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A new Photolysis Module for COSMO-ART

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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

Validation

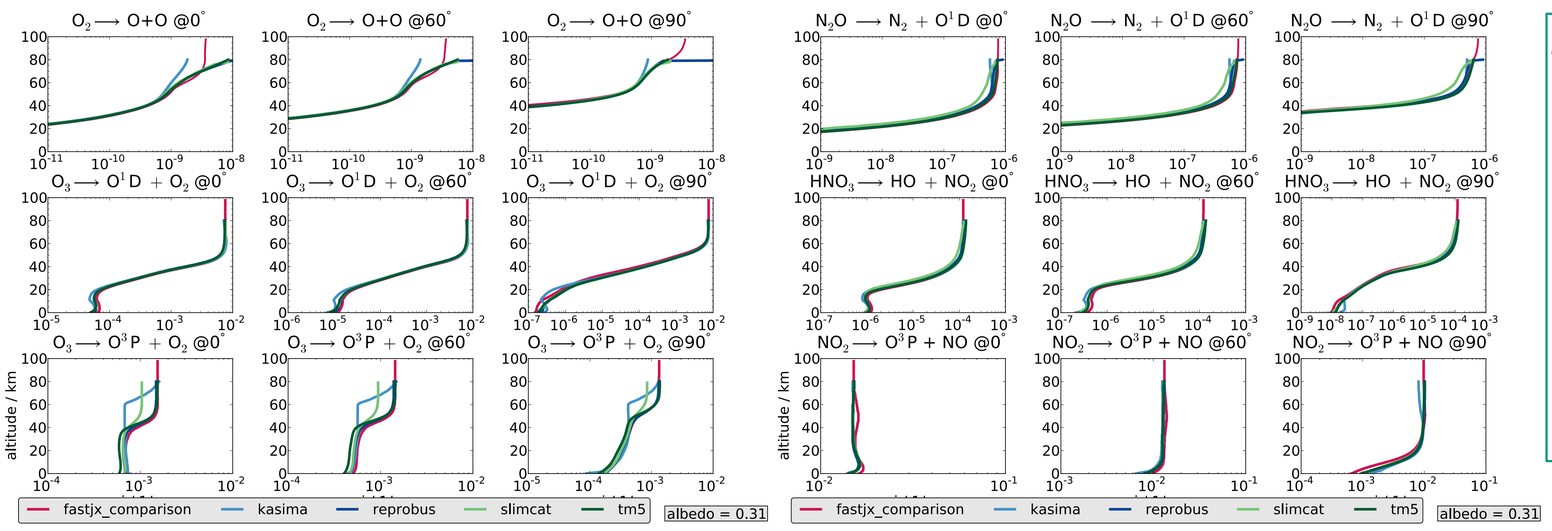
- For validation j-values calculated by FastJx[1] were compared to those being calculated for a j-value-intercomparison, done in 2002
- Different photolysis codes in global 3D-CTMs (KASIMA[2], REPROBUS[3], SLIMCAT[4] and TM5[5]), with different input of absorption cross sections and quantum yields (mainly 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

Information about COSMO-ART

- Regional Chemistry-Transport Model (CTM)
- Gas-phase chemistry (KPP) and aerosol processes
- Radiation transport model: GRAALS[6]
- Old Photolysis Modul: PAPA[7] ➜ uses look-up-table generated with STAR[8]

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

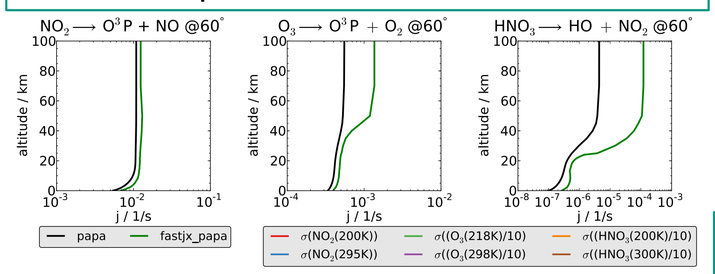


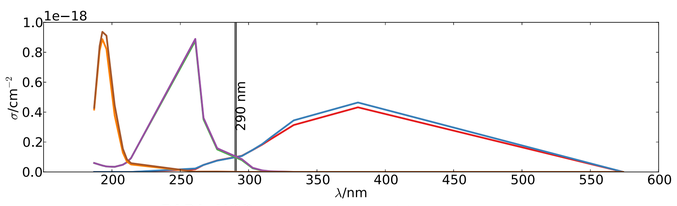
Result of Validation

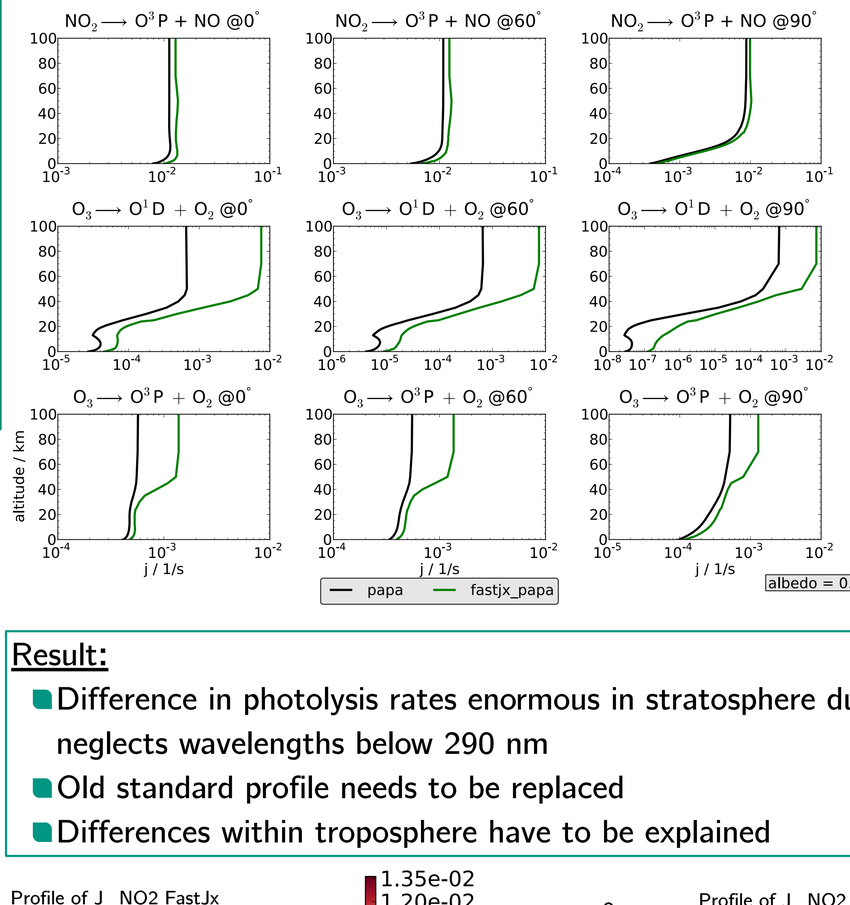
- Agreement of photolysis rates for most substances
- Differences in radiation transfer model, non equal incoming solar flux
- Usage of different quantum yields and cross sections
  ➜ main part of deviation
- Previous result of inter-model comparison still holds for FastJx
- Validation shows capability of FastJx usage

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

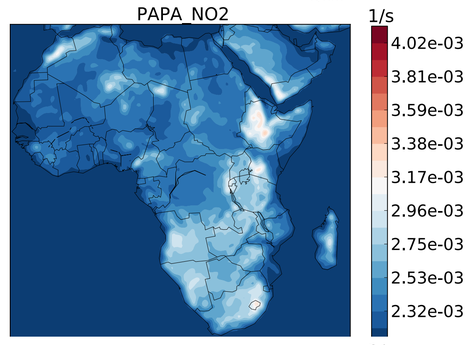


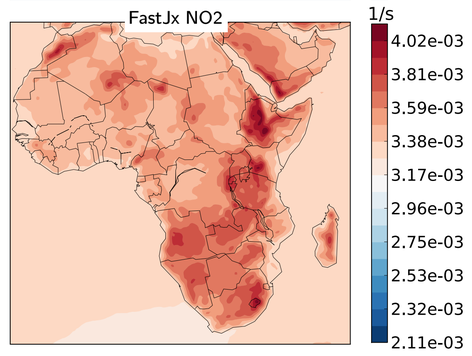


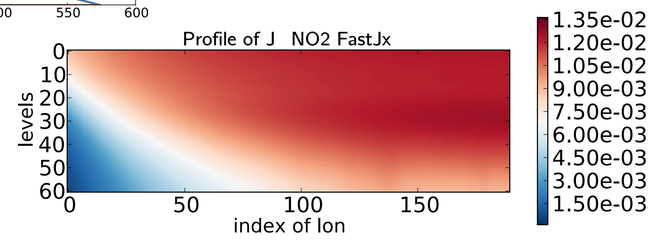


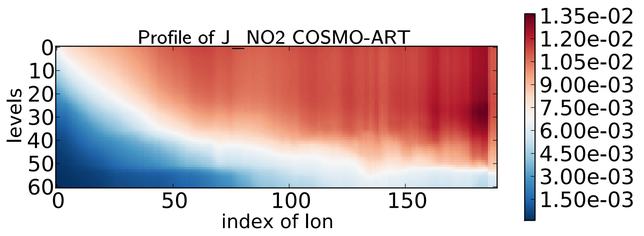
Result:

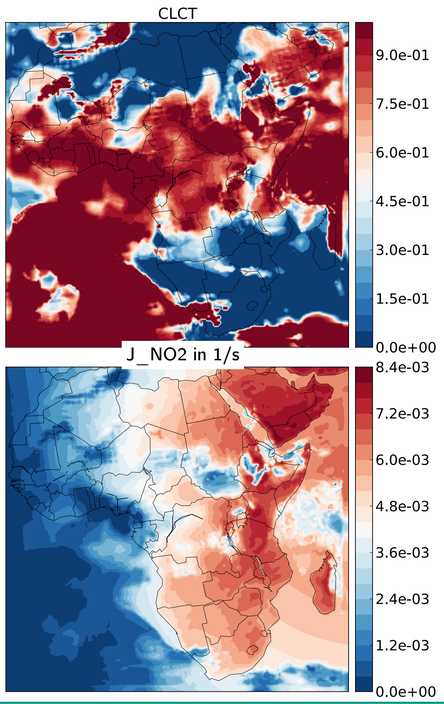
- Difference in photolysis rates enormous in stratosphere due to the fact that STAR neglects wavelengths below 290 nm
- Old standard profile needs to be replaced
- Differences within troposphere have to be explained











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

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.