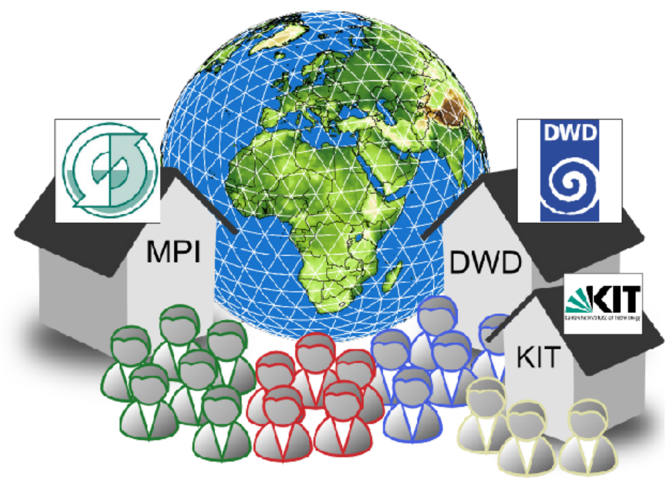
Karlsruhe Institute of Technology

Institute for Meteorology and Climate Research - Atmospheric Trace Gases and Remote Sensing

Simulation of volantile organic compounds with ICON-ART

Michael Weimer[1], D. Rieger, J. Schröter, C. Stassen, R. Ruhnke, B. Vogel

[1]E-mail: michael.weimer@student.kit.edu



Introduction

We have extended the global **ICON** (ICOsahedral Nonhydrostatic) modelling framework. ICON is a joint development by the German Weather Service (DWD) and the Max-Planck-Institute for Meteorology (MPI-M). We added modules for gas-phase chemistry and aerosol dynamics (ART, Aerosols and Reactive Trace gases) [1].

ICON allows a regional grid refinement with two-way interactions between the different horizontal grids. In January 2015, it replaced GME as operational model for numerical weather predictions at DWD with resolution R3B07 and will be used by MPI-M for climate projections [2].

The extended modelling framework **ICON-ART** is developed in an analogous way to its predecessors COSMO-ART [3], so that aerosol and chemical composition feedbacks can be considered in a comprehensive way. Up to now, ICON-ART accounts for volcanic ash tracers, radioactive tracers, sea salt and mineral dust aerosols. Additionally, several gaseous tracers have been introduced. For the dynamics (transport and diffusion) of aerosol and 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.

The ICON model

- Global nonhydrostatic model
- No singular points at poles
- Unstructured triangular grid
  - Resolution: R<n>B<k> (see Fig. 1)
  - Examples:
    - R2B05: mesh size of ~ 80 km
    - R2B06: mesh size of ~ 40 km
    - R3B07: mesh size of ~ 13 km

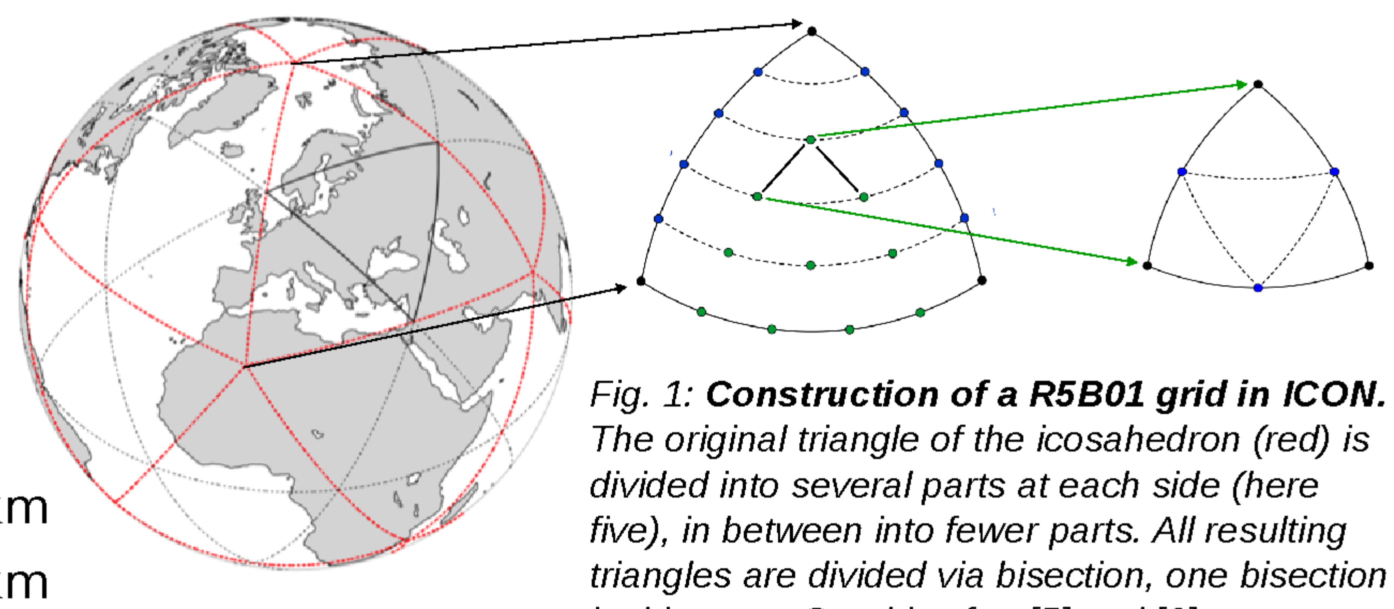


*Fig. 1: **Construction of a R5B01 grid in ICON.** The original triangle of the icosahedron (red) is divided into several parts at each side (here five), in between into fewer parts. All resulting triangles are divided via bisection, one bisection in this case. Graphic after [5] and [6]*

Emission database: ECCAD

- ECCAD (see [7]): **E**missions of atmospheric **C**ompounds & **C**ompilation of **A**ncillary **D**ata
- Emission data available ...
  - ... from different projects (e.g. MACCity, MEGAN-MACC, POET)
  - ... for a lot of compounds
  - ... for different types: anthropogenic, biogenic and biomass burning

Recent development

- New module to include external emission data in ICON-ART
  - Data is spatially interpolated to ICON grid (with DWD ICON tools)
  - Emission is linearly interpolated between two neighboured timesteps in emission file
  - Data is converted to volume mixing ratio (vmr) and added to vmr at surface level

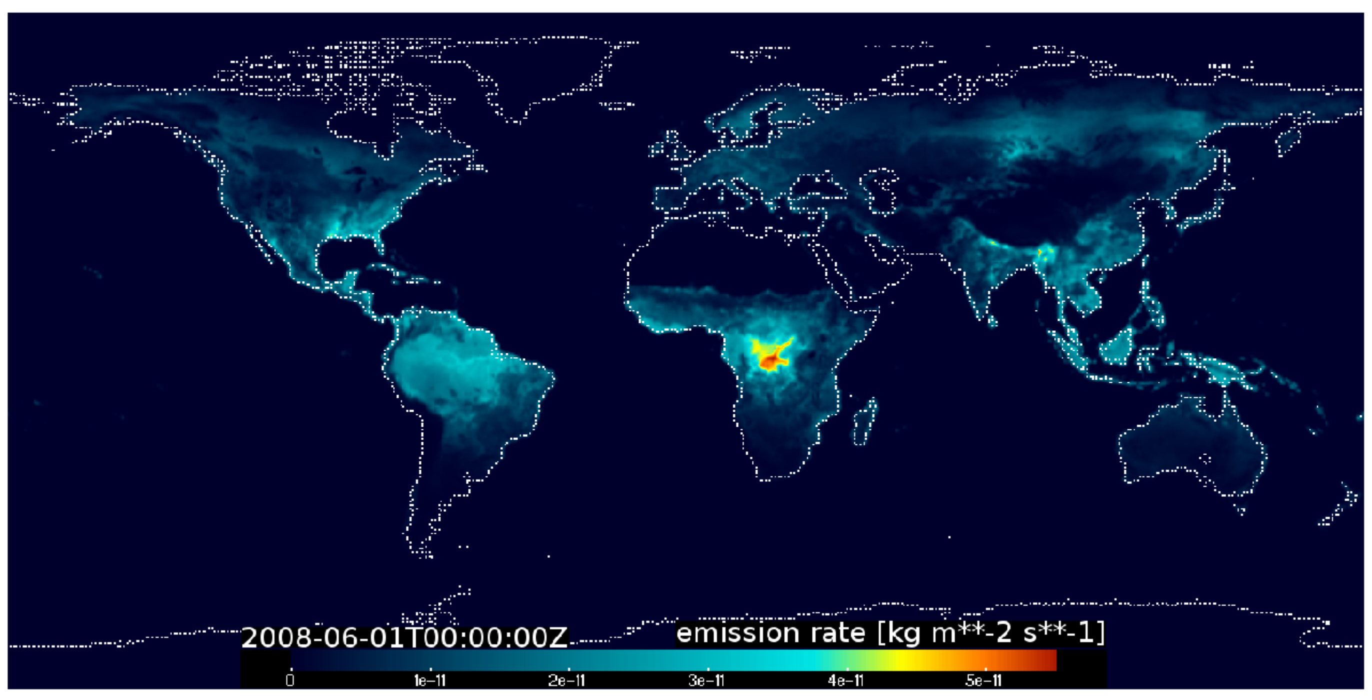


*Fig. 2: **Biogenic emission of acetone from project MEGAN-MACC.** Original emission data in units of kg m^{-2} s^{-1} at 2008/06/01 00 UTC where this simulation with ICON-ART begins. These values are converted to volume mixing ratio with temperature and pressure calculated by ICON at simulation time. Then, the vmr is added to surface vmr at simulation time. Colour bar ranges from 0 to $5.5 \cdot 10^{-11}$ kg m^{-2} s^{-1}.*

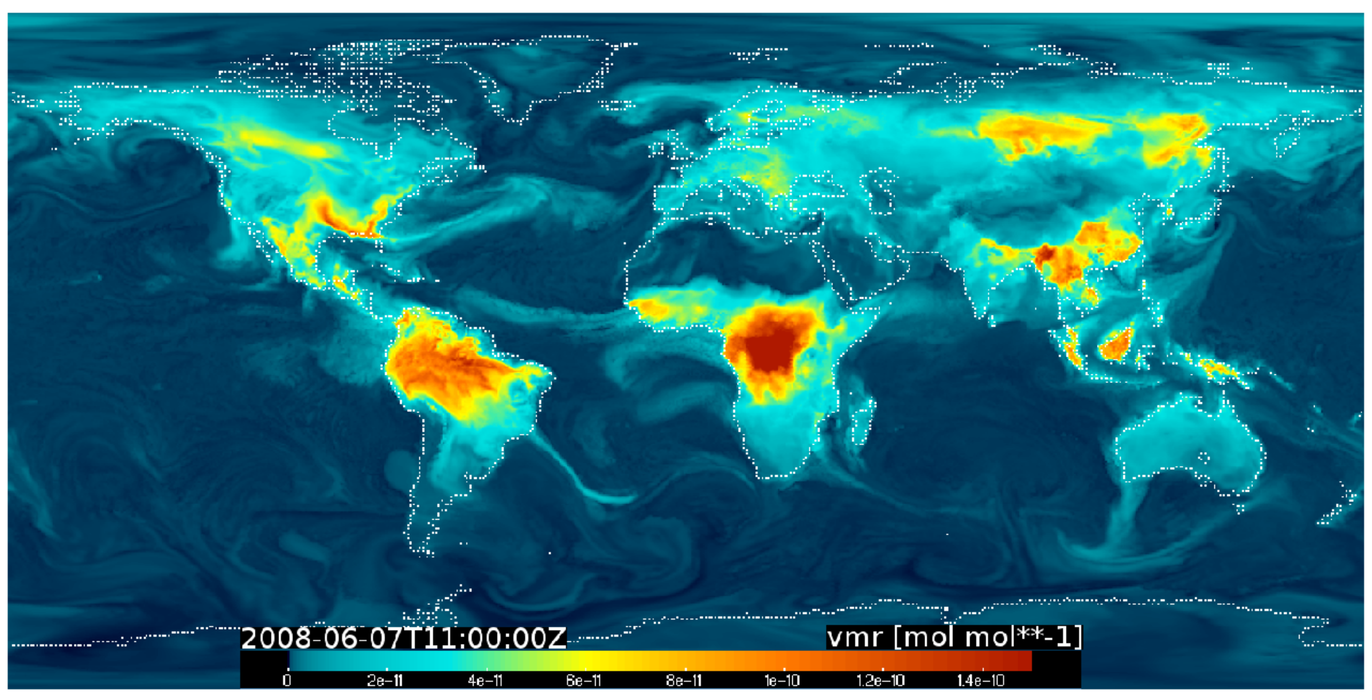


*Fig. 3: **Acetone volume mixing ratio due to biogenic emissions from MEGAN-MACC in ICON-ART with resolution R2B06 at model level 84.5 (about 500 m above surface)** at 2008/06/07 11 UTC, 6.5 days after date of Fig. 2. Lifetime based chemistry is used to calculate depletion of acetone. The lifetime is set to the constant value of 20 days. Colour bar ranges from 0 to $1.5 \cdot 10^{-10}$ mol mol^{-1} with emphasis on low values. This is a snap-shot of a video that can be watched via QR code in the middle of the resulting website: http://icon-art.imk-tro.kit.edu/*

Why acetone?

1. O_3: high radiative impact in upper troposphere (UT)
2. Both OH and HO_2 regulate O_3 budget in UT
3. Volatile organic compounds (VOC): Important source of OH and HO_2 in UT

➔ Acetone: VOC with significant influence on O_3 budget [4]

Outlook

- Insertion of a steady-state OH chemistry in ICON-ART to simulate loss of acetone more accurately
- Comparison between acetone tracer in ICON-ART due to different types of emissions and CARIBIC measurements [4] in upper troposphere
- Comparison between the data of different projects in ECCAD

References

[1] Rieger, D., et al. (2015), ICON-ART - A new online-coupled model system from the global to regional scale, Geosci. Model Dev. Discuss., 8, 567-614
[2] Zängl, G., et al. (2014), The ICON (ICOsahedral Non-hydrostatic) modelling framework of DWD MPI-M: Description of the non-hydrostatic dynamical core. Q.J.R. Meteorol. Soc., doi:10.1002/qj.2378
[3] Vogel, B., et al. (2009), The comprehensive model system COSMO-ART - Radiative impact of aerosol on the state of the atmosphere on the regional scale, Atmos. Chem. Phys., 9, 8661-8680
[4] Neumaier, M., et al. (2014), Impact of acetone (photo)oxidation on HOx production in the UT/LMS based on CARIBIC passenger aircraft observations and EMAC simulations, Geophys. Res. Lett., 42
[5] Reinert, D. (2014), ICON - towards operational numerical weather prediction, presentation at EMS ECAC Prague
[6] Wan, H. (2009), Developing and testing a hydrostatic atmospheric dynamical core on triangular grids, PhD thesis
[7] http://eccad.sedoo.fr