Fast stratospheric ozone chemistry for climate models: The polar SWIFT model

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Motivation

Importance of ozone-climate interactions has long been recognized

- E.g. Effect of changes in polar stratospheric vortex and ozone on surface temperature trends in Antarctica (Thompson and Solomon, Science, 296, 895, 2002)
- E.g. Changes in tropospheric wave driving and the Brewer-Dobson circulation (Rex et al., GRL, 33, doi:10.1029/2006GL026731, 2006)

Ozone is usually prescribed in climate models, since a detailed calculation is computationally very expensive.

- E.g. In the IPCC CMIP5 models (IPCC, 2013)

It is desirable to account for ozone-climate interactions on a decadal scale in climate models.

Existing approaches

Chemistry Climate Models (CCMs): Coupling of a full stratospheric chemistry model to a GCM (slow)

- Not applicable to scenarios where long-term runs and multiple scenarios are needed

Existing fast ozone schemes like the Cariolle scheme (e.g. Cariolle and Deque, JGR, 91, 10825, 1986) or Linoz (e.g. McLinden, JGR, 105, 14653, 2000) based on Taylor series expansion around mean state have several disadvantages

- Do not model the actual physical and chemical processes
- Only based on current state of atmosphere and not on history
- Can't cope well with non-linearities

The SWIFT model

SWIFT is a fast yet accurate chemistry scheme for calculating the chemistry of stratospheric ozone in climate models which consists of two parts:

- The polar SWIFT model is based on a small set of differential equations, which simulate time evolution of polar vortex averaged mixing ratios of ozone and key species
- Extrapolar SWIFT (see poster Kreyling et al.) is based on evaluating a polynomial for the rate of change of ozone (lower stratosphere) or ozone itself (upper stratosphere), which is a function of 9 parameters (including latitude, temperature and chemical families like HOx or NOx).

SWIFT can run with three transport schemes:

- No transport and temperature-based transport parameterization (finished)
- Transport by the ECHAM6 GCM (W. Dorn, in development)
- Lagrangian transport and mixing from the ATLAS CTM (in development)

SWIFT has been successfully coupled to two models, preliminary results are available, development is ongoing

- Coupling to ECHAM6 at AWI (see poster Dorn et al.)
- Coupling to EMAC at FU Berlin

Advantages Polar SWIFT

- **Fast**
- **Parameterization based on real atmospheric processes**
- **Behaves realistically under wide range of conditions**
- **Able to cope with non-linearities**
- **Takes meteorological history into account**

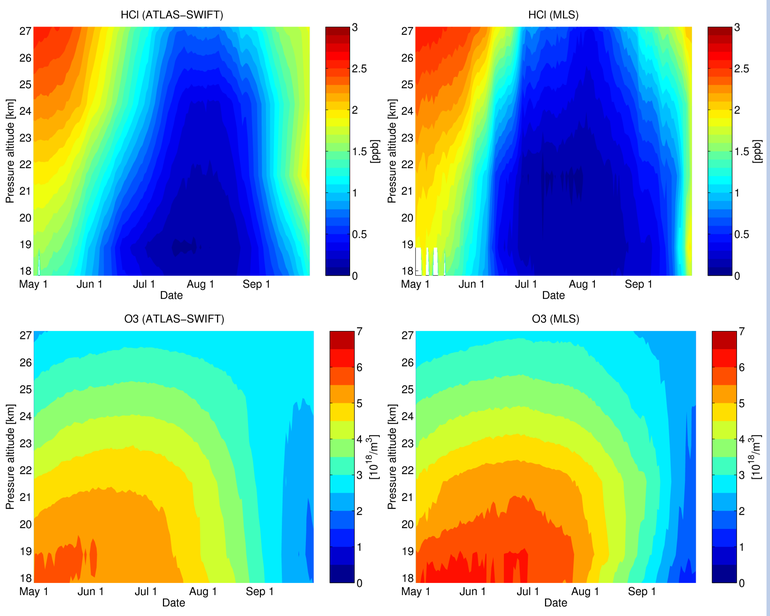
Polar SWIFT: Overview

- Model for vortex averaged polar ozone loss
- Only 4 prognostic equations per altitude (vortex means)
- Large time step possible (1 day)
- Fast: seconds per model year on 1 processor
- Solves system of differential equations for key species
  - O_3
  - HNO_3 (total)
  - HNO_3 (gas phase)
  - HCl
  - $ClONO_2$
  - ClO_x
- Includes terms for the overall net effect of chemical and physical mechanisms rather than one term for each reaction. Equations are physically justified (no Taylor expansions etc.). Terms include e.g.
  - Chlorine activation by heterogeneous reaction $HCl + ClONO_2$
  - Ozone loss by ClO dimer cycle
  - Denitrification by sedimenting particles
  - Deactivation of chlorine in the southern hemisphere by $Cl + CH_4$
  - ...
- Proportionality constants of the individual terms are empirical parameters trained on chemical reaction rates from a Chemistry Transport Model (ATLAS CTM) for two Arctic and two Antarctic winters
- Driven by only 2 time series: FAP (fraction of vortex where polar stratospheric clouds can form) and FAS (fraction of vortex exposed to sunlight)

References:

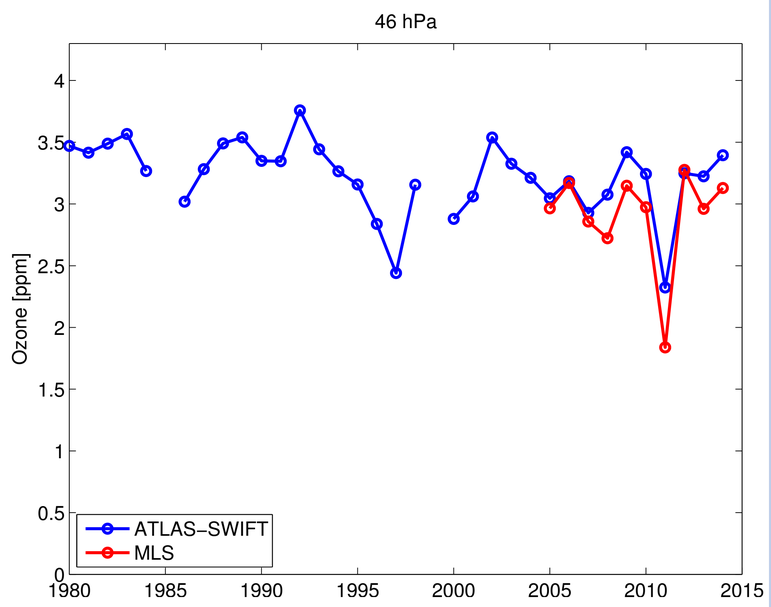
- Original version: Rex et al., Atmos. Chem. Phys., 14, 6545, 2014
- This version: Wohltmann et al., in preparation

Results for SH winter 2006



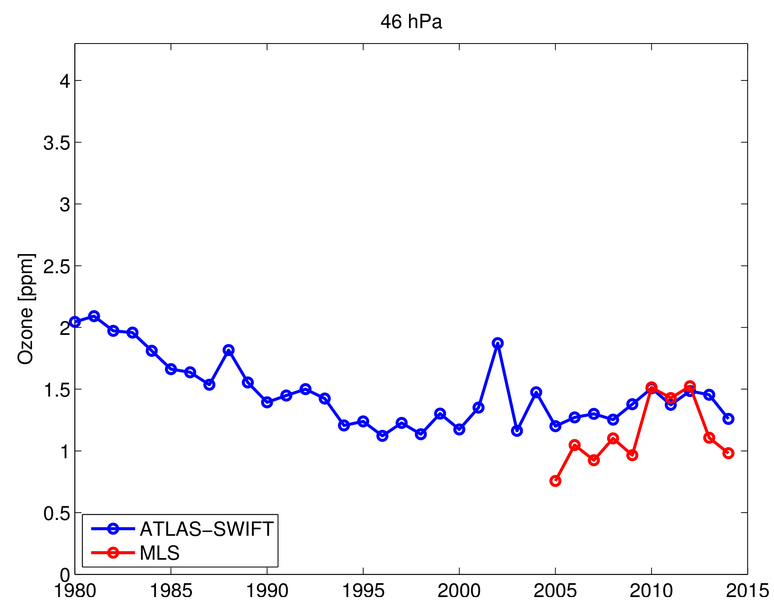
Validation of Polar SWIFT as a chemistry module in the ATLAS Chemistry and Transport Model driven by ECMWF ERA Interim reanalysis data. Vortex means for the southern hemisphere winter 2006. Left: Time evolution of the vortex means for the ATLAS-SWIFT model. Right: Time evolution from MLS satellite measurements. Top: HCl volume mixing ratios. Bottom: Ozone concentrations.

Interannual variability Northern hemisphere



Interannual variability of vortex averaged ozone mixing ratios in early spring shortly before vortex breakup in the northern hemisphere at 46 hPa. Ozone mixing ratios simulated by Polar SWIFT as a chemistry module in ATLAS driven by ECMWF ERA Interim reanalysis data (blue) and observed mixing ratios by the MLS satellite instrument (red). Dates in different years differ due to the different breakup dates of the vortex and availability of satellite data. Chlorine loading changes according to EESC.

Interannual variability Southern hemisphere



Interannual variability of vortex averaged ozone mixing ratios on 1 October in the southern hemisphere at 46 hPa. Ozone mixing ratios simulated by Polar SWIFT as a chemistry module in ATLAS driven by ECMWF ERA Interim reanalysis data (blue) and observed mixing ratios by the MLS satellite instrument (red). Chlorine loading changes according to EESC.

Details: The differential equations

Prognostic

$d[O_3]/dt = -d[ClO_x]FAS$ — Ozone depletion by ClO+ClO and ClO+BrO cycle

$d[ClONO_2]/dt = b[ClO_x][HNO_3gas]FAS$ — Net effect of $ClONO_2$ photolysis / ClO+NO_2

$-a\{[HCl]\}[ClONO_2][HNO_3total]^{2/3}FAP$ — Chlorine activation by HCl+$ClONO_2$ (heterogeneous)

$-h[ClONO_2][HNO_3total]^{2/3}FAP$ — Chlorine activation by $ClONO_2$+H_2O (heterogeneous)

$d[HCl]/dt = c_1[ClO_x]FAS^2/[O_3] + c_2[ClONO_2]FAS^3/[O_3]$ — Chlorine deactivation by Cl+CH_4 into HCl (SH)

$+f[ClO_x][OH_{day}]FAS$ — HCl formation by ClO+OH

$-a\{[HCl]\}[ClONO_2][HNO_3total]^{2/3}FAP$ — Chlorine activation by HCl+$ClONO_2$ (heterogeneous)

$-l[ClO_x][H_2O]FAS[HCl][HNO_3total]^{2/3}FAP$ — Chlorine activation by HOCl+HCl (heterogeneous)

$-k[HCl][OH_{day}]FAS$ — Activation by HCl+OH (gas phase)

$d[HNO_3total]/dt = -e[HNO_3total]FAP_s$ — Effect of denitrification

Diagnostic

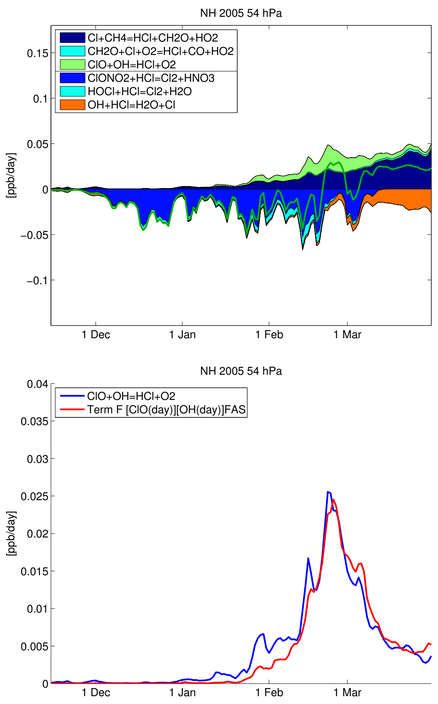
$[ClO_x] = [Cl_y] - [HCl] - [ClONO_2]$ — ClO_x is everything not in reservoir gases

$[HNO_3gas] = [HNO_3total](1-FAP_s) + z[HNO_3total]FAP_s$ — Partitioning HNO_3 (gas / clouds)

$[OH_{day}] = sqrt([H_2O][NO_{day}]FAS)$ — OH in sunlit part

$[NO_{day}] = [HNO_3gas]FAS^4/([O_3] + \alpha FAS)$ — NO in sunlit part

Details: Training method



SWIFT terms fitted to vortex averaged chemical rates of ATLAS CTM

Advantages:

- No transport effects are fitted
- Needs no measurement data. Availability for species like $ClONO_2$ limited
- Detailed look into processes

Disadvantage:

- Fit is not based on observational data, but on model results
- ... but ATLAS validated with observations, agreement is good

Left: Example training of Term F.

Top: Vortex averaged rates of all significant reactions changing HCl in the northern hemisphere winter 2004/2005 deduced from a full chemistry run of the ATLAS CTM. The green line is the net chemical change of HCl.

Bottom: Vortex averaged rate of the ClO+OH reaction from a full chemistry run of the ATLAS CTM (blue) and the fitted parameterization for Term F (red).

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