Helmholtz Climate Initiative

Regional Climate Change

REKLIM Helmholtz-Verbund Regionale Klimaänderungen

HELMHOLTZ | ASSOCIATION

Session 5 Atmospheric composition and climate: interactions from global to regional scales

Simulating the Ozone Distribution over Europe in May 2008 with a new Photolysis Module for COSMO-ART

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1. General information about COSMO-ART

- Regional Chemistry Transport Model (CTM) based on COSMO model of DWD (German Weather Service)
- Gas-phase chemistry and aerosol processes included
- Chemistry based on RADM (Regional Acid Deposition Model) mechanism
- Radiation transport model: GRAALS[1]

2. Model version

- Domain: Central Europe, May 2008, COSMO 5.0 ART 3.0 (39 level up to 20km, horizontal resolution: 0.0625° about 7 km)
- Fixed boundary conditions for chemical tracers, prescribed emissions[2] e.g. NO, CO, NO_2, SO_2.

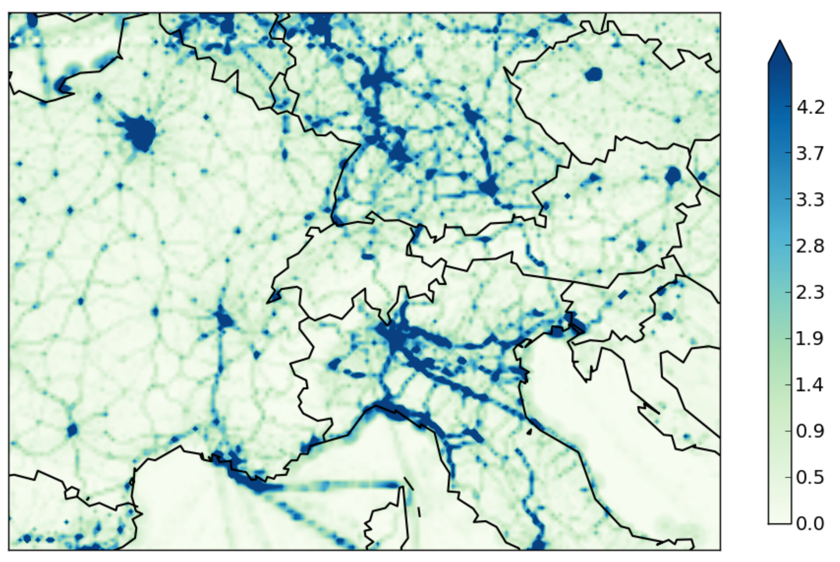

Fig. 1: Emission of NO at ground level, date: 27/05/2008 13:00, given in units of kg/h/cell

3. Why do we need a Photolysis Module?

- Stratospheric / tropospheric chemistry is mainly driven by solar radiation, thus the photolysis rate (j-value) calculation is important for atmospheric chemistry modeling.
- Differences in j-values cause major differences in detailed results of chemical model.

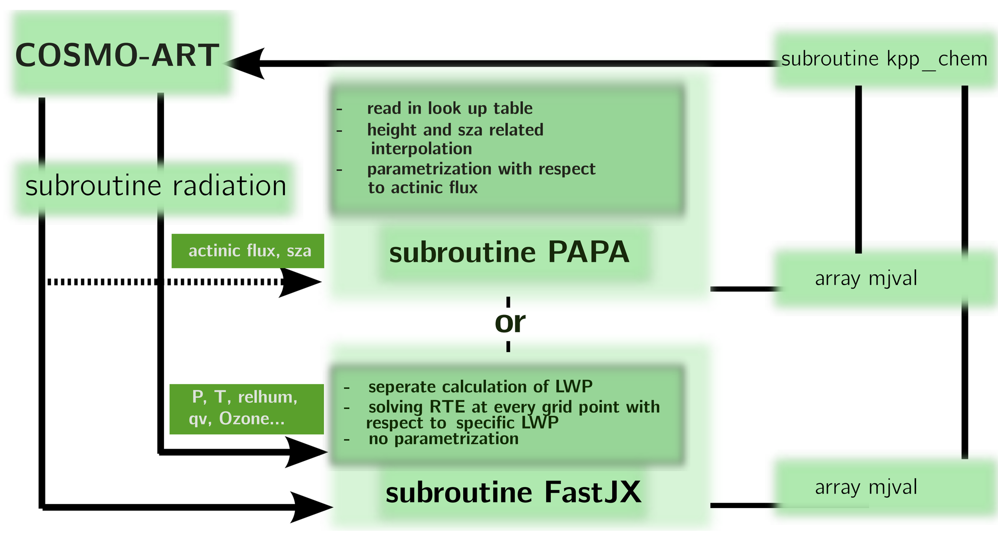

Fig. 2: Process diagram to illustrate the technical structure of Photolysis Module integration

4. What about the old Photolysis Module?

- Up to now PAPA[3] (parametrization of photolysis frequencies for atmospheric modeling) was used
- Uses standard j-value profiles (look up table generated with STAR[4] - System for Transfer of Atmospheric Radiation)
- Correction of standard profiles of 21 species with online calculated factors (**parametrization**)
- Wavelength range: **270 nm up to 750 nm** (not valid for stratospheric chemistry)

Not accurate enough for detailed chemistry modeling

5. ... and the new?

Online coupled version of FastJX[5]:

- 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: **170 nm up to 850 nm**
- Solar spectrum divided into 18 wavelength bins

6. Research question

It should be investigated whether chemistry modeling with a more accurate photolysis module would change chemical dominating processes within the HOx cycle. This change could lead to a shift in Ozone production rates.

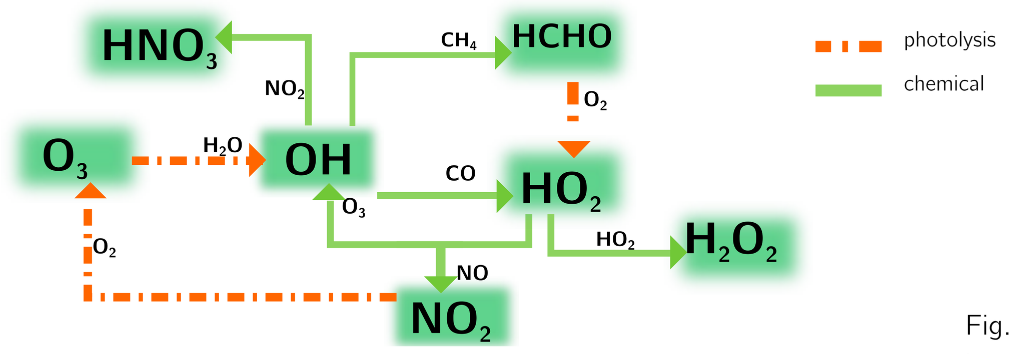

Fig. 3: Diagram of chemical and photolytic processes important for Ozone construction and destruction

7. Results

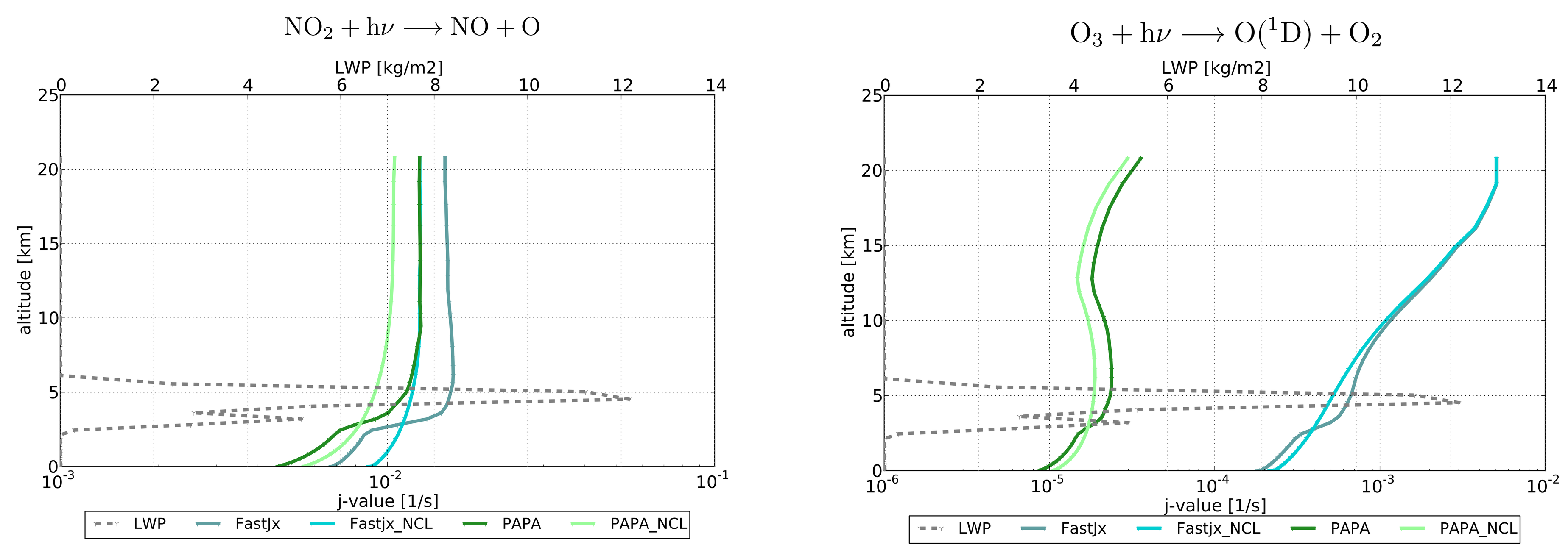

Fig. 4: Photolysis rates of NO_2 on the left, and Ozone ($O(^1D)$) channel) on the right. Values in dark blue and dark green are taken from a grid point, where a low cloud was indicated, which can be seen in the grey colored liquid water path (LWP). Values in light green and light blue represent a cloud free grid point.

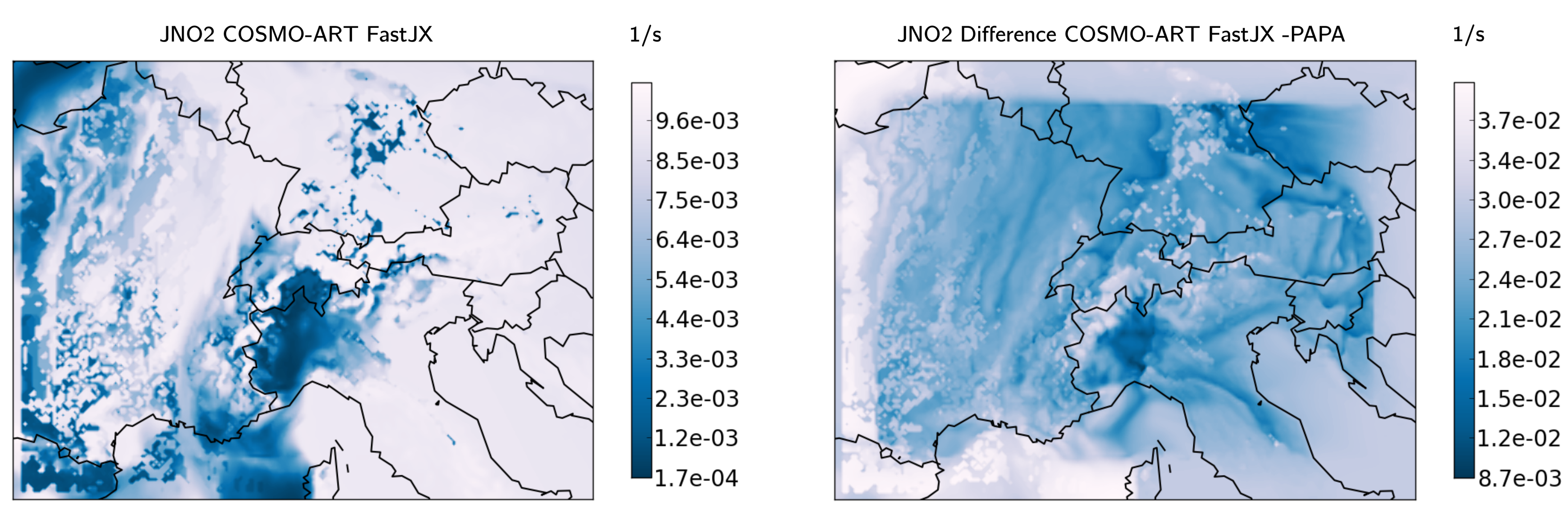

Fig. 5: Photolysis rates of NO_2 at 28/05/2008 13:00h at 1000 hPa, calculated with new COSMO-ART FastJX at the left, On the right, difference between old COSMO-ART simulation with PAPA and the new simulation with FastJX is shown. Impact of different cloud treatment can easily be seen.

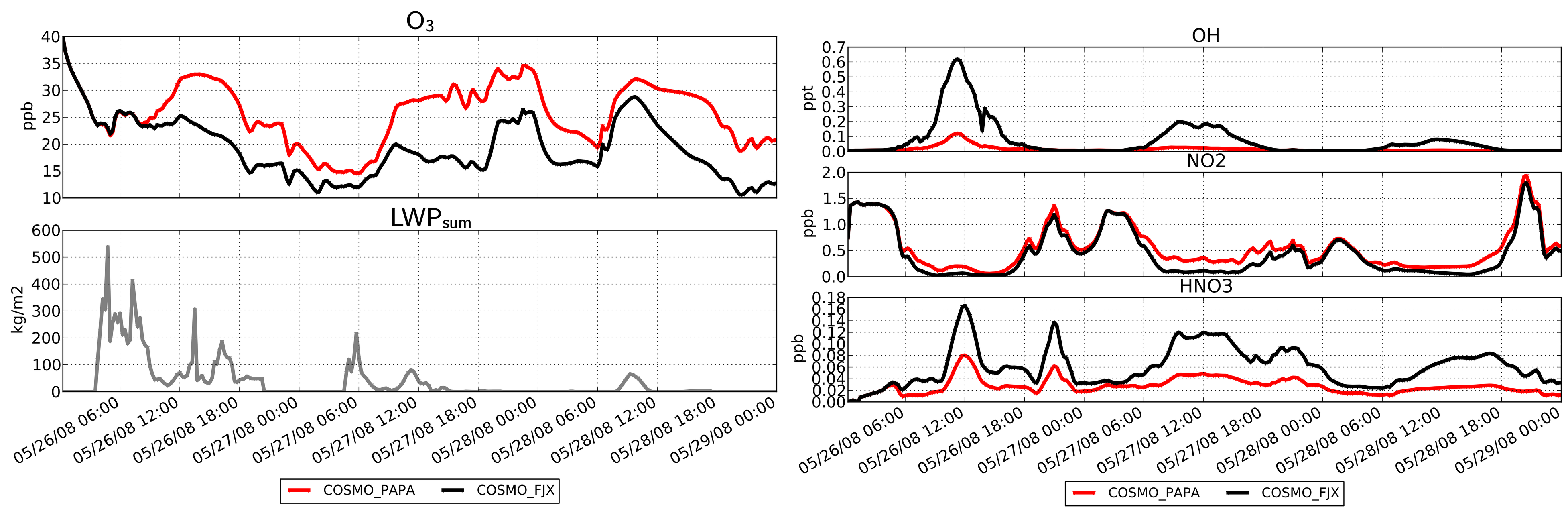

Fig. 6: On the left: resulting Ozone VMR simulated with COSMO-ART PAPA (red) and COSMO-ART FJX (black) with respect to the liquid water path summed up over all model levels.
On the right: resulting HNO_3, OH and NO_2 VMR. All results are taken from the ground level at the model grid point representing Karlsruhe.

8. Conclusion and Outlook

J-values calculated with COSMO-ART FJX differ from those calculated with the old PAPA module. J-Values of the $O(^1D)$ channel of O_3 are up to ten times higher at the ground level than those of PAPA, which leads to an increase of OH production.
In addition to that, NO_2 production rates are modified too, which yield lower Ozone VMR, since HNO_3 is generated instead of a catalytic oxidation of CO which would end up in net production of Ozone.

These results have to be validated with measurements in the future.

1: Ritter, B., & Geleyn, J. F. (1992). *Monthly Weather Review*, *120*(2). , 2: for further information please contact: heike.vogel@kit.edu, 3: Bangert, M. (2006) 4: Ruggaber, A., Dlugi, R., & Nakajima, T. (1994).*Journal of Atmospheric Chemistry*, *18*(2), 171-210.
5: 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)

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