FAST-O3: Fast stratospheric ozone chemistry for climate models with the SWIFT model

Ingo Wohltmann[1], Daniel Kreyling[1], Ralph Lehmann[1] Markus Rex[1], Janice Scheffler[2], Ulrike Langematz[2]

[1]Alfred Wegener Institute for Polar and Marine Research, Potsdam
[2]Freie Universität Berlin

ALFRED-WEGENER-INSTITUT
HELMHOLTZ-ZENTRUM FÜR POLAR- UND MEERESFORSCHUNG

Freie Universität Berlin

Motivation

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

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

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)

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

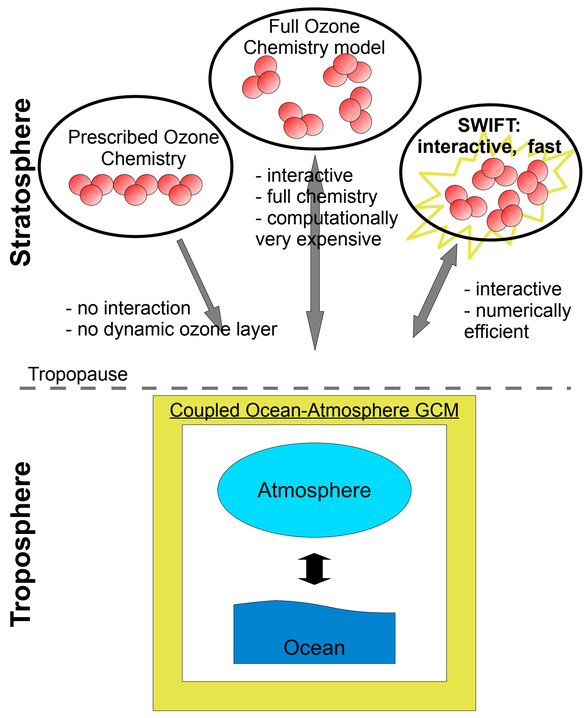
Existing approaches

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



References

- First version: Rex et al., Atmos. Chem. Phys., 14, 6545–6555, 2014
- Version shown here: Wohltmann et al., Atmos. Chem. Phys., in preparation

FAST-O3

The FAST-O3 project in Module B aims at the development of a fast scheme for calculating stratospheric ozone chemistry and transport

- Further development of existing AWI SWIFT model for fast calculation of polar ozone depletion
- Development of extrapolar chemistry model for SWIFT
- Addition of a Lagrangian transport module from the ATLAS CTM to the SWIFT model
- Coupling to the the state-of-the-art CCM EMAC for validation

The SWIFT model

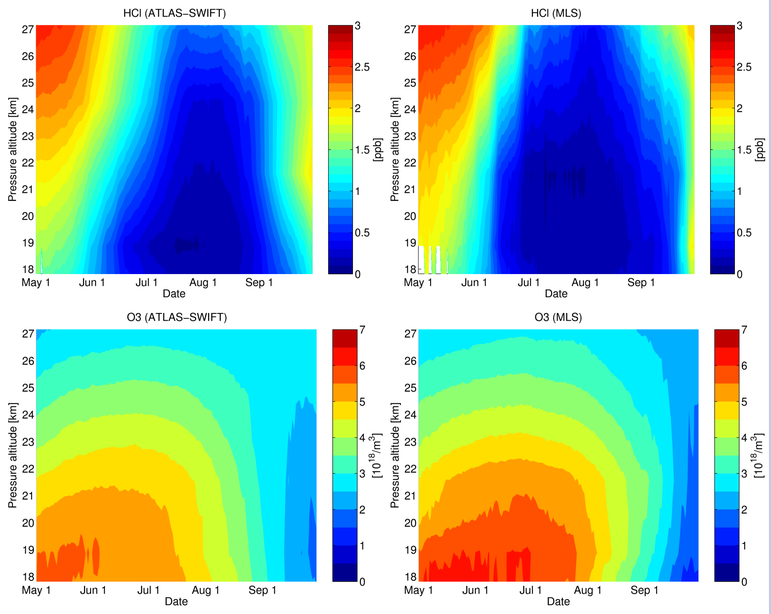
SWIFT is a fast yet accurate chemistry scheme for calculating the chemistry of stratospheric ozone which consists of two parts

- 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 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).

Polar SWIFT: Overview

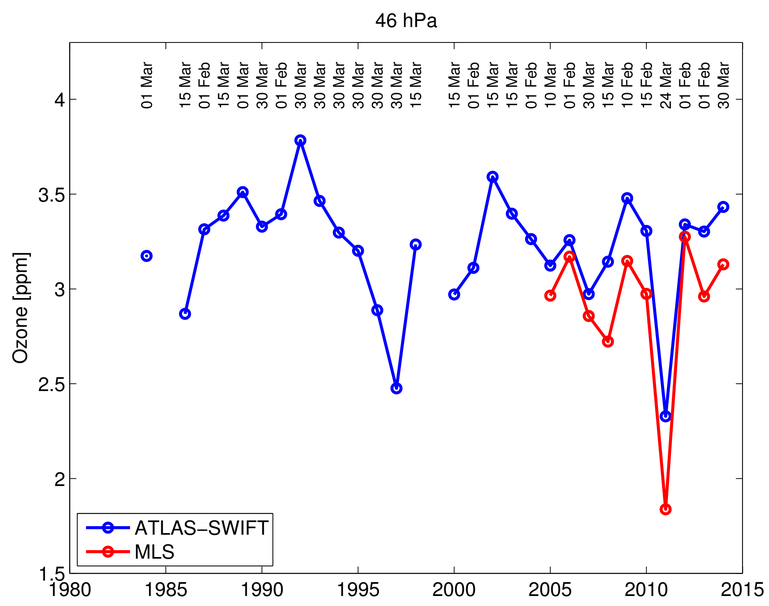
- Fast model for vortex averaged polar ozone loss
- Only 6 equations per altitude (vortex means)
- Large time step possible (1 day)
- Solves system of differential equations for key species
  - O_3
  - HNO_3 (total)
  - HNO_3 (gas phase)
  - HCl
  - $ClONO_2$
  - ClO_x
- Includes terms for the overall net effect of chemical and physical mechanisms rather than one term for each reaction. Equations are physically justified (no Taylor expansions etc.). Terms include
  - 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 $Cl + CH_4$
  - ... (5 more)
- Proportionality constants of the individual terms are empirical parameters trained on chemical reaction rates from a Chemistry Transport Model (ATLAS CTM) for one Arctic and one Antarctic winter
- Driven by only 2 time series: FAP (fraction of vortex where polar stratospheric clouds can form) and FAS (fraction of vortex exposed to sunlight)

Polar SWIFT: Results for one winter



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.

Polar SWIFT: Interannual variability



Interannual variability of vortex averaged ozone mixing ratios in early spring. 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. Dates in different years differ due to the different breakup dates of the vortex and availability of satellite data (top).

Extrapolar SWIFT: Overview

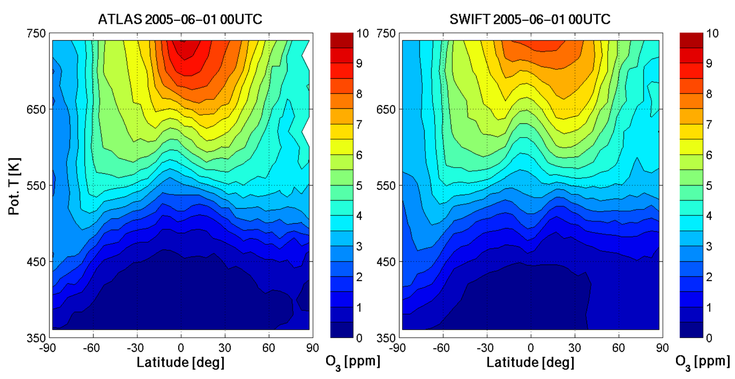
- **Repro-modeling** is the parameterization of complex reaction mechanisms by explicit algebraic functions via numerical fitting
- Fit is applied to full chemistry model output of the ATLAS Chemistry and Transport Model

Benefits:

- Extremely efficient and fast calculaton
- Few effective parameters

Repro-modeling has been successfully applied to chemical models, e.g. Turanyi, Computers and Chem., 18, 1, 45 (1994) or Lowe and Tomlin, Environmental Modelling & Software, 15, 6–7, 611 (2000)

Extrapolar SWIFT: Results



Simulations with the extrapolar module yield promising results. Comparison of zonal mean ozone mixing ratios simulated by the ATLAS CTM with the full chemistry model (left) and by the ATLAS CTM with the SWIFT extrapolar module as the chemistry module (right). Stable simulation run for 5 months (starting date: 1 Jan 2005). Simulation run employs an extrapolation prevention mechanism.

Extrapolar SWIFT: Lower stratosphere module

One explicit function per month (polynomial) for global ozone loss and production rates:

$$O_3(t) = O_3(t - 24\mathrm{h}) + \frac{\Delta O_3}{24\mathrm{h}}$$

$$\frac{\Delta O_3}{24\mathrm{h}} = F(x_1, x_2, \ldots, x_9) : \mathbb{R}^9 \to \mathbb{R}$$

$\Delta O_3/24\mathrm{h}$ can be sufficiently described by only 9 parameters:

Geographic and atmospheric variables:

- Latitude
- Altitude
- Temperature
- Overhead ozone column

Mixing ratios of chemical families:

- Chlorine family (Cl_y)
- Bromine family (Br_y)
- Nitrous-oxides family (NO_y)
- Water vapor (substitutes HO_y family)
- Odd-oxygen family (O_x)

- $\Delta O_3/24\mathrm{h}$ rates as a function of these 9 parameters, taken from the ATLAS model yield a rather compact 9-D hypersurface.
- $F(x_1, x_2, \ldots, x_9)$ is fittted with orthonormal polynomials of 4th to 6th order. Quality of the fit is determined by the order of the polynomial and the number of polynom terms (typically 100 to 200). Reduces the complex differential equation system of chemical reaction mechanisms in the stratosphere to one explicit polynomial function per month.

SWIFT in a general circulation model

The ECHAM/MESSy Atmospheric Chemistry (EMAC) model (Jäckel et al., ACP, 6, 5067–5104, 2006) is a CCM that can also be used as a GCM. The polar SWIFT has been implemented into this GCM (EMAC-SWIFT).

In EMAC-SWIFT the following steps are carried out:

- Temperature, potential vorticity, solar zenith angle, ozone delivered by GCM
- Calculation of vortex area with modified PV (Lait, J. Atm. Sci., 51, 1754–1759, 1994)
- SWIFT calculations performed once a day

EMAC-SWIFT is now being tested. So far, the computing time for a simulation of one month with EMAC-SWIFT is similar to the computing time needed by EMAC in GCM mode.

Next, longtime simulations will be performed. The performance of EMAC-SWIFT will be validated by comparing with simulations of EMAC in CCM mode. SWIFT chemistry and full chemistry will also be compared in the EMAC version that is coupled to an ocean (EMAC-O, see MiKlip project STRATO).

ingo.wohltmann@awi.de