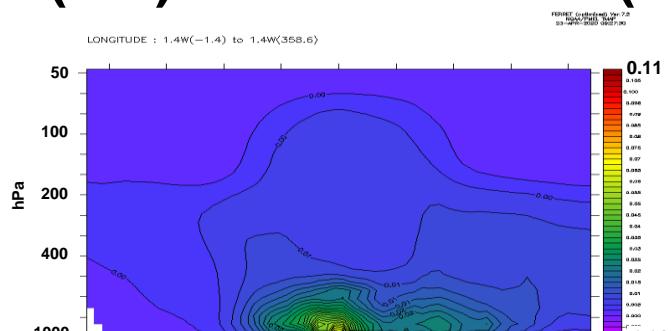
PAN (ppbv)
Difference to
1960-1969



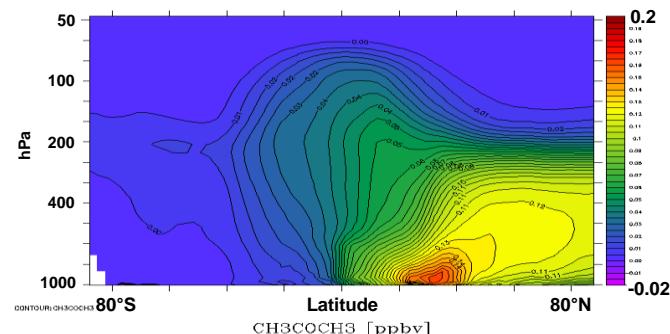
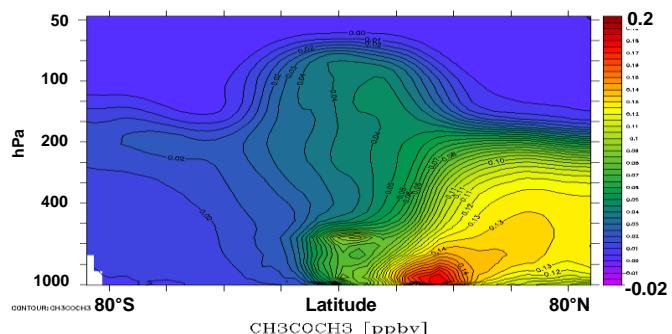
2020-29

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

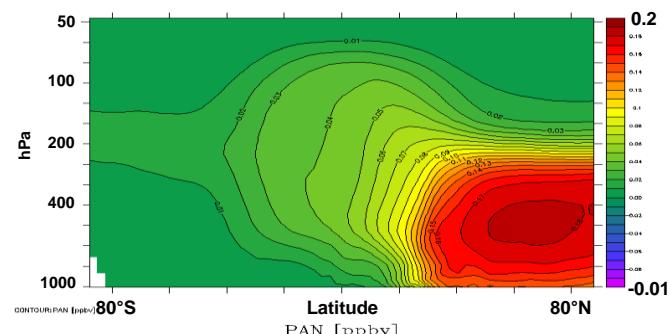
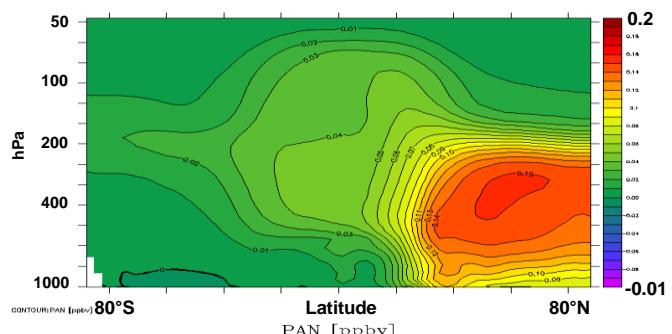
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



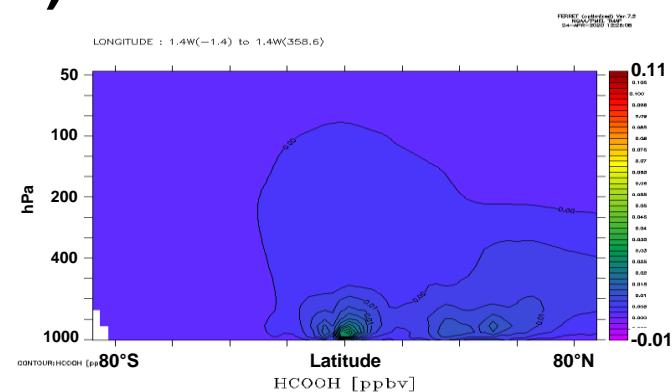
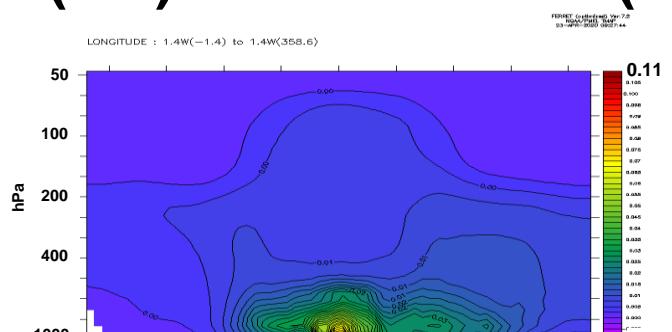
PAN (ppbv)
Difference to
1960-1969



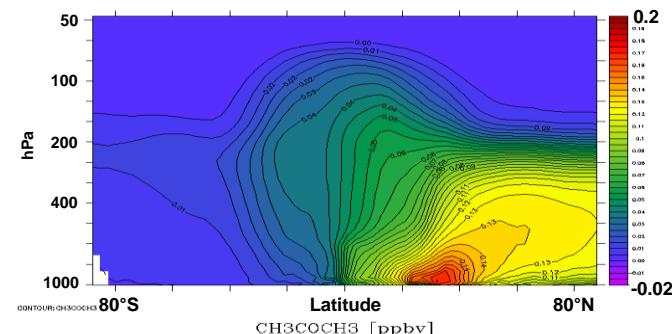
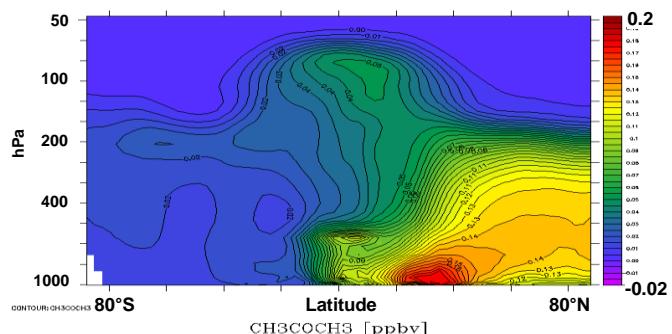
2030-39

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

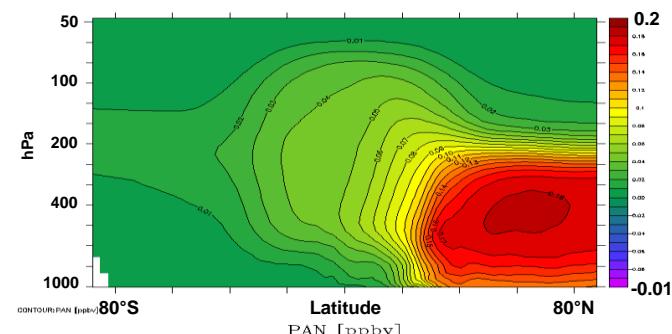
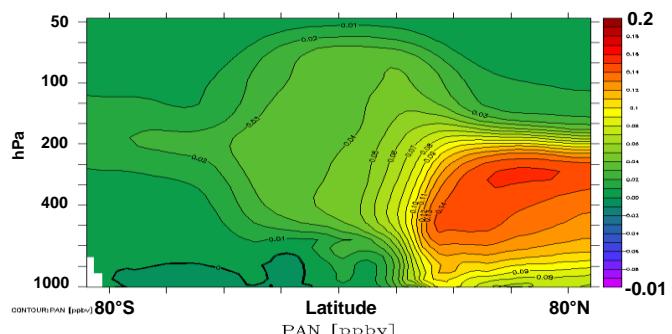
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



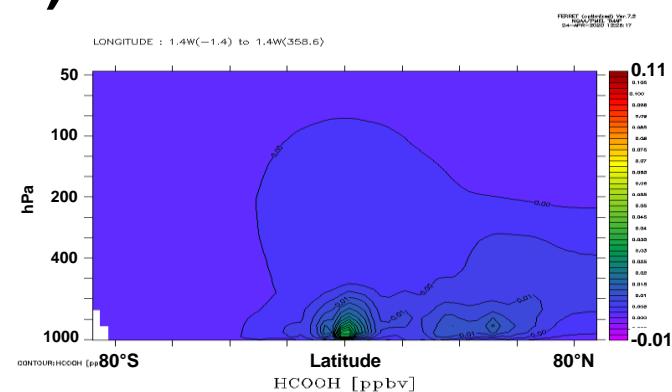
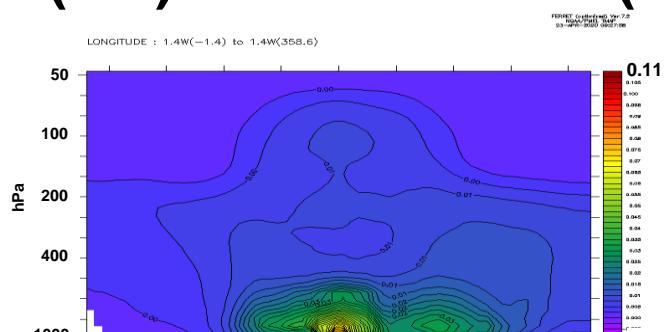
PAN (ppbv)
Difference to
1960-1969



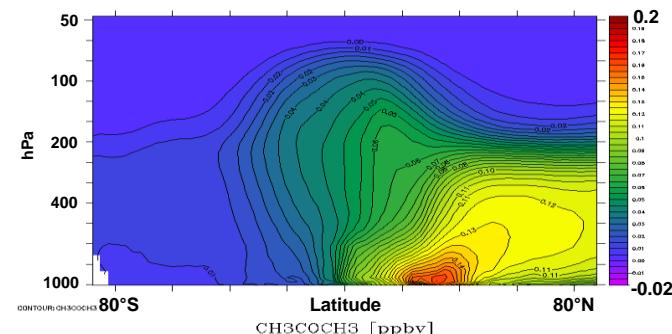
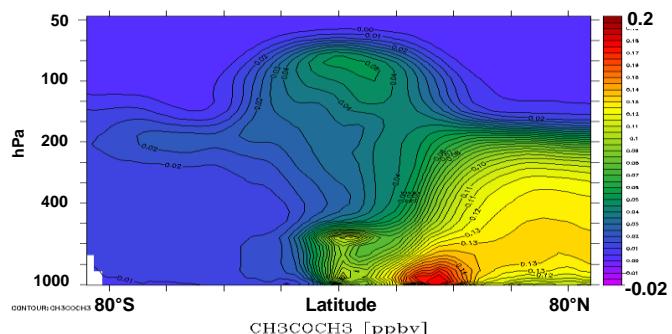
2040-49

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

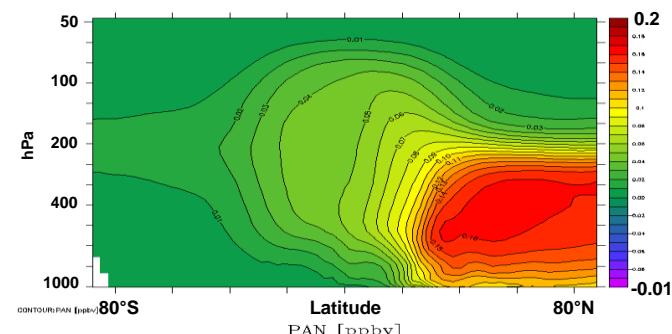
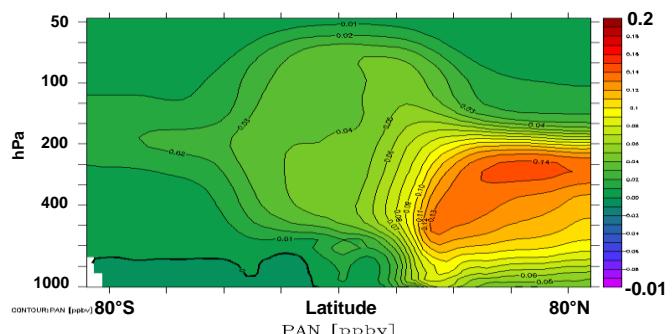
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



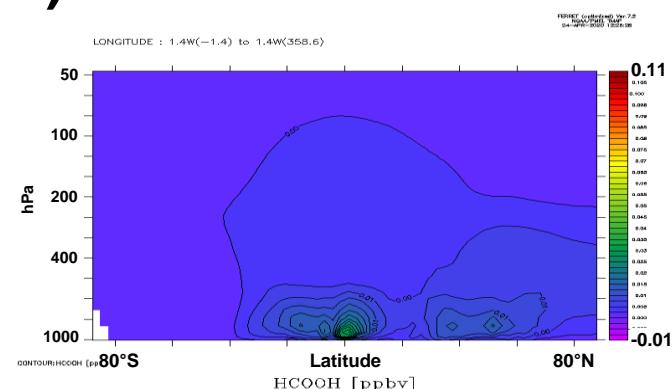
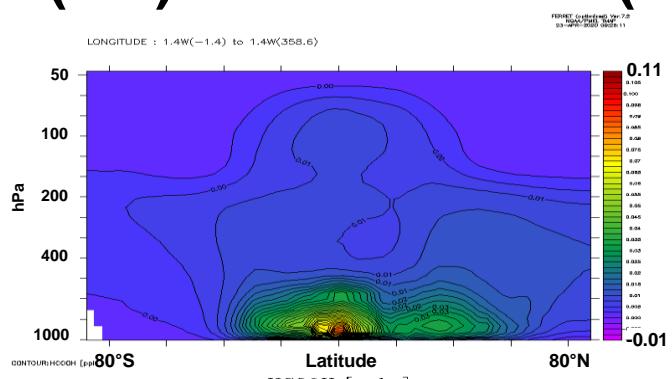
PAN (ppbv)
Difference to
1960-1969



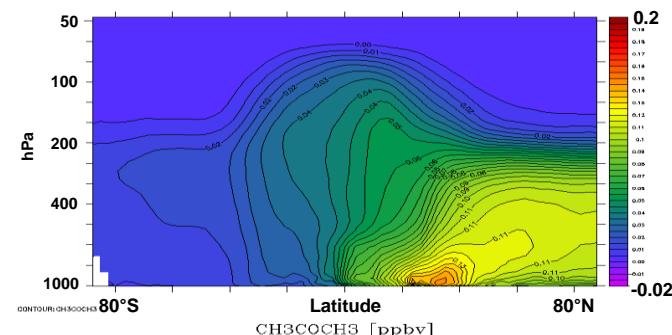
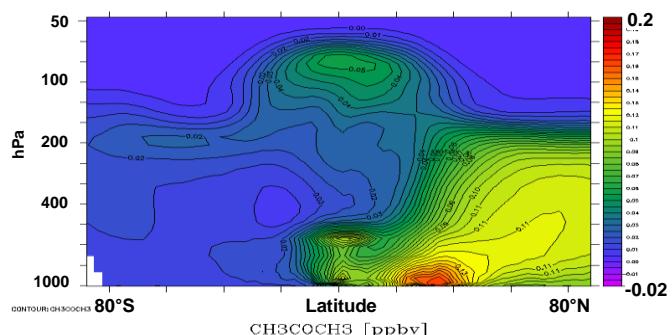
2050-59

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

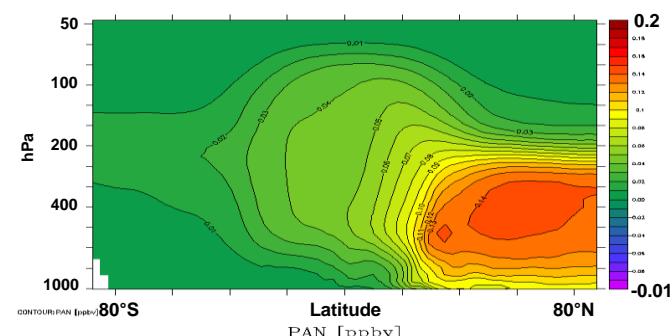
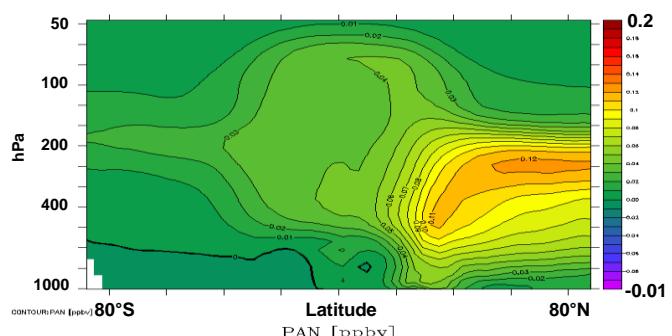
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



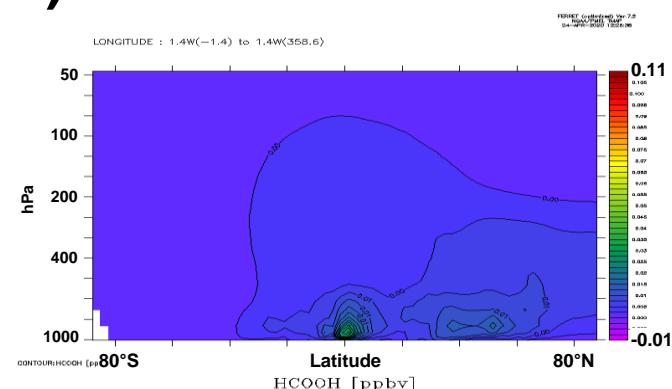
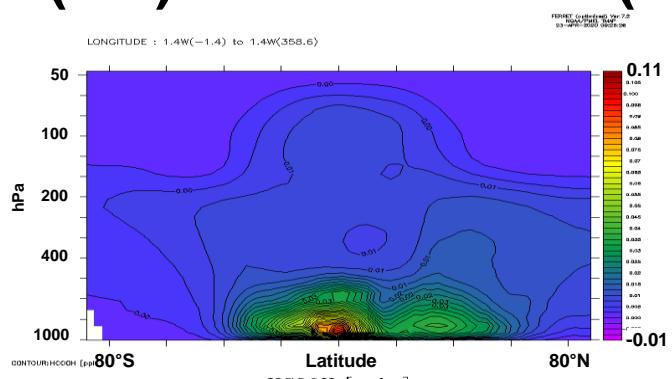
PAN (ppbv)
Difference to
1960-1969



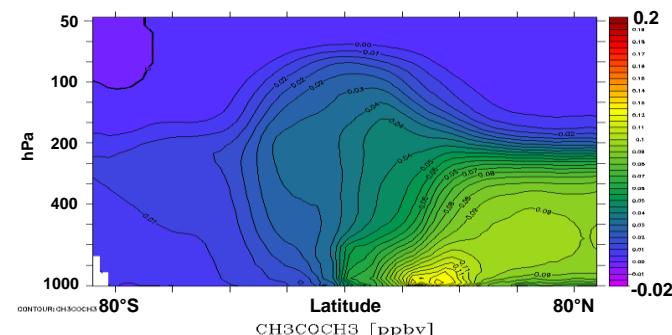
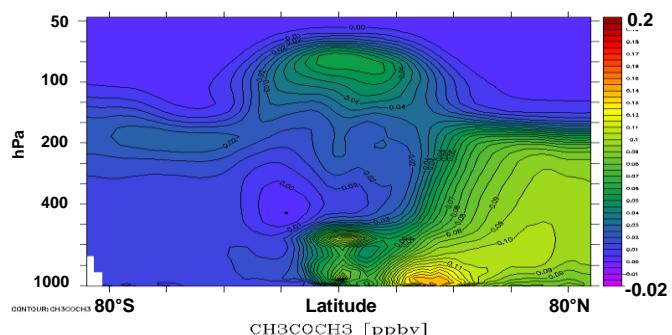
2060-69

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

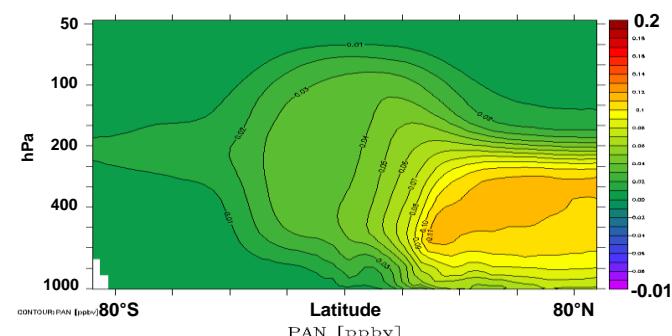
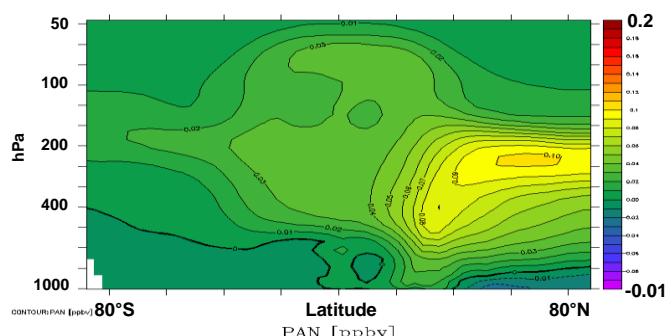
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



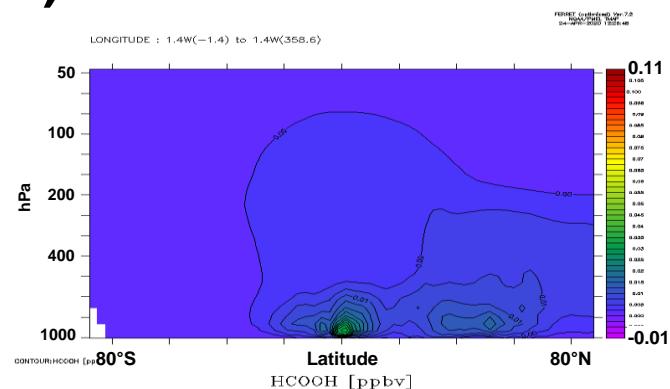
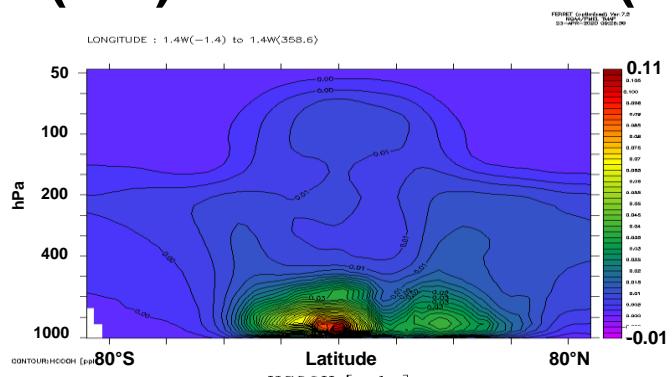
PAN (ppbv)
Difference to
1960-1969



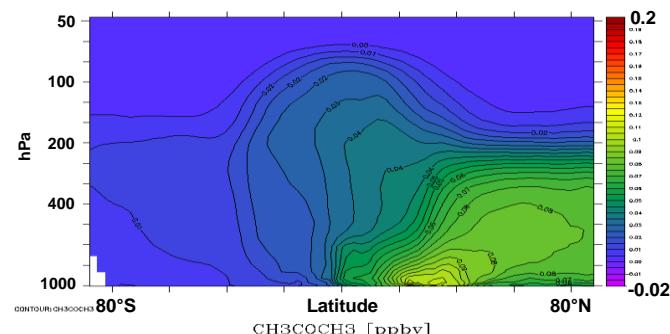
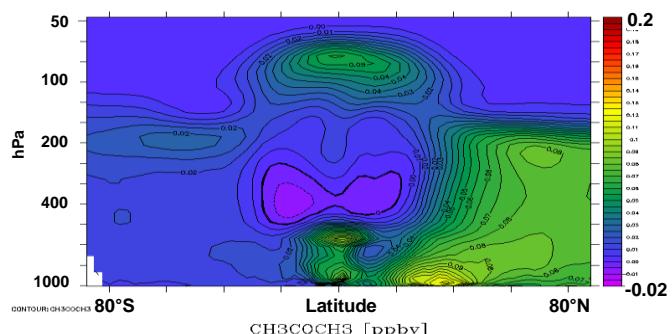
2070-79

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

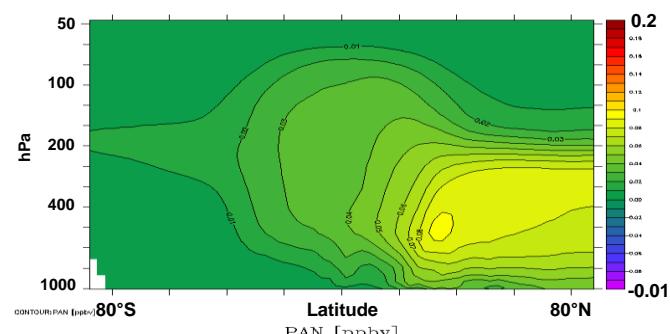
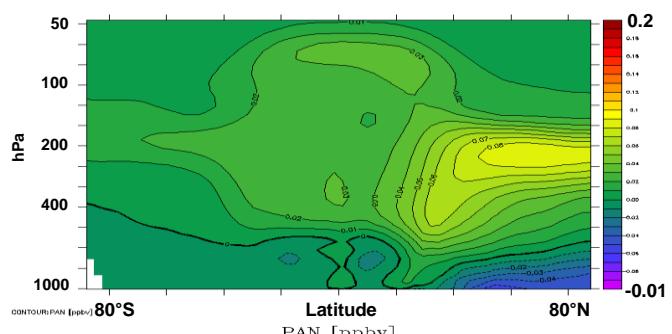
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



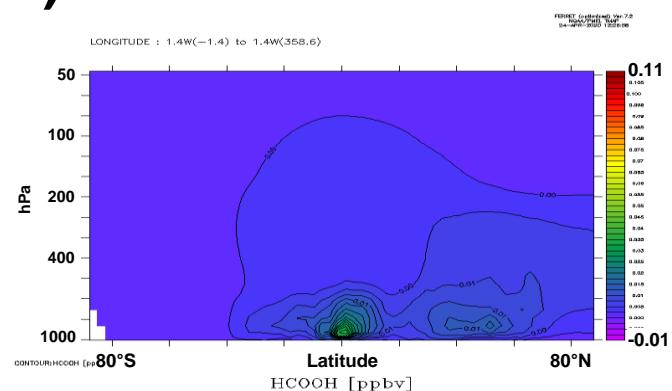
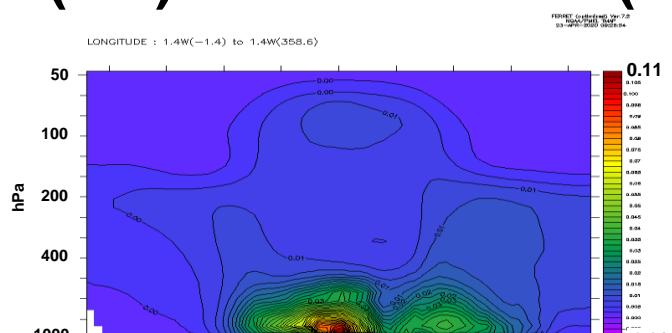
PAN (ppbv)
Difference to
1960-1969



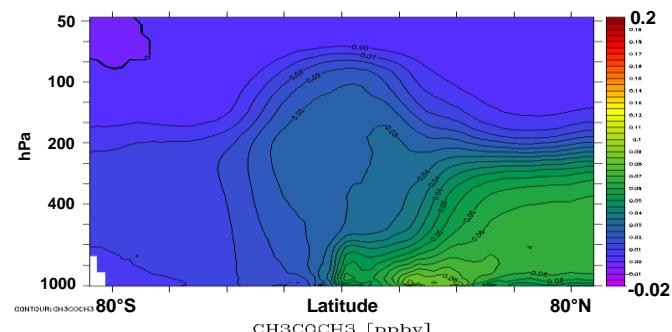
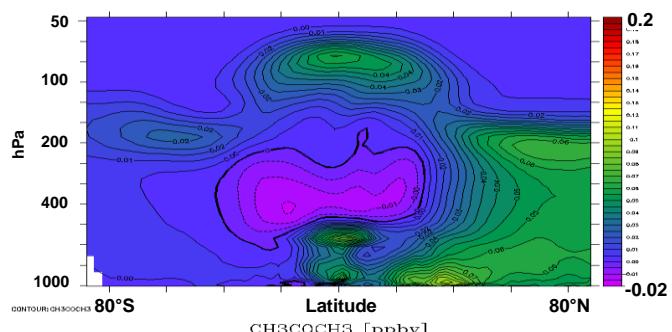
2080-89

Development of formic acid, acetone, and PAN in RC2-base (left) and SC2-fGHG (right) from 1960-2099

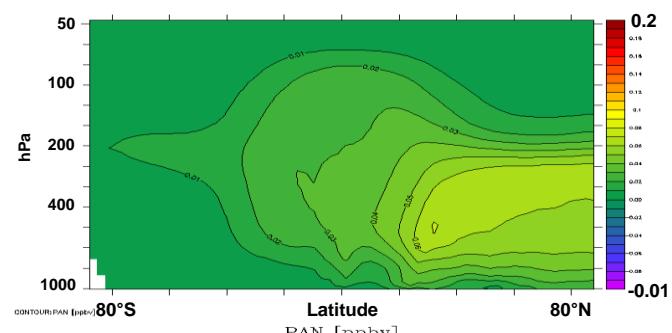
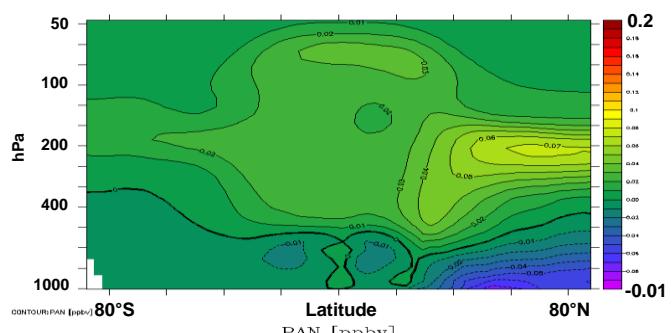
HCOOH (ppbv)
Difference to
1960-1969



CH₃COCH₃ (ppbv)
Difference to
1960-1969



PAN (ppbv)
Difference to
1960-1969



2090-99

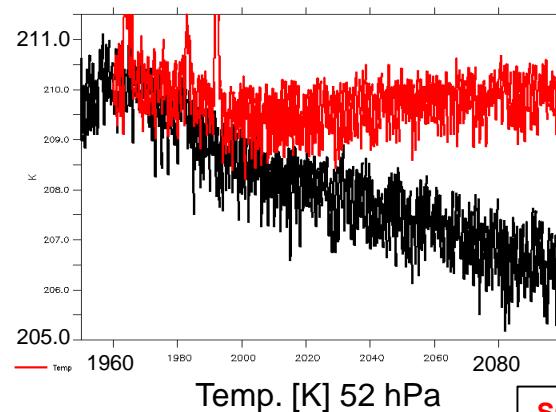
Climate Change

- The average global surface temperature change in RC2-base-04 is approx. 4 K (in the Northern High Latitudes over 10 K) (see slides 6 to 19).

There is no climate change simulated in SC2-fGHG-01.

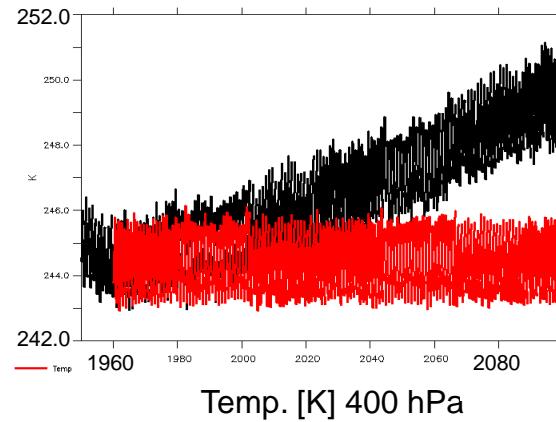
- In SC2-fGHG-01 the temperature change in the lower stratosphere is related to the ozone development. There is no additional cooling due to the greenhouse gases simulated. This cooling effect is clearly visible in RC2-base-04.

FDNET (corrected), Ver.7.2
01-MAR-2020 1541:32
DATA SET: FH2_ECHAM5.mrc



SC2-fGHG-01
RC2-base-04

FDNET (corrected), Ver.7.2
01-MAR-2020 1554:47
DATA SET: FH2_ECHAM5.mrc

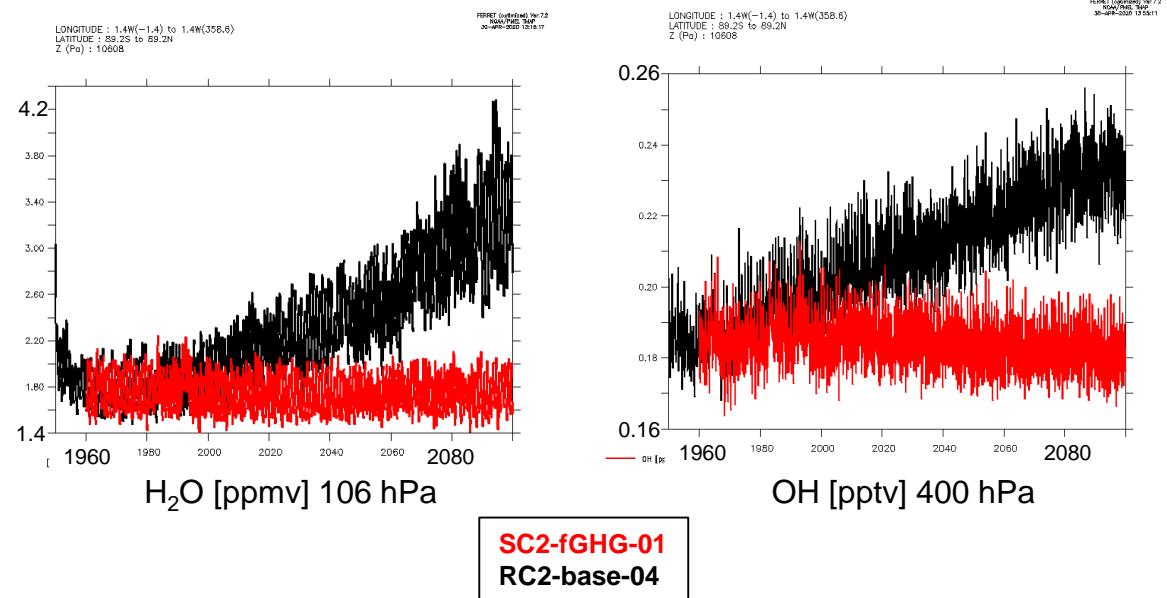


Hydroxyl radical (OH) and water vapour (I)

The trend of the hydroxyl radical (OH) is influenced by two main effects: The development of CH_4 as OH sink ($\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$) and the development of H_2O as OH source ($\text{H}_2\text{O} + \text{O}(1\text{D}) \rightarrow 2 \text{ OH}$). But is also influence by the trend of many other substances.

In RC2-base-04 a positive OH trend is simulated in the lower stratosphere (around 100 hPa, see slides 21 to 34). This is caused by the increase of H_2O due to the methane oxidation.

In SC2-fGHG-01 this trend doesn't exist.

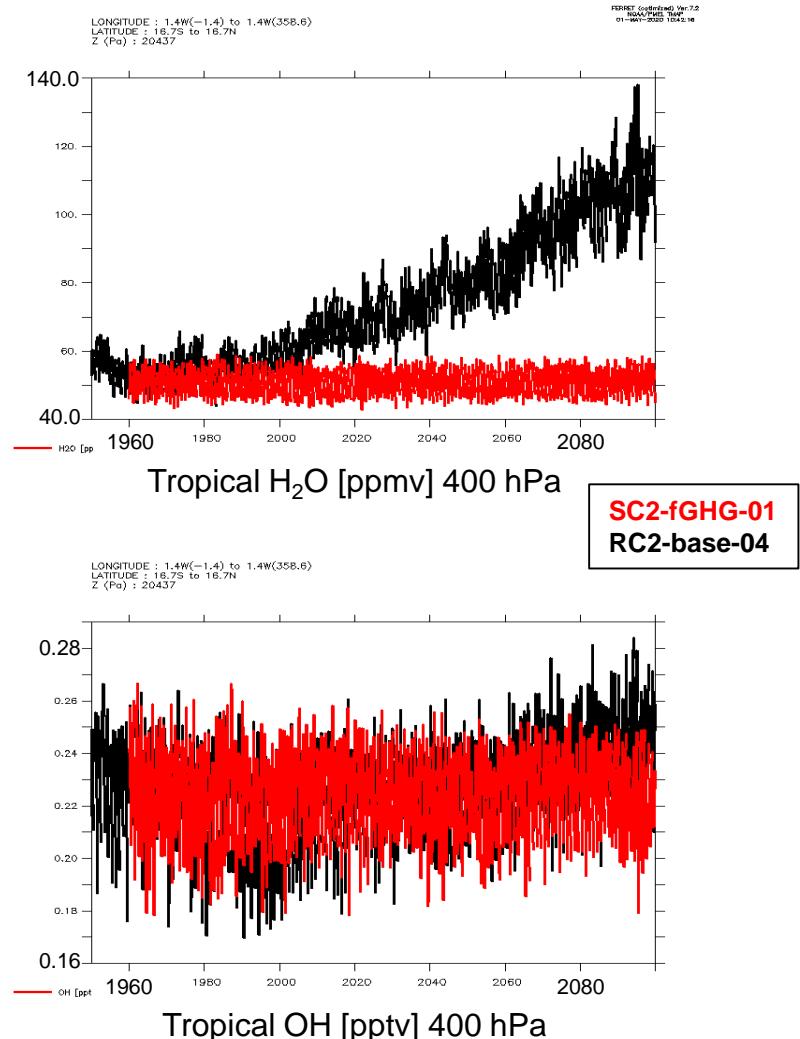


Hydroxyl radical (OH) and water vapor (H_2O) (II)

In the troposphere, especially in the tropical region, first a decrease in OH (1960 to 2010), and later (2010 to 2099) an increase is simulated.

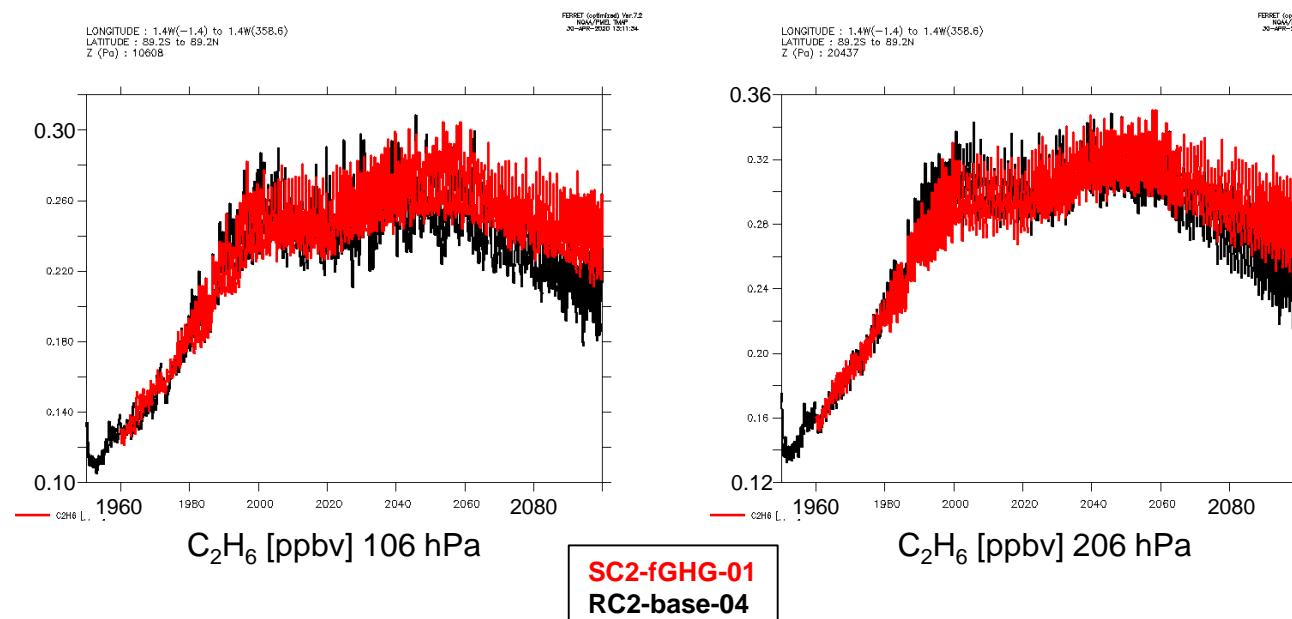
The decrease is caused by the additional reaction of OH with methane, the increase is caused by the H_2O increase, probably due to a intensified tropical upwelling through convection.

In SC2-fGHG-01 is no significant trend simulated.



Ethane (C_2H_6)

The trend of ethane is mainly influenced by the emissions as main source, but there is a small sink due to the reaction with OH ($C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$). Because of the different OH trends this sink is particularly visible in the upper troposphere. Here different ethane trends are simulated in RC2-base-04 and SC2-fGHG-01. Because of the higher OH mixing ratios in RC2-base-04, smaller C_2H_6 mixing ratios are simulated in the second half of the 21st century.

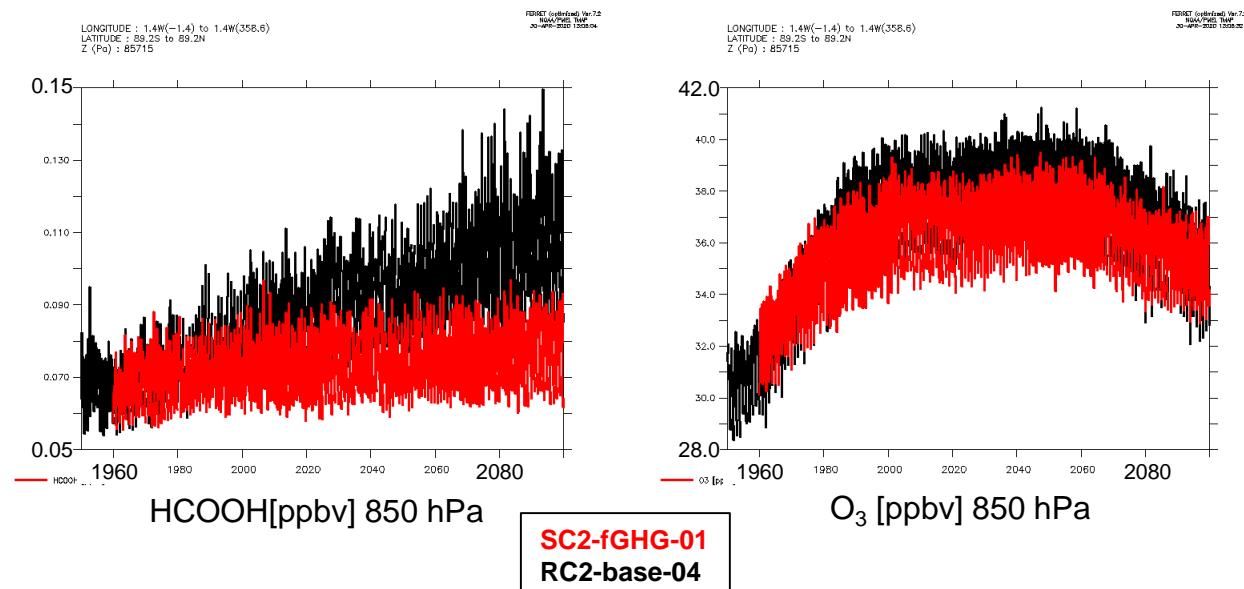


Formic acid (HCOOH)

The trend of HCOOH is very strong influenced by the temperature change. The sources of HCOOH are, besides emissions, different temperature-dependent reactions with other substances (for example $C_2H_4 + O_3$, or $C_3H_6 + O_3$, or MVK + O_3). The higher the temperature, the higher are the reaction rate of these reactions. The distribution of HCOOH is also influenced by the mixing ratios of tropospheric ozone.

In RC2-base-04 a positive HCOOH trend is simulated, mainly caused by the climate change.

In SC2-fGHG-01 only a slight positive HCOOH trend is visible from 1960 to 2000, probably due to the increase in tropospheric ozone.

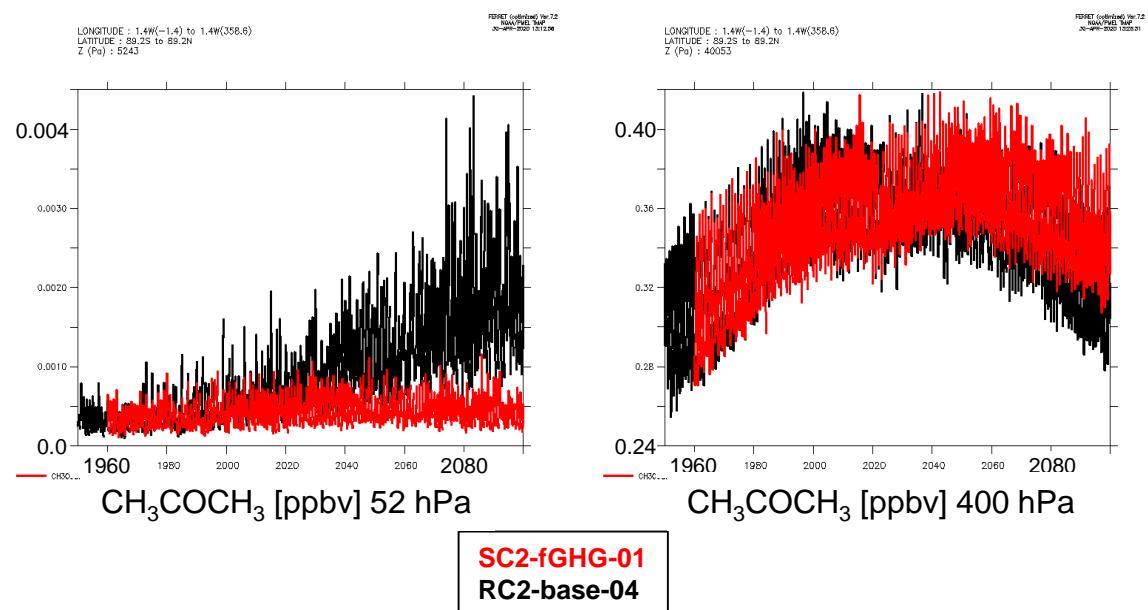


Acetone (CH_3COCH_3)

Acetone is mainly formed by secondary formation from substances as propane, isopropylnitrat or isobutane and emitted due to biomass burning. In EMAC the reaction $\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$ is one of the source reactions. Beside the photolysis, the reaction $\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$ is the main sink. Both reactions are temperature dependent: the higher the temperature the higher the reaction rates.

Depending on latitude and altitude, temperature and OH trend, the acetone trend shows different signs (see slides 36 to 49).

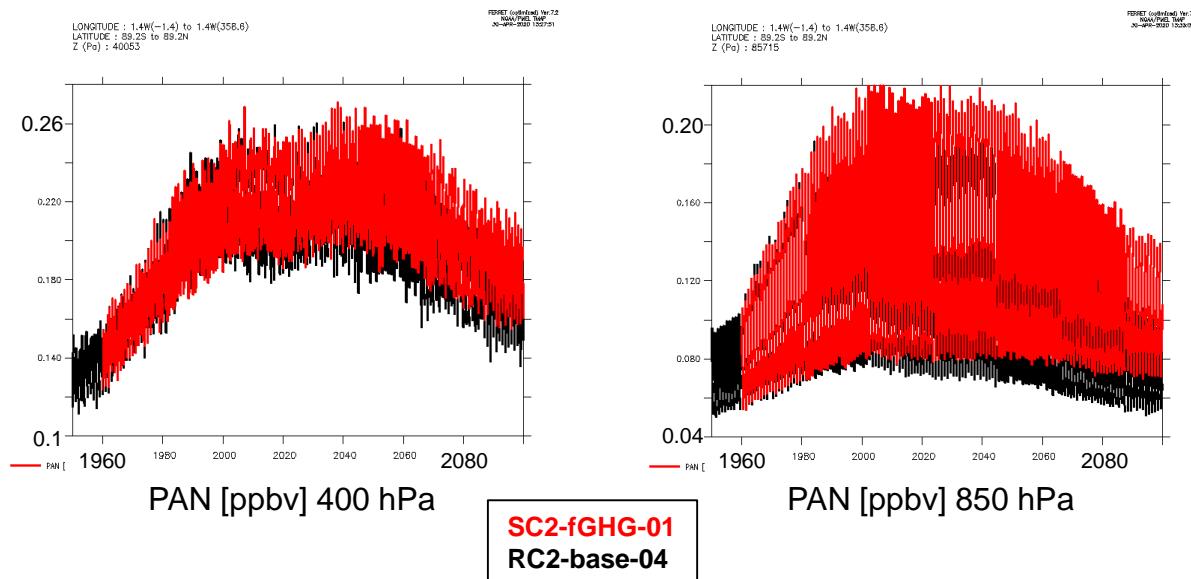
In RC2-base-04 in 50 hPa a positive trend exists (no trend exists in SC2-fGHG-01), whereas at 400 hPa a negative trend during the second part of the 21st century is simulated (in SC2-fGHG-01 weaker).



PAN ($\text{CH}_3\text{COOONO}_2$)

The chemistry of PAN is relatively complex. There are many reactions involved in the formation of PAN. The main sources are the oxidation of acetaldehyde (CH_3CHO), as well the photolysis of acetone ($\text{CH}_3\text{C(O)CH}_3$) and methylglyoxal (CH_3COCHO) to $\text{CH}_3\text{C(O)OO}$ and the following reaction: $\text{CH}_3\text{C(O)OO} + \text{NO}_2 \rightarrow \text{PAN}$. The main sink is the thermal decomposition of PAN $\rightarrow \text{CH}_3\text{C(O)OO} + \text{NO}_2$, the higher the temperature the stronger is this decomposition.

Due to the climate change and the resulting higher temperatures, this thermal decay is becoming one of the dominant factor in the PAN trend. Therefore in RC2-base-4, a negative trend is simulated in the troposphere within the 21st century (see slides 36 to 49).



Conclusions

- In RC2-base-04 a realistic climate change corresponding to RCP6.0 is simulated in EMAC. In SC2-fGHG-01 no climate change exists.
 - Water vapour is increasing in RC2-base-04 due to methane oxidation.
 - In RC2-base-04 an OH increase in the stratosphere is simulated, but also in some regions in the troposphere, e.g. in the upper tropical troposphere, due to increasing H₂O mixing ratios (methane oxidation and intensified tropical upwelling). Decrease due to reaction with CH₄.
 - The trend of C₂H₆ depends mainly on the development of emissions, but also shows a dependence on the OH trend.
 - HCOOH shows a high temperature dependency. In RC2-base-04 the trend is more positive than in SC2-fGHG-01.
 - The trends of acetone depend on OH distribution and temperature and is regionally different.
 - The trend of PAN is highly dependent on climate change.
- **The tropospheric chemistry is changing due to climate change and the increase of CH₄ and N₂O. This could be of great importance.**