Helmholtz Climate Initiative

Regional Climate Change

Topic 9: Climate change and air quality

A new Photolysis Module for the Regional Chemistry-Transport Model COSMO-ART

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1. Introduction

- Chemistry throughout troposphere and stratosphere is mainly driven by solar radiation
- Calculation of photolysis rates: important role in modelling stratospheric chemistry
- Commonly used: precalculated look-up-tables since actinic flux calculation is a time consuming procedure
- Differences in j-values ➜ major differences in detailed results of chemical model

2. General Information

Information about COSMO-ART

- Regional Chemistry-Transport Model (CTM) based on COSMO model of DWD
- Gas-phase chemistry (KPP) and aerosol processes
- Chemistry based on RADM (Regional Acid Deposition Model)
- Radiation transport model: GRAALS[6]
- Old Photolysis Modul: PAPA[7] ➜ not suitable for stratosphere

Information about FastJx:

- Fast and accurate numerical method for calculating j-values
- **Solution** of radiative transfer equation (**RTE**) for plane-parallel isotropic atmosphere by expanding scattering phase function in Legendre and associated Legendre functions, finished by integration with discrete ordinate method (**4-Gauss-Points**)
- Wavelength range from **170 nm up to 850 nm**
- Solar spectrum divided into 18 wavelength bins

Information about PAPA:

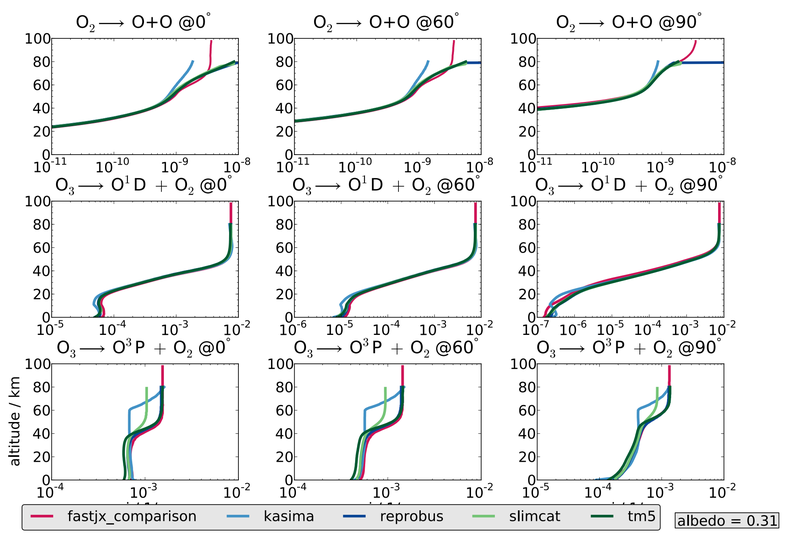
- „Parametrization of photolysis frequencies for atmospheric modelling“
- Correction of standard profiles of 21 species with online calculated factors (**parametrization**)
- Standard profile: read in via look-up-table generated with STAR
- STAR wavelength range: **270 nm up to 750 nm**

New Photolysis Module

- Should replace PAPA Module
- Valid for stratosphere and troposphere
- More accurate calculation of j-values for more than 21 species
- Online calculation of impact by clouds and aerosols

3. Validation

- For validation, j-values calculated by FastJx[1] were compared to those being calculated for a j-value-intercomparison, done in 2002
- Different photolysis codes in global 3D-CTMs (KASIMA[2], REPROBUS[3], SLIMCAT[4] and TM5[5]), with different input of absorption cross sections and quantum yields (mainly from JPL 1997 (REPROBUS, TM5), JPL 2000 (SLIMCAT) or selected spectra (KASIMA)). Albedo (0.31), ozone and temperature profiles (US Standard Atmosphere, 1976) were prescribed for input independence



Result of Validation

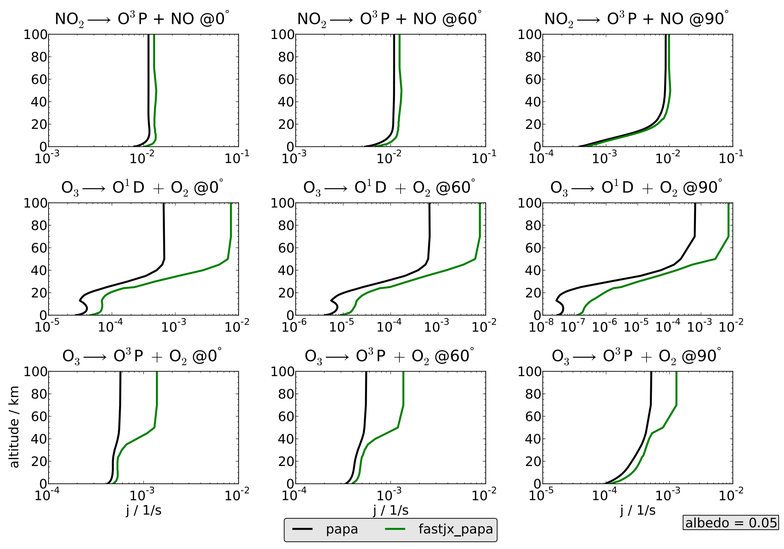
- Agreement of photolysis rates for most substances
- Differences in radiation transfer model, non equal incoming solar flux
- Usage of different quantum yields and cross sections

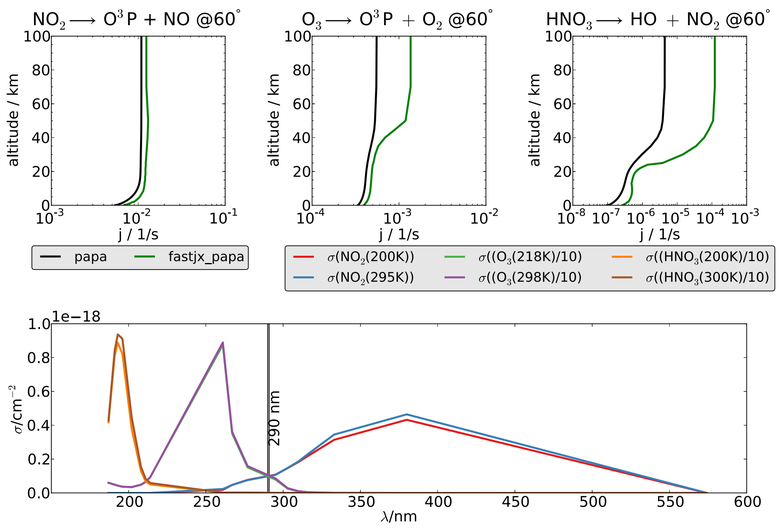
  ➜ main part of deviation

- Previous result of inter-model comparison still holds for FastJx
- Validation shows capability of FastJx usage

4. Generating standard profile

- Comparison between standard profile generated by STAR and FastJx
- Investigation of 21 species
- Prescription:
  - cloud free and aerosol free atmosphere
  - **albedo, vertical ozone, temperature, pressure** and **relative humidity** distribution
  - distributions based on **US Standard Atmosphere**
  - cross sections (FastJx) mainly from JPL10



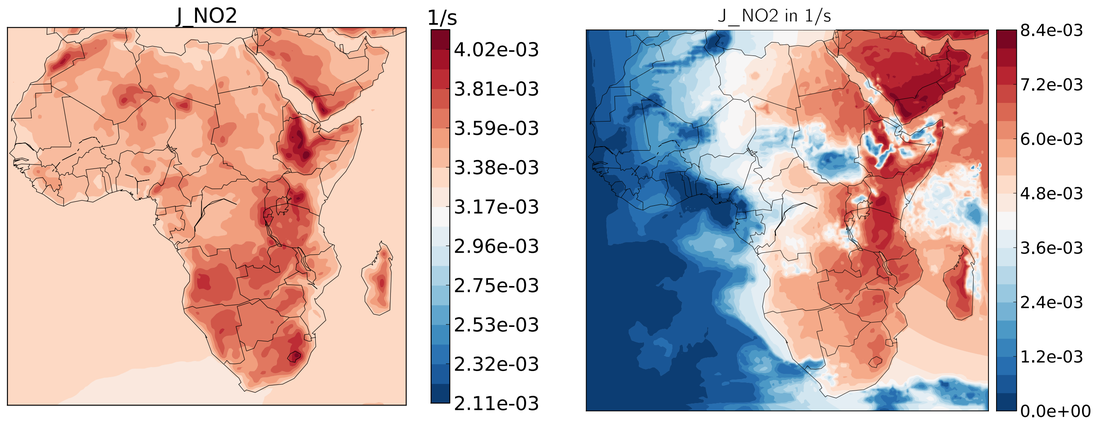


Result:

- Difference in photolysis rates enormous (up to 3 orders of magnitude) in stratosphere due to the fact that STAR neglects wavelengths below 290 nm
- Old standard profile needs to be replaced
- Differences within troposphere have to be explained

5. Extension of FastJx

- Successfully implemented 3D-Interface of FastJx for COSMO-ART
- Calculation of photolysis rates of 72 species with altitude dependence for every grid point at every radiation time step
- With additional information about cloud water path FastJx is ready to replace the PAPA Module
- Even better description of photolysis and thus chemical processes in stratosphere
- More accurate representation of processes of halogen substances
- Possibility to add more species to FastJx



left: Photolysis Rate of NO2 at ground level for constant SZA; no impact of clouds and aerosols; calculated by FASTJx-COSMO-ART interface

right: Photolysis Rate of NO2 at ground level at 7 p.m.; impact of clouds and aerosols; Calculated by PAPA Module

1: Bian, H. and Prather, M. (2002) Journal of Atmospheric Chemistry, 41(3), Wild, O., Zhu, X., and Prather, M. (2000). Journal of Atmospheric Chemistry, 37(3) 2: Röth, E.-P. (2002), Berichte des FZJ Jül-3960.

3: Madronich, S. and Flocke, S. (1999). Environmental photochemistry 4: Lary, D. and Pyle, J. (1991). Journal of Atmospheric Chemistry, 13(4) 5: Landgraf, J. and Crutzen, P. (1998).Journal of the Atmospheric Sciences, 55(5)

6: Ritter, B., & Geleyn, J. F. (1992). *Monthly Weather Review*, *120*(2). 7: Bangert, M. (2006) 8: Ruggaber, A., Dlugi, R., & Nakajima, T. (1994).*Journal of Atmospheric Chemistry*, *18*(2), 171-210.

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