Supplement to "Implications of Lagrangian transport for simulations with a coupled chemistry-climate model" by Stenke et al.

Parameterisation of bromine chemistry

In contrast to E39C, E39C-A considers a parameterisation for bromine chemistry (ClO/BrO-cycle). The parameterisation is based on a scaling of the ozone destruction via the ClO-ClO-cycle. The implementation of the parameterisation is given below (Markus Rex, personal communication):

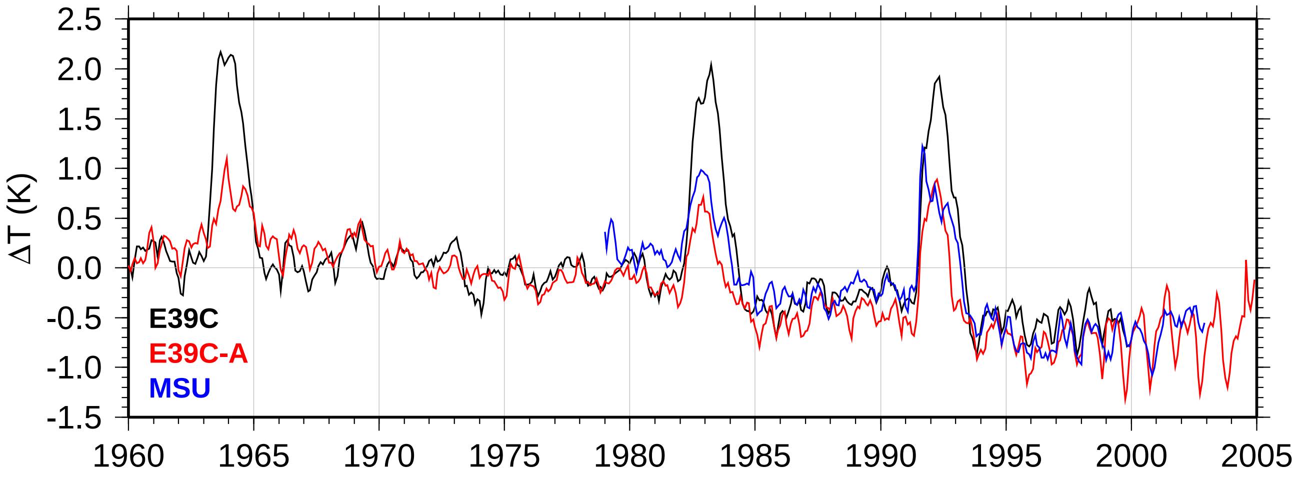
```
if ((clox .ge. 0.25) .and. (p .le. 80.) .and. (p .ge. 20.) then
   t = t + max(p - 60., 0.)/2.
   factor = abs( &
     exp(-0.064996 - 0.8939601*log(clox)) + &
     exp(-3.760605 - 0.9998547*log(clox)) * (t - 195.) - &
     exp(-3.674095 - 1.0190500*log(clox)) * (p -50.) )
else
   factor = 0.
end if

deltao3 = factor * 2. * photcl2o2
```

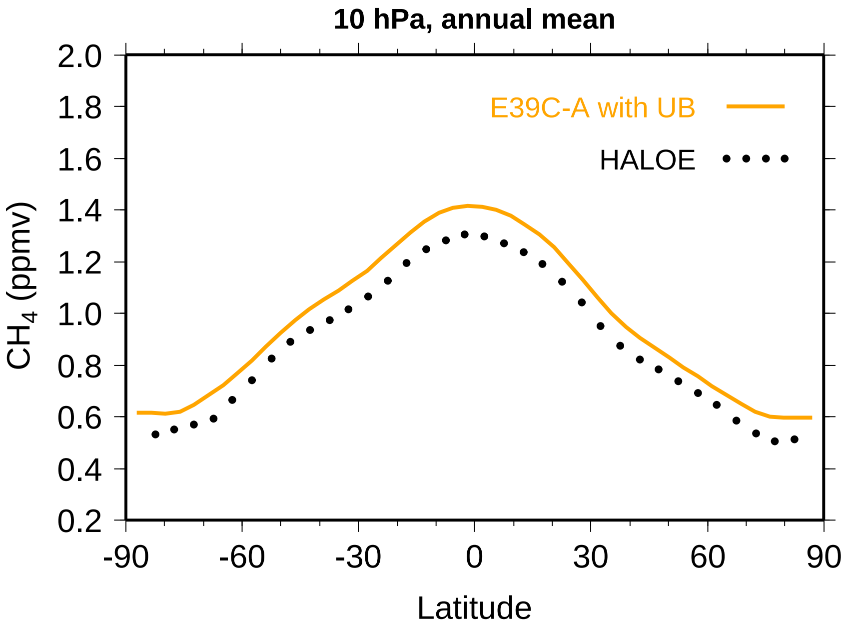
p: pressure [hPa], with $20\ hPa \leq p \leq 80\ hPa$
t : temperature [K], with $170\ K \leq T \leq 250\ K$
clox: mixing ratio of ($ClO+2*Cl_2O_2$) [ppbv], with $0.25\ ppbv \leq clox \leq 4\ ppbv$
photcl2o2: number of Cl_2O_2 molecules photolysed during one timestep [molec/cm^3]
deltao3: number of ozone molecules destroyed by ClO/BrO-cycle during one timestep [molec/cm^3]

The parameterisation is adapted for chemical conditions in polar winter. It is based on in-situ measurements of BrO:

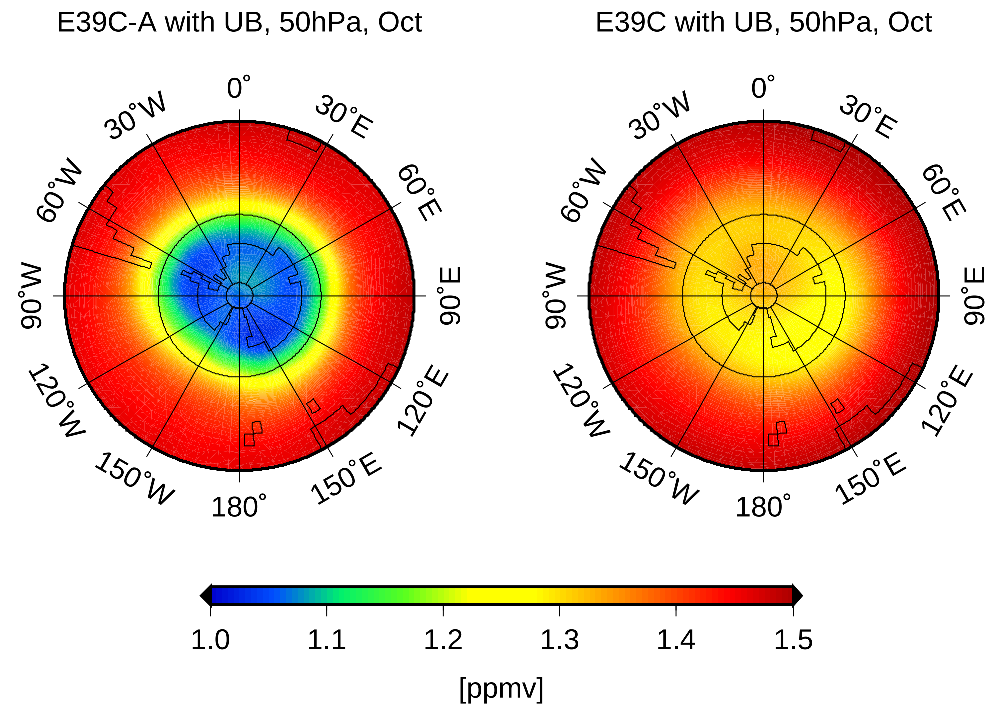
Avallone, L. M., D. W. Toohey and K. R. Chan, In situ measurements of BrO during AASE II, Geophys. Res. Lett., 22, 831-834, 1995.



S 1: Comparison of global mean temperature anomalies in the lower stratosphere (15 to 23 km) derived from observations (MSU Channel 4, blue) and equivalent values calculated from results of the model simulations with E39C (black) and E39C-A (red).



S 2: Climatological zonal mean CH_4 mixing ratios [ppmv] at 10 hPa for E39C-A using an upper boundary condition with a meridionally varying CH_4 gradient (orange) and HALOE observations (black). The HALOE climatology is normalised to the CH_4 mixing ratio in the inner tropics (10°N-10°S). The normalised CH_4 gradient is prescribed at the model top. At each time step the normalised gradient is multiplied with the acutal simulated CH_4 mixing ratio in the inner tropics to receive the upper boundary condition in the model. The upper boundary condition is based on annual mean values and does not consider the annual cycle.



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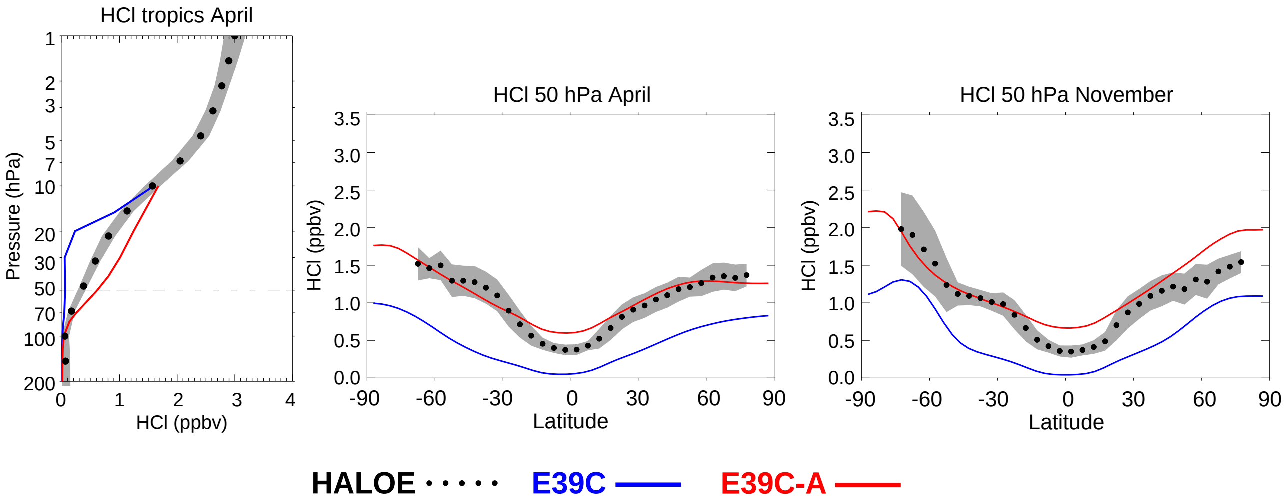
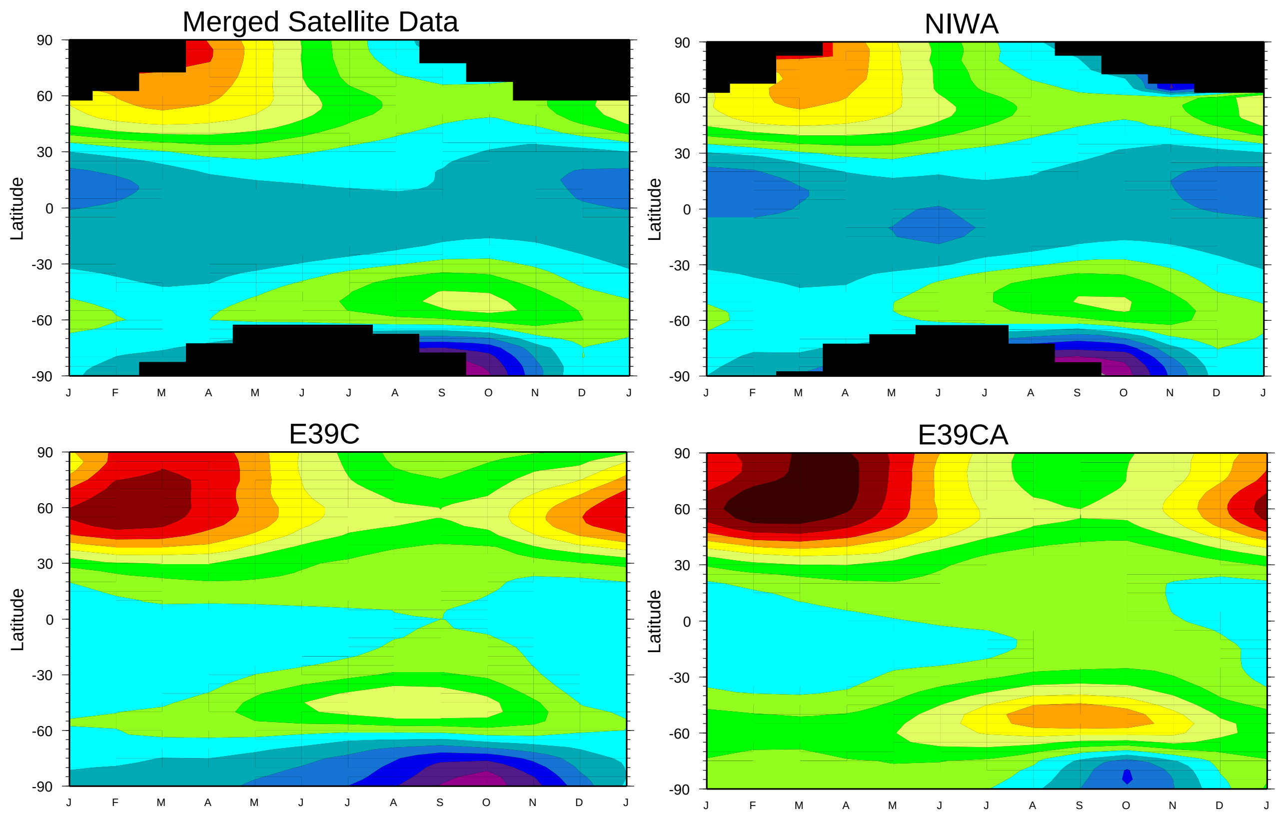
S 3: Climatological mean CH_4 mixing ratios [ppmv] at 50 hPa in October for E39C-A (left) and E39C (right) including the upper boundary condition for CH_4.



S 4: Climatological mean HCl vertical profile at the Equator in April and zonal mean mixing ratios [ppbv] at 50 hPa in April (left) and November (right). The grey areas show HALOE plus and minus 1 standard deviation about the climatological zonal mean. Observations taken from Eyring et al. (2006), their Fig. 11.



S 5: Modeled total column ozone climatologies (1980 to 1999) for E39C and E39C-A compared to merged satellite and NIWA assimilated data (taken from Eyring et al. (2006), their Fig. 14).