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CO_2 variability and seasonal cycle in the UTLS: insights from EMAC model and AirCore observational data

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Table S 1. Properties of the different AirCore setups. Note that tubing lengths and total volume may vary slightly between the individual AirCores of the same design.

AirCore design approach	Individual AirCore ID's (almost identical in construction)	Tubing Length of the different sections [m]	Inner diameter of the different sections [mm]	Total volume [ml]
NOAA 1st generation AirCore (Karion et al., 2010)	BIG002	152	5.8	4000
NOAA 1st generation StratoCore (dual-dimension coil)	GML001-GML004	26, 37	5.8, 2.7	1000
NOAA 2nd generation AirCore (standard design)	GML007-GML013, ROO001-ROO004	91	2.9	600
NOAA 2nd generation StratoCore (dual-dimension coil)	GML014-GML017	21, 28	5.8, 2.9	750
GUF AirCore (three sections) (Engel et al., 2017)	GUF003, GUF005	20, 40, 40	7.6, 3.6, 1.76	1400

Table S 2. MESSy submodels used for the EMAC simulation for this work.

Submodel	**Description**	**Citation**
AEROPT	Aerosol optical properties	(Dietmüller et al., 2016)
AIRSEA	Emission and deposition over the ocean	(Pozzer et al., 2006)
BIOBURN	Biomass burning emissions	(Kaiser et al., 2012)
CLOUD	ECHAM5 cloud scheme	(Roeckner et al., 2003)
CLOUDOPT	Cloud optical properties	(Dietmüller et al., 2016)
CONVECT	ECHAM5 Tiedtke convection scheme with Nordeng closure	(Roeckner et al., 2003)
CVTRANS	Convective tracer transport	(Tost, 2006)
DDEP	Dry deposition	(Kerkweg et al., 2006a)
E5VDIFF	ECHAM5 Land-Atmosphere exchange (not for tracers) and vertical diffusion	(Roeckner et al., 2003)
GMXE	Tropospheric aerosol microphysical processes	(Pringle et al., 2010)
GWAVE	ECHAM5 non-orographic gravity wave scheme	(Roeckner et al., 2003)
JVAL	Photolysis rate coefficients	(Sander et al., 2014)
LNOX	NOx production by lightning	(Tost et al., 2007)
MECCA	Atmospheric chemistry	(Sander et al., 2019)
MSBM	Heterogeneous reactions in polar stratospheric clouds and stratospheric background aerosols	(Jöckel et al., 2010)
OFFEMIS	Tracer tendencies from offline emission files	(Kerkweg et al., 2006b)
ONEMIS	Tracer tendencies from online calculated emissions	(Kerkweg et al., 2006b)
ORBIT	Earth's orbit parameters	(Dietmüller et al., 2016)
OROGW	ECHAM5 subgrid scale orographic wave drag parameterisation	(Roeckner et al., 2003)
PTRAC	Add prognostic tracers	(Jöckel et al., 2008)
QBO	Assimilation of QBO zonal wind observations	(Jöckel et al., 2006)
RAD	ECHAM5 radiation scheme with new features and extensions	(Dietmüller et al., 2016)
S4D	Temporal high resolution model output along moving observation	(Jöckel et al., 2010)
SCAV	Wet deposition and liquid phase chemistry in precipitation	(Tost et al., 2006)
SCALC	Online calculations	(Jöckel et al., 2016)
SEDI	Sedimentation scheme for aerosol particles	(Kerkweg et al., 2006a)
SURFACE	ECHAM5 surface subroutines	(Roeckner et al., 2003)
TNUDGE	Tracer nudging to defined fields	(Kerkweg et al., 2006b)
TREXP	Add prognostic tracers with lifetime or point sources	(Jöckel et al., 2010)
TROPOP	Tropopause diagnostics	(Jöckel et al., 2006)
UBCNOX	Effect of energetic particles on NOx	(Funke et al., 2016)

Table S 3. MESSy infrastructure framework.

CHANNEL	Data exchange between submodels, control of output and restart files	(Jöckel et al., 2010)
GRID	Grid definition and transformation	(Kerkweg et al., 2018)
IMPORT	Data import from external files	(Kerkweg and Jöckel, 2015)
QTIMER	Simulation wall-clock time and restart trigger	(Jöckel et al., 2010)
TENDENCY	Tendency per process for prognostic variables	(Eichinger and Jöckel, 2014)
TIMER	Time and date control	(Jöckel et al., 2010)
TRACER	Data and meta data handling for chemical species	(Jöckel et al., 2008)

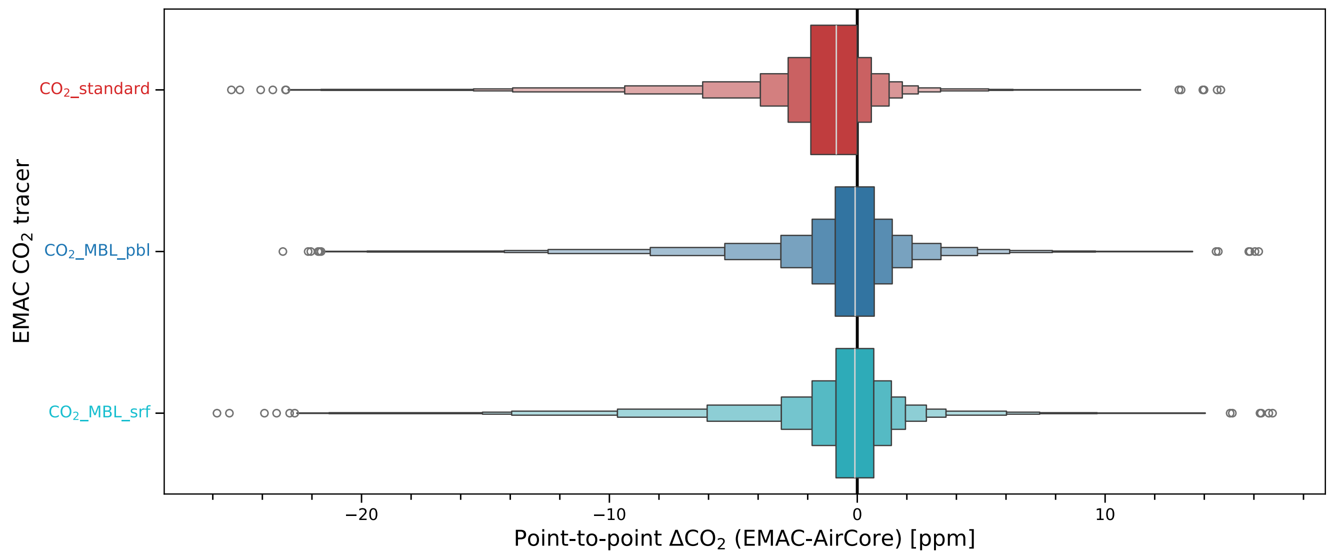


Figure S 1. Letter-value plot of the point-to-point deviations from the comparison of the different EMAC CO_2 tracers with respect to the corresponding AirCore observations.

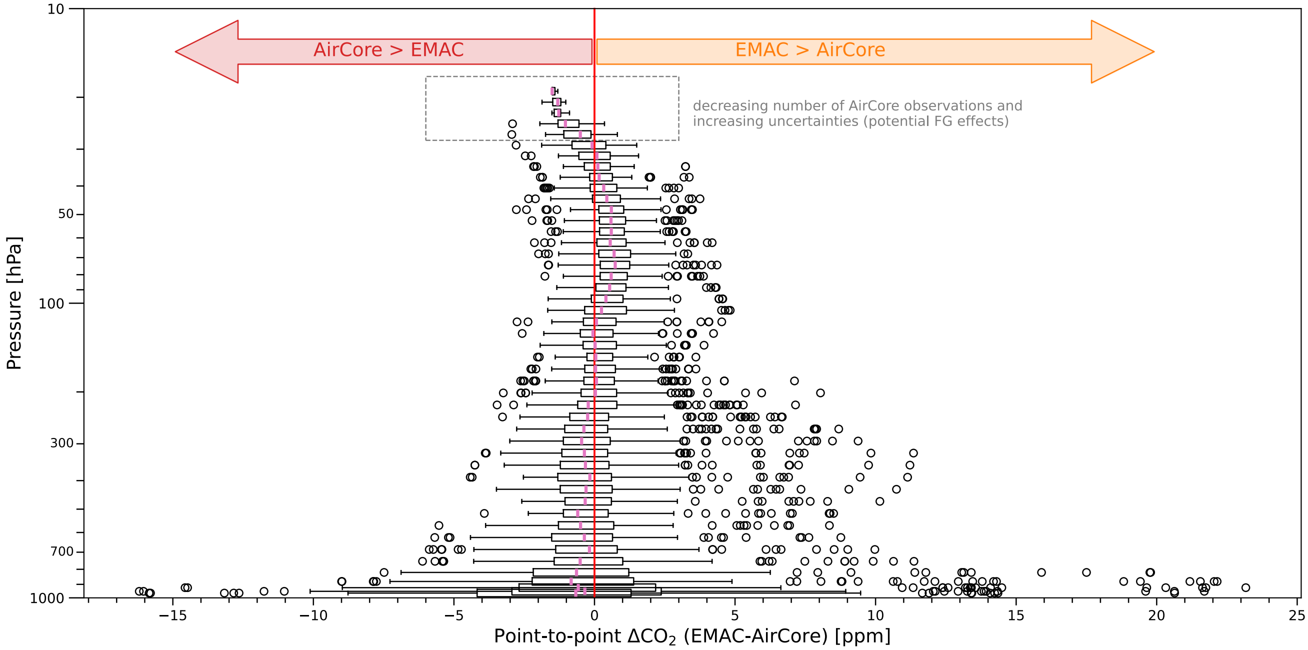
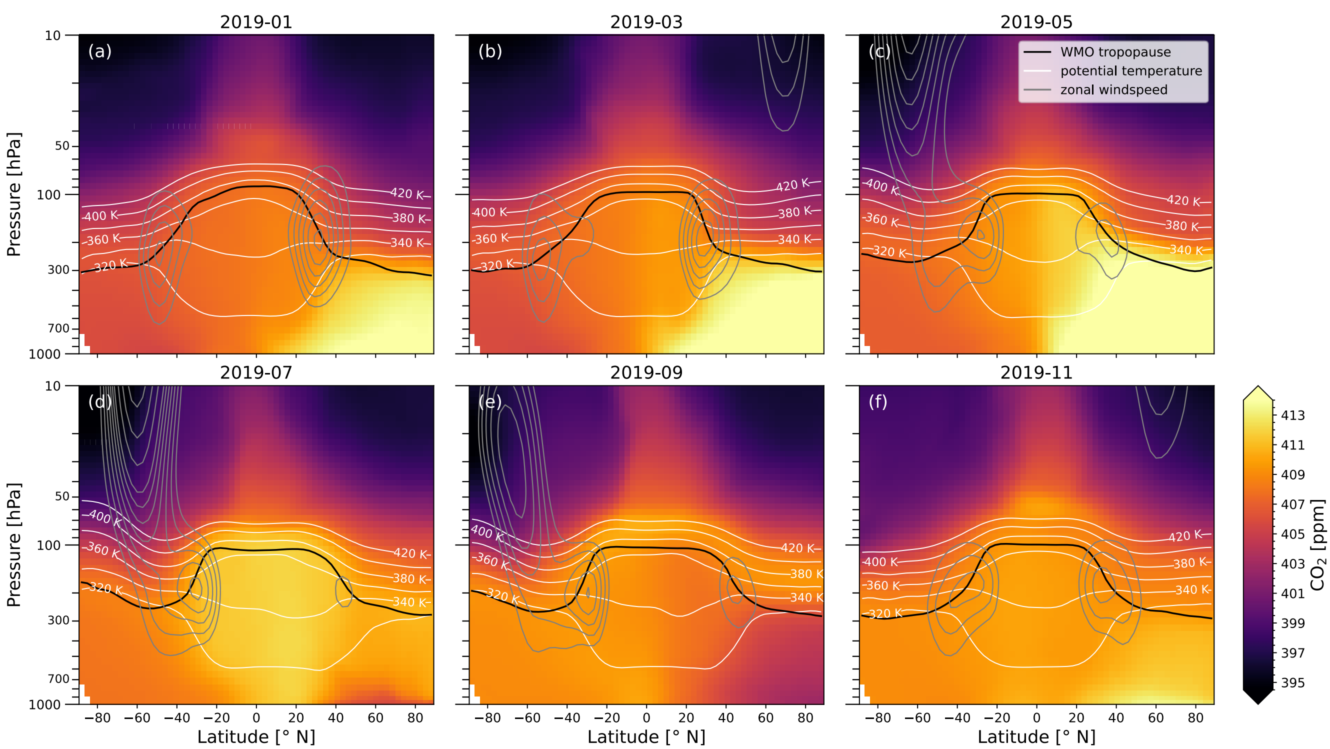


Figure S 2. Vertical profile of point-to-point deviations from the comparison of EMAC CO₂_MBL_pbl and AirCore observations (boxplots of all data for 10 hPa bins). Note that AirCore data from 30 hPa upwards are sparse and may be affected by the remaining FG.



35 **Figure S 3.** Same as Fig. 4 but for odd months of 2019: monthly averaged zonal mean latitude-pressure cross section plots of EMAC CO_2_MBL_pbl with WMO tropopause (black line), jet positions (grey contour lines) and potential temperature surfaces (white lines).

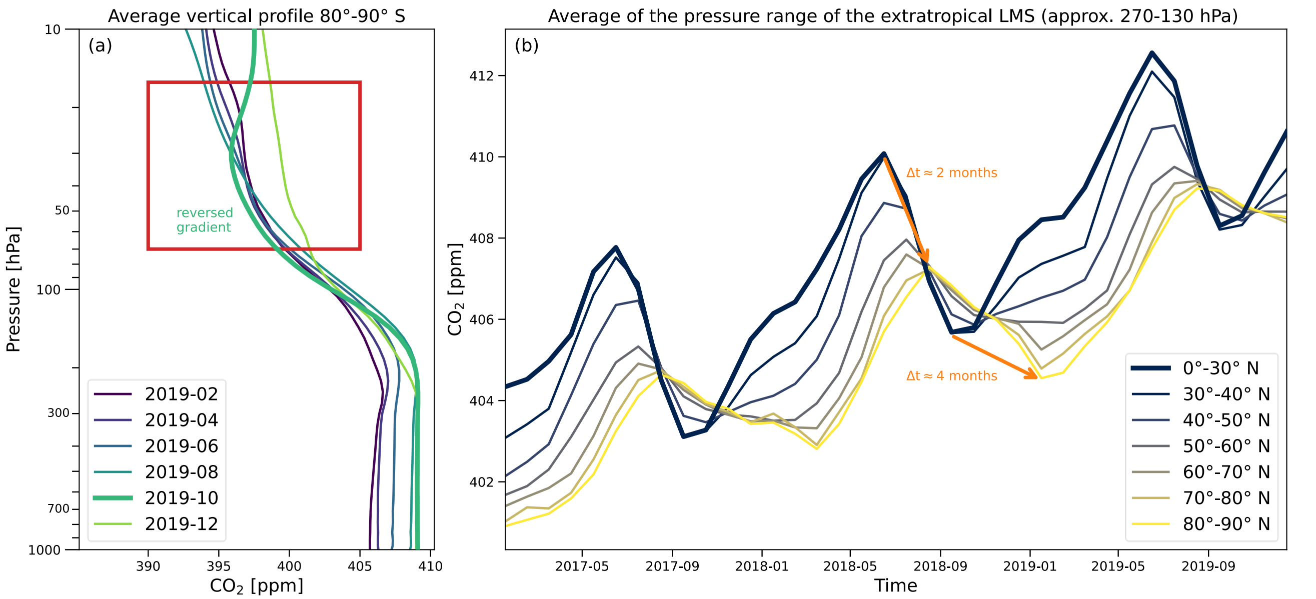


Figure S 4. Detailed visualisation of specific features of the global CO_2 distribution (EMAC CO2_MBL_pbl simulation results). (a) CO_2 vertical profiles at SH polar latitudes (average of 80°-90° S) for even months of 2019. The red box is the same as in Fig. 4e and highlights the stratospheric pressure range where the reversed CO_2 gradient during SH winter is observed. (b) Temporal evolution of CO_2 zonally averaged over the 270-130 hPa pressure range for different latitudinal bands. The orange annotations illustrate the CO_2 expansion from the tropical tropopause layer to the mid-latitude LMS and shows the different timescales that it takes in summer or winter.

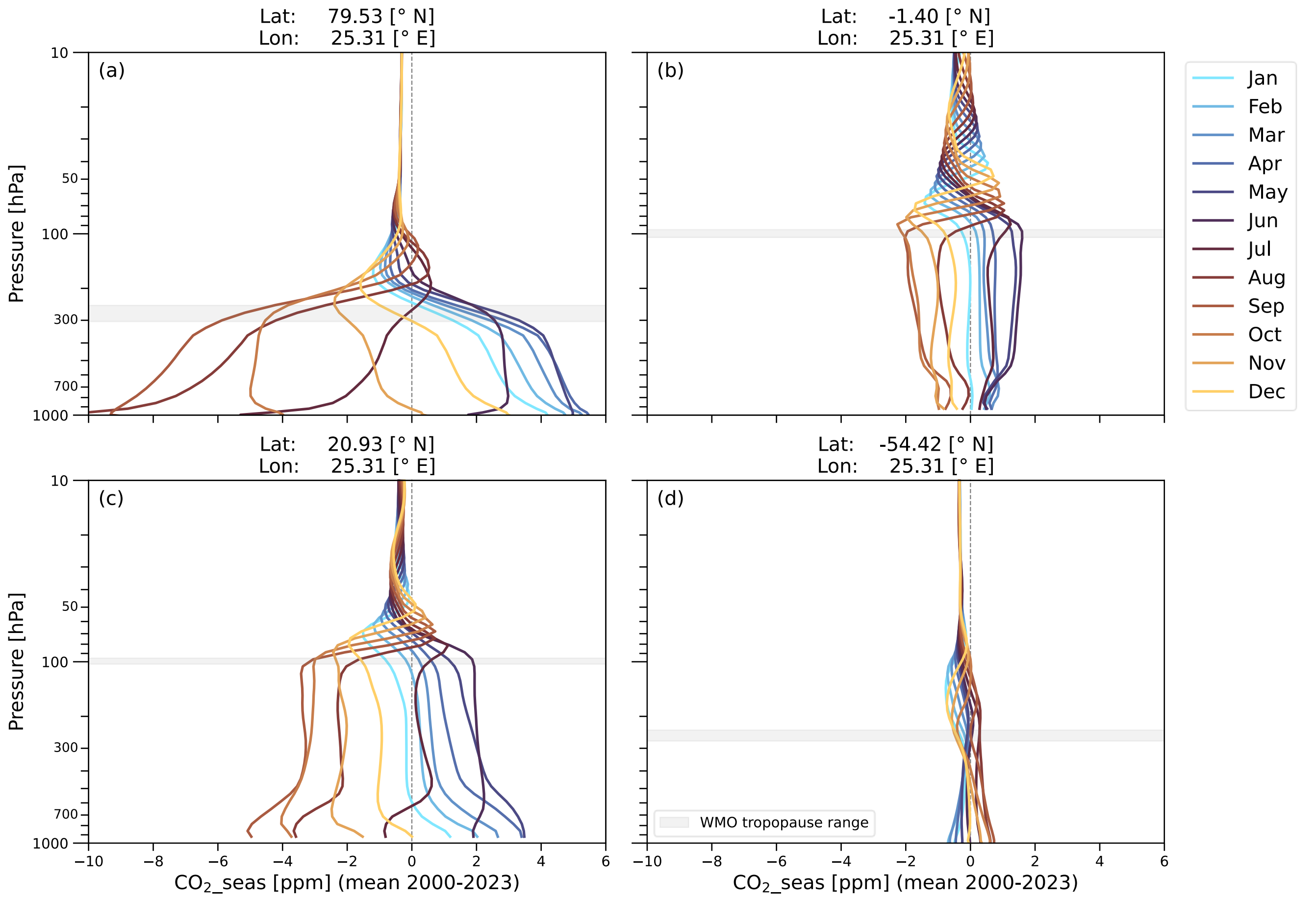


Figure S 5. As in Fig. 6, climatological EMAC-derived CO_2 seasonal signal vertical profiles per calendar month for (a) NH polar latitudes, (b) tropics, (c) NH subtropics and (d) SH mid-latitudes.

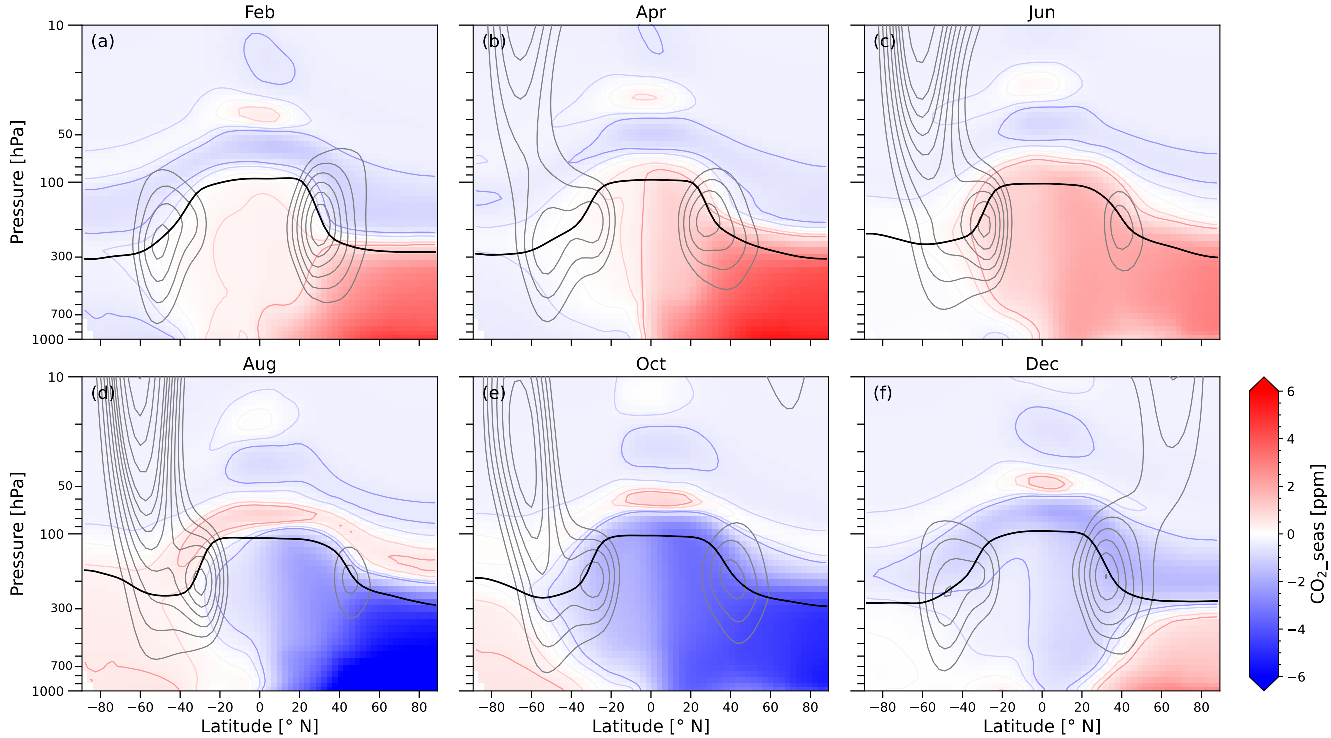


Figure S 6. Same as Fig. 8 but for even months: zonal mean latitude-pressure cross-sections of the EMAC-derived climatological average of the CO_2 seasonal signal. The black line indicates the WMO tropopause. Grey contour lines indicate jet positions (zonal windspeed; lower threshold is 20 m s^{-1}, 5 m s^{-1} spacing).

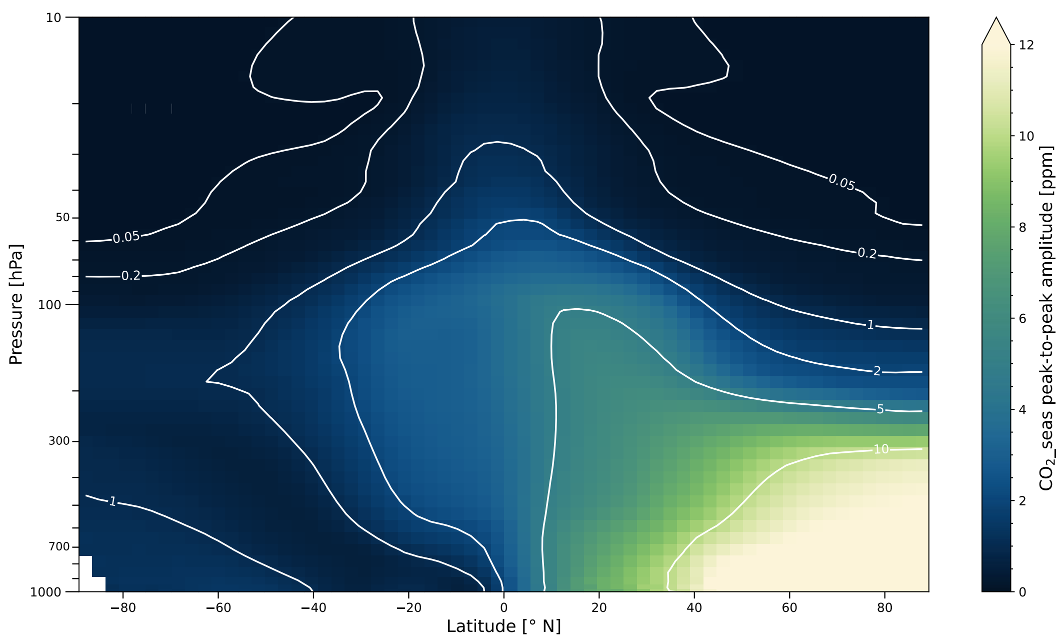


Figure S 7. Zonal mean latitude-pressure cross-section of the EMAC-derived climatological average of the CO_2 seasonal signal peak-to-peak amplitude.

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