

Simulating the global ozone distribution with ICON-ART

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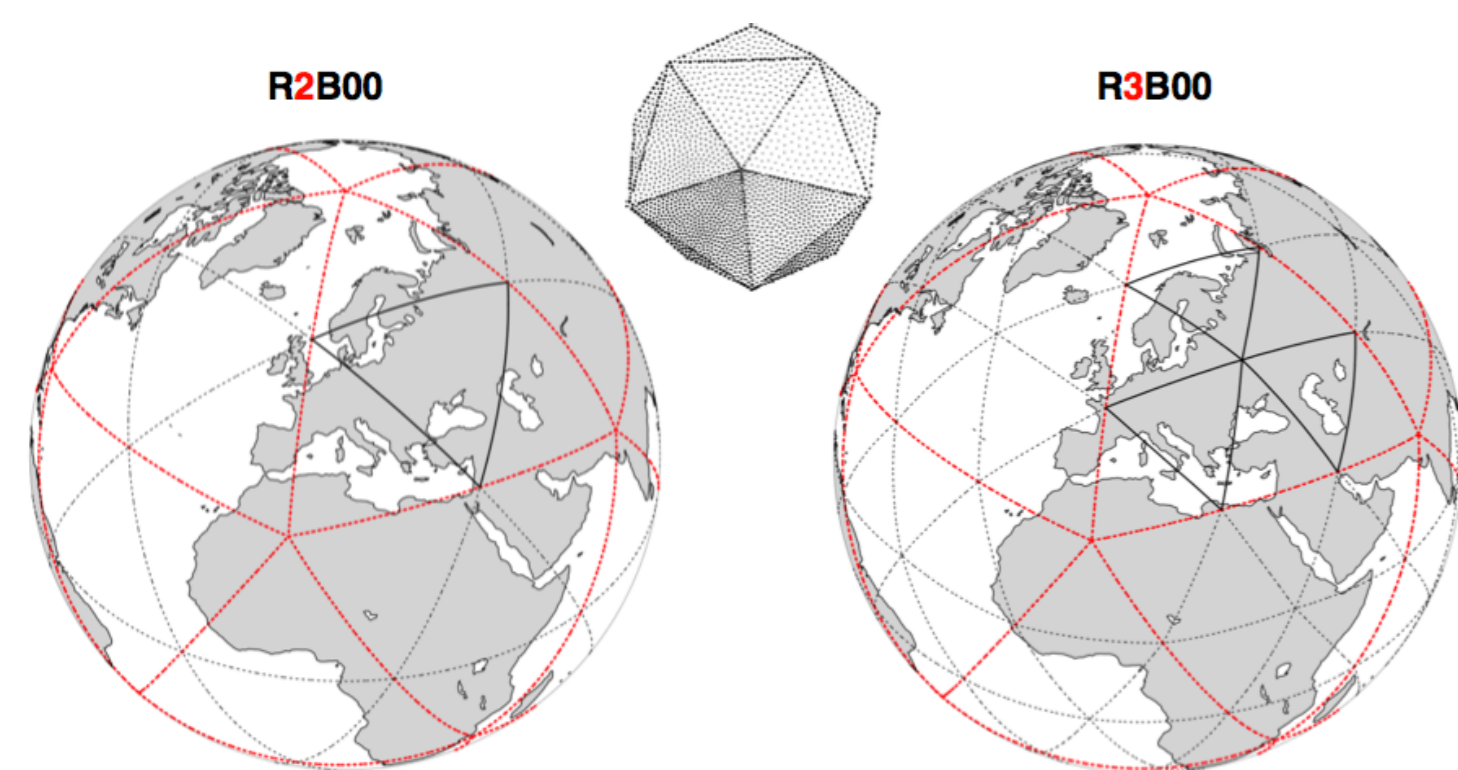
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Introduction

The ICON-ART[1] model is an extension of the non-hydrostatic modelling framework ICON[2], jointly developed by the German Weather Service (DWD) and Max-Planck-Institute for Meteorology (MPI-M), and is used for numerical weather prediction as well as for future climate predictions. ICON-ART is developed at KIT with the goal to simulate interactions between trace substances and the state of the atmosphere. We will present first simulations of global ozone distribution by using the new gas-phase chemistry module and photolysis module to show the ability of ICON-ART to investigate chemical mechanisms and transport of chemical trace gas constitutions on a global scale.

General information about ICON

ICON = ICOSahedral Nonhydrostatic modelling framework

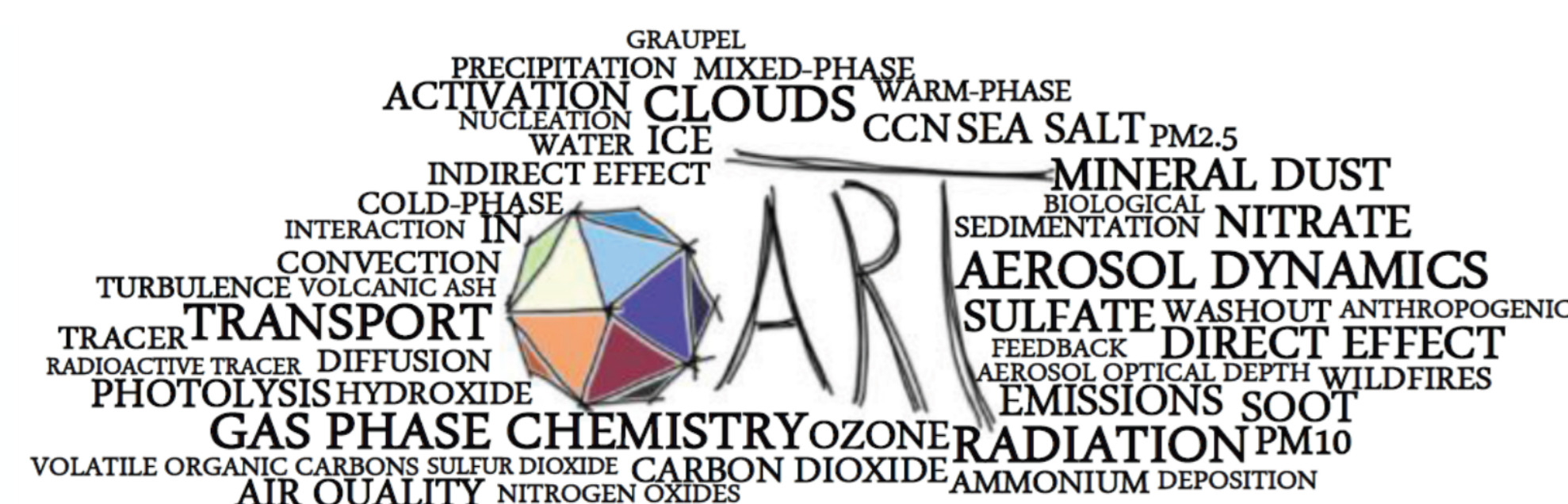


Development Goals

- Conservation of mass
- Applicability on scales from 100km to 1km
- scalability and efficiency on massively parallel computer architectures

General information about ICON-ART

ART = Aerosols and Reactive Trace substances



The extended modelling framework ICON-ART is developed in an analogous way to its predecessors COSMO-ART. For the dynamics (transport and diffusion) of gaseous tracers, the original ICON tracer framework is used. For the model physics, numerical time integration follows a process splitting approach separating physical processes. Each process is called independently via an interface module. Currently, the processes of emission, dry and wet deposition, sedimentation, and first order chemical reactions are included.

We developed a photolysis module for ICON-ART, based on FastJx[3] which was extended by an interface which allows to interact with ICON-ART. In general, stratospheric / tropospheric chemistry is mainly driven by solar radiation, thus the photolysis rate (j-value) calculation is important for atmospheric chemistry modelling. The gas-phase chemistry module is based on KPP[4].

First simulations

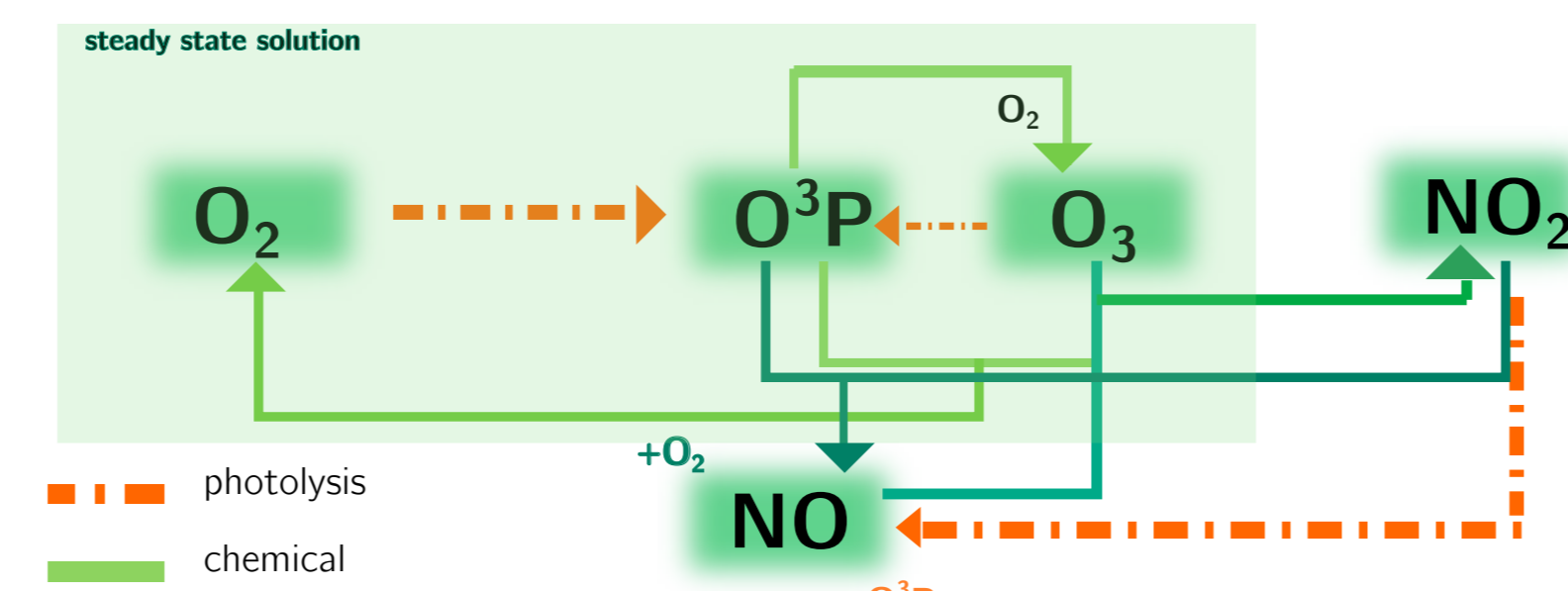
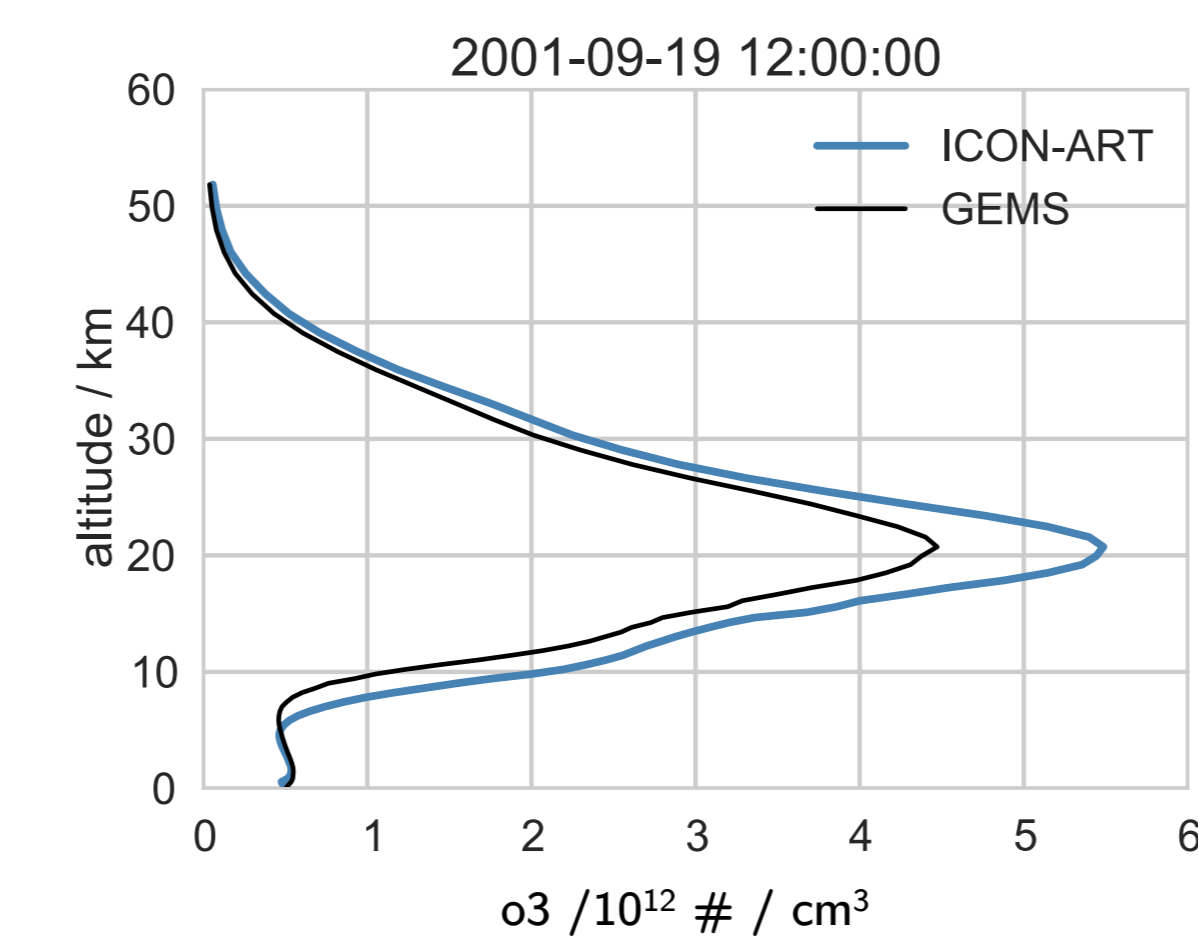


Fig. 3 Extended Chapman Mechanism - the steady state represents the original Chapman Cycle (green background) and is extended by NOx reactions

Ozone is one of the most important trace gases within the Earth's Atmosphere. The peak of the vertical ozone distribution is found at approximately 20km. The foundation for current understanding of stratospheric ozone lays at the so called Chapman mechanism (Fig. 3), proposed 1930 by S.Chapman.

The multi-day simulation with online photolysis rate calculation and gas phase chemistry was initialised with IFS Data. Ozone volume mixing ratios are prescribed by the internal ozone climatology (GEMS -ECMWFs IFS 37r2). Other chemical compounds are vertically fixed at initialisation time.



Setup

Init Date	19.09.2002
Init Data	IFS
Grid	R02B06
hor. res./ # level/ max height	40km / 90 / 75km
number of cells	492520

Initialisation values

O3P	8.9E-11 mol/mol
O2	210.E-03 mol/mol
NO2	2.9E-11 mol/mol
NO	2.7E-9 mol/mol

Fig. 4 Vertical profile of Ozone number concentration simulated with ICON-ART (blue) and given by GEMS climatology (black) at the grid box corresponding to (-65°, -155°) latitude, longitude.

The extended Chapman mechanism within ICON-ART reproduces the general shape of ozone distribution throughout the stratosphere and troposphere, with a maximum at approximately 20 km very well (see Fig.4).

The discrepancy between the GEMS and ICON-ART ozone number concentration is caused by missing sinks of ozone, for example the catalytic loss cycle with HOx or halogens.

This can also be seen in Fig. 5. ICON-ART shows the ability to forecast large scale stratospheric dynamics, it has been used to simulate the unprecedented event of the Antarctic stratospheric vortex split in September 2002.

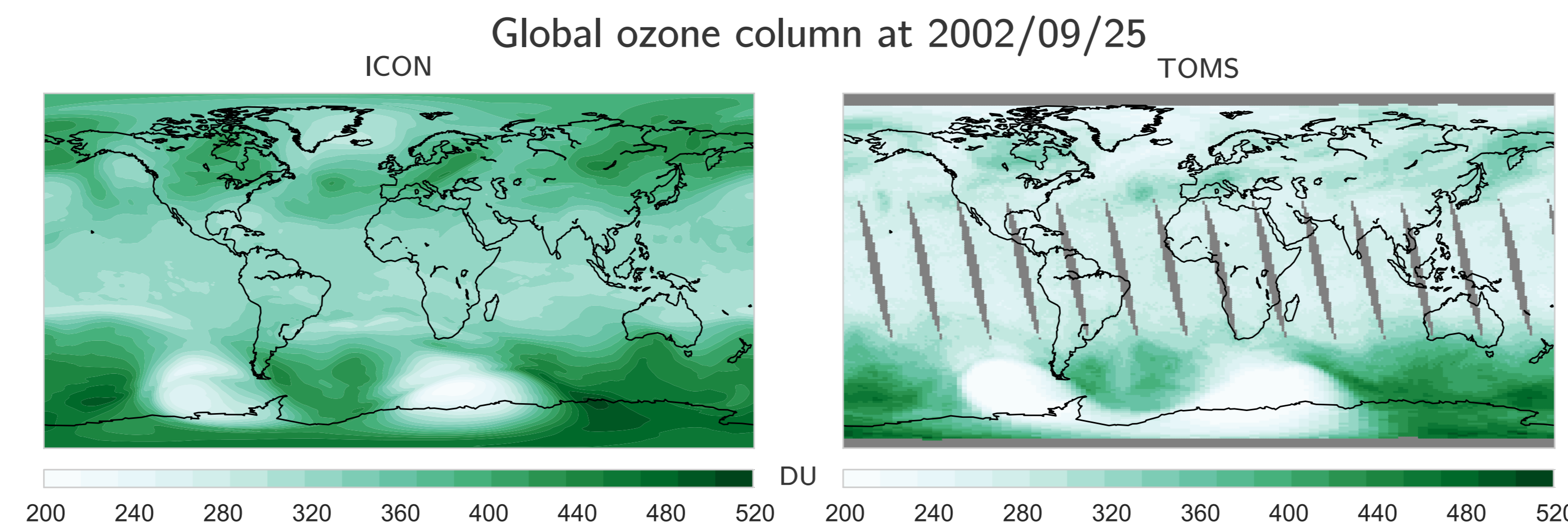


Fig. 5 Global total ozone column given in Dobson Units (DU) simulated with ICON-ART (left) gas phase chemistry (extended Chapman mechanism) and measured by the Total Ozone Mapping Spectrometer (TOMS) (right).

Comparison of zonal mean

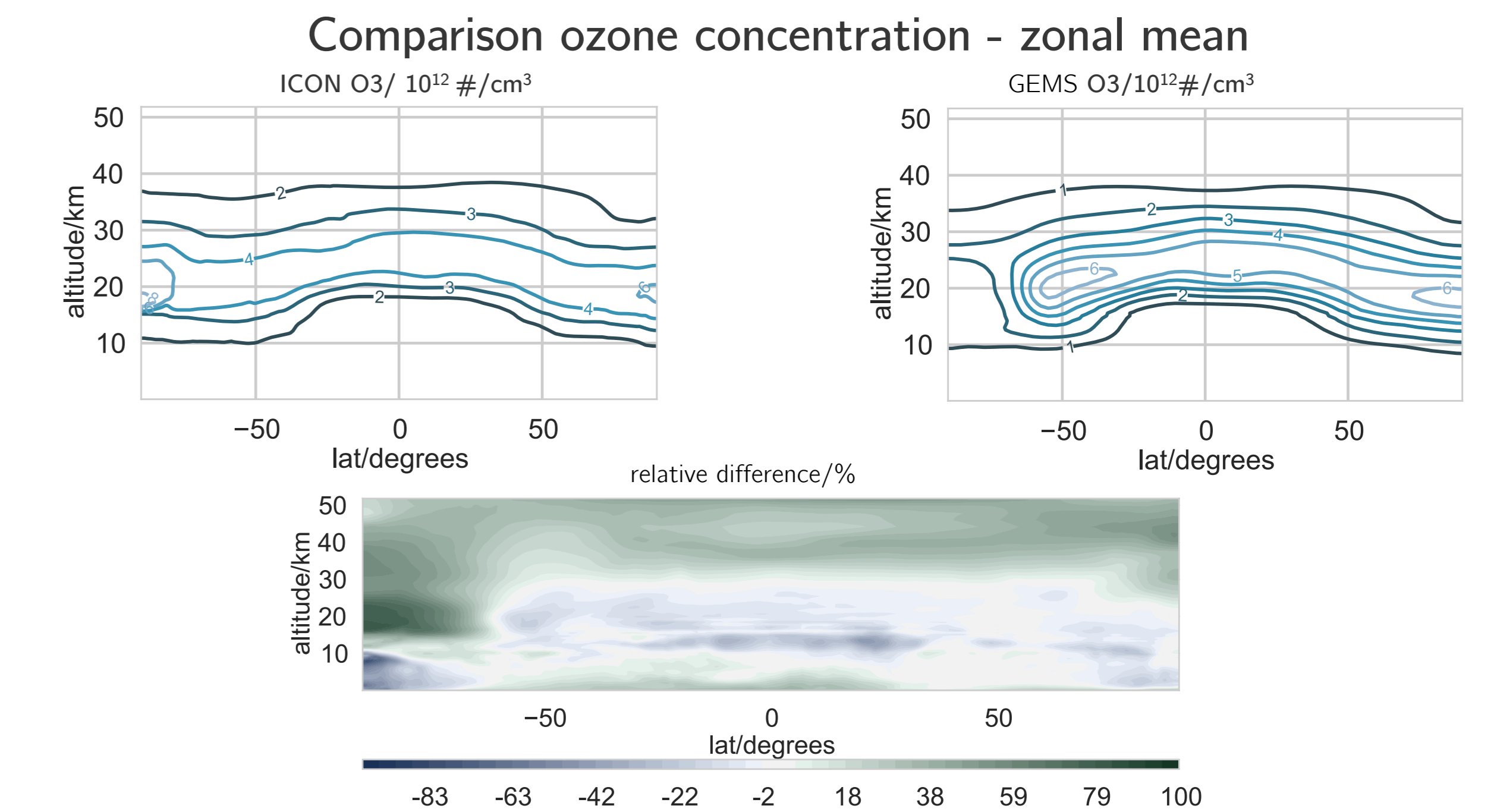


Fig. 6 Zonal mean of ozone distribution, top left simulated with ICON-ART, top right given by GEMS climatology and bottom relative difference between both, color coded at 2002/09/25.

The global zonal mean comparison shows that the general characteristics like the maximum in the tropics is well reproduced. Differences occurring especially in the polar latitudes are mainly caused by missing ozone loss by catalytic cycles with e.g. ClOx, BrOx and heterogenous processes.

Conclusion

In this model study we introduced a new gas-phase module, coupled with the online photolysis module within ICON-ART. This model sets the framework for simulating atmospheric chemistry reaching from global to regional scale and from the ground up to about 80 km.

With a reduced chemical mechanism, describing basic gas-phase and photolytic processes forming an extended Chapman mechanism, we simulated the global ozone distribution.

We could show that, using the internal ICON GEMS ozone climatology, we are able to reproduce important unprecedented events within the stratosphere. The global zonal mean and vertical distribution reproduces the general characteristics of the measured ozone distribution.

In the future we will extend the chemical mechanism by for example heterogeneous chemical processes. These are ozone sinks and their absence is causing the main differences between simulation and measurement in polar latitudes.

References

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