

ICON-ART: Modelling the Atmosphere – from Weather to Greenhouse Gas Emissions

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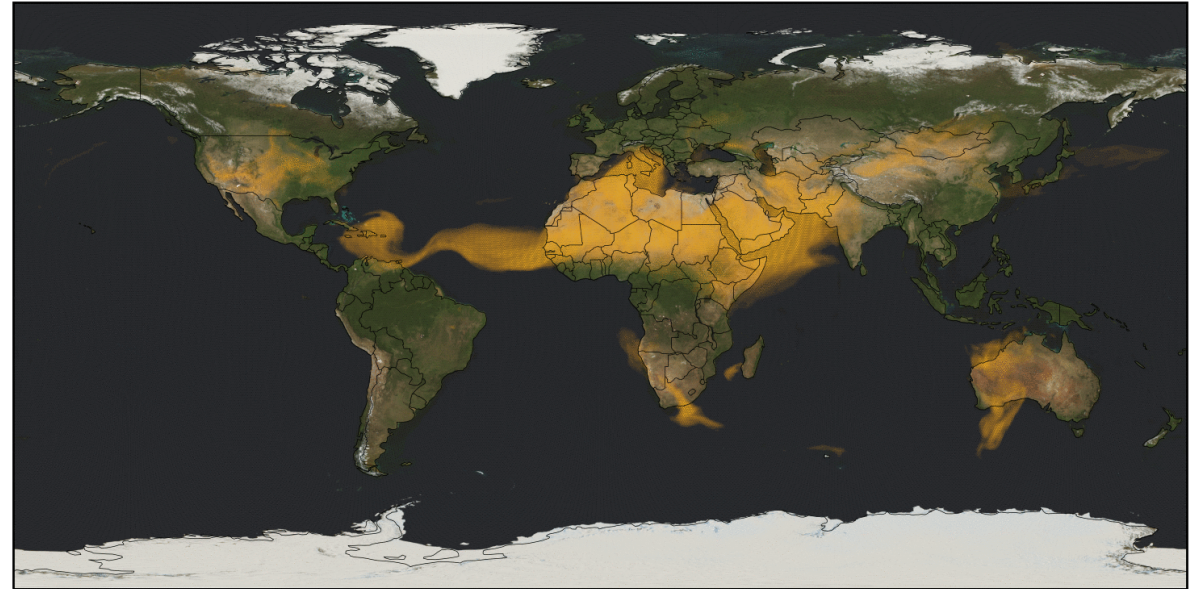
21st edition, 2nd Visiting scholar lecture · ME Forum
School of Mechanical Engineering and Robotics, Tongji
University, Jiading Campus, Kaiwu Hall A101



Global ICON-ART simulation of mineral dust (yellow), biomass burning aerosol (white), and sea salt (blue) during the period June 22, 2019 - July 22, 2019.

animation by Anika Rohde

22-06-2019 00:00



With the help of my colleagues Lena Feld, Stefan Versick, Valentin Hanft, Peter Braesicke, Frank Hase, Sabine Barthlott, Ali Hoshyaripour, the ARTists and the IMKASF team and [claude.ai](https://www.claude.ai) for the layout

Karlsruhe Institute of Technology

1825
**Universität
Karlsruhe**

2006
**Success in the first
round of the
Excellence Initiative**

2012
KIT Further Development Act (KIT-WG)

- Capacity of employer
- Builder status (Campus East)
- Right to appoint

2021
KIT 2.0
End of the separation
into University Sector and
Large-scale Research Sector

1825 - 2008

2009 - 2011

2012 - 2020

2021 →

1956
**Forschungs-
zentrum
Karlsruhe GmbH**

2009
**Foundation of
Karlsruhe Institute of
Technology**

2016
**New Vice
President
Transfer and
International
Affairs**

2019
**Success in the
Excellence Strategy**
e.g. 100 professorships program
with a focus on tenure-track
professorships

2023
**New Vice President
Digitalization and
Sustainability**

KIT in Figures

2025

424

Professors

23 083

Students

10 131

Employees

68

New spin-offs
and start-ups

6

Locations
(200 ha area)

1 773

International
scientists

3 544

Doctoral
researchers

319

Trainees

38

Patent
applications

Budget

1,216.2 million euros

32 %

state
funds

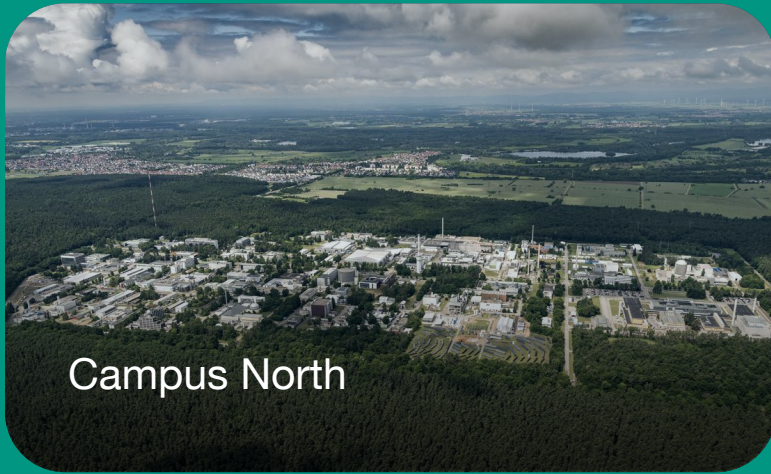
32 %

federal
funds

36 %

third-party funds

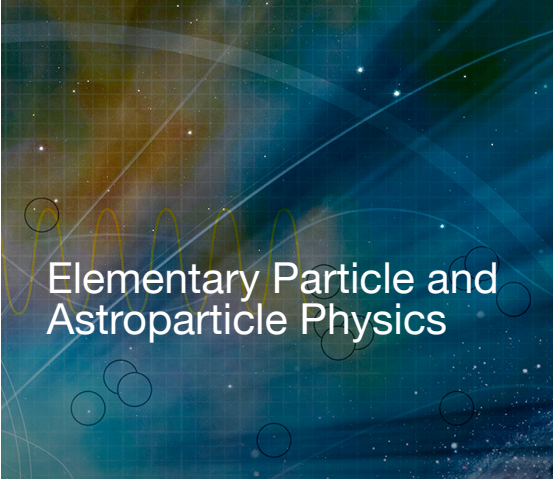
One KIT – Multiple Locations



Our Scientific Profile

Focus on major societal challenges -
founded on sound fundamental
research.

Nine interdisciplinary KIT Centers
interlink research on important topics



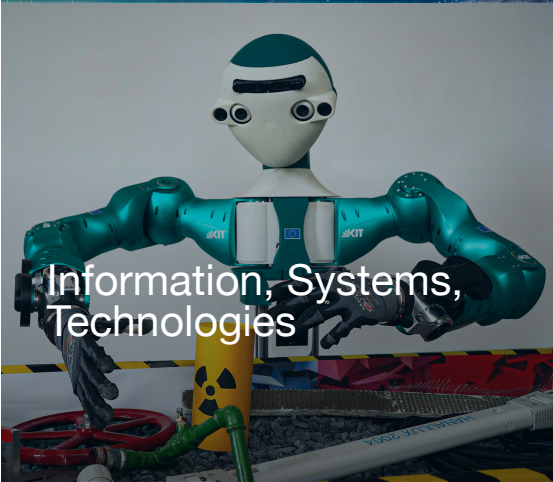
Elementary Particle and
Astroparticle Physics



Energy



Health
Technologies



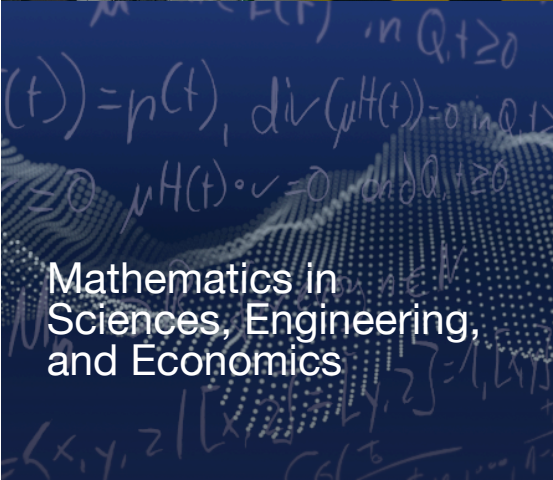
Information, Systems,
Technologies



Climate and
Environment



Materials in Technical
and Life Sciences



Mathematics in
Sciences, Engineering,
and Economics



Humans and
Technology



Mobility Systems

Our KIT Departments

Studying and teaching are organized in eleven KIT Departments, which are assigned to five Divisions.



Architecture



Chemical and Process Engineering



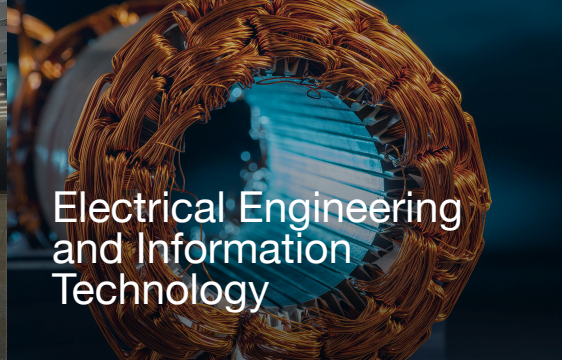
Chemistry and Biosciences



Civil Engineering, Geo- and Environmental Sciences



Economics and Management



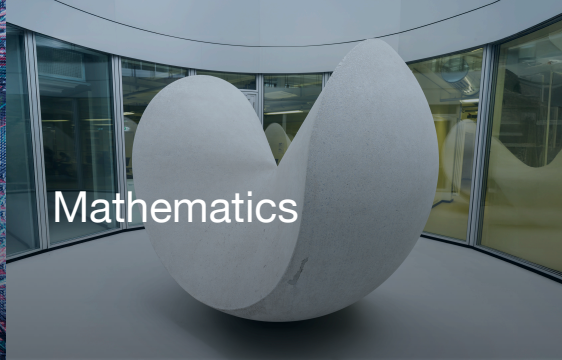
Electrical Engineering and Information Technology



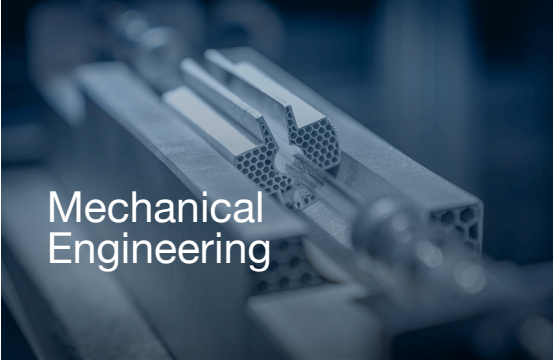
Humanities and Social Sciences



Informatics



Mathematics



Mechanical Engineering



Physics

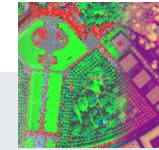
Science for Impact

Become Part of Our Vision

Agenda

1. Why model the atmosphere? (10 min)
2. ICON and ICON-ART: background (20 min)
3. Case study: Thessaloniki CO₂ emissions (25 min)
4. COCCON and data management at IMKASF (15 min)
5. Outlook (5 min)
6. Discussion (15 min)

IMKASF at a glance



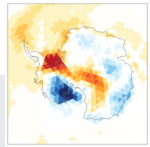
Urban air- and spaceborne
remote sensing



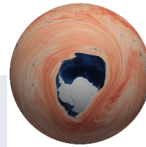
Balloons, aircraft, satellites

**Surface stations and
meteorological satellites**

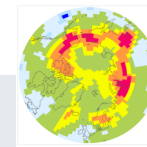
**Modelling the atmospheric
system**



Data management



Global modelling



**Middle atmosphere, solar
variability, climate**



**Remote sensing from
aircraft and balloons**

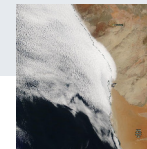
**Aircraft measurements in
the tropopause region**



**Remote sensing of trace
gases from satellites**



Satellite climatology



**Ground-based remote
sensing**



Source: Peter BRAESICKE and imkasf.kit.edu: 3 departments and 8 research groups (Institute of Meteorology and Climate Research, Atmospheric Trace Gases and Remote Sensing)

1 Why model the atmosphere?

10 min

What should a weather service predict?

1970s: the day-ahead weather forecast

Today: hours to months — weather, environment, and climate

Energy, health, aviation and emergencies all depend on it



Pictures: slide material Valtentin HANFT, IMKASF

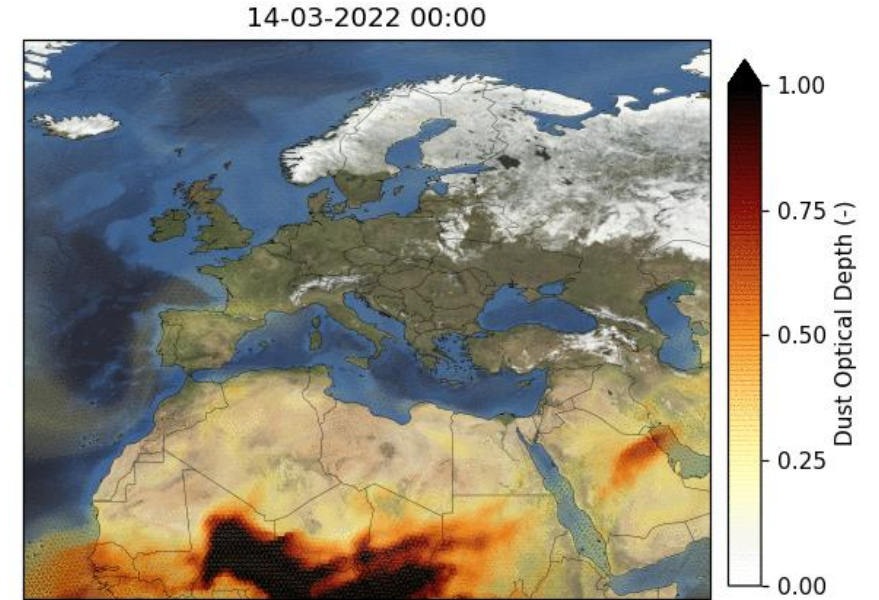
Saharan dust and solar power

Dust episodes change the sunlight that reaches the ground

Example: Saharan dust over Europe, mid-March 2022

Day-ahead solar forecast too high by about 5000 MWh ($\approx$ € 1 Mio) on 17 March 2022, TransnetBW area

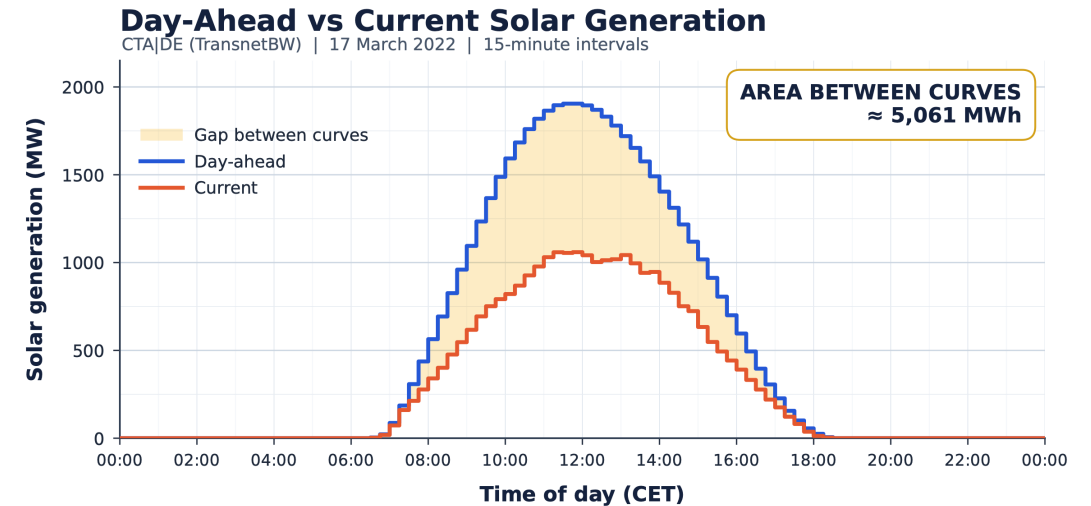
Forecasts need aerosol and composition, not only weather



Electricity prices around 17 March 2022: 220€/MWh

5061 MWh x 220 €/MWh $\approx$ €1.11 million

Source: Valentin HANFT (IMKASF); data DWD, transparency.entsoe.eu



Energy-gap estimate = $\sum [\text{Day-ahead} - \text{Current}] \times 0.25 \text{ h}$ | Signed net (Day-ahead - Current): +5,061.35 MWh
Source: ENTSO-E Transparency Platform export. Estimate uses the supplied 15-minute MW values as interval averages.

The atmosphere is a fluid we compute

Governing equations: fluid dynamics, thermodynamics, radiative transfer and chemistry

Discretize the atmosphere into a 3D grid

Step forward in time at every grid point

Same as CFD, at planetary scale

Vilhelm Bjerknes (1862-1951): a set of seven *primitive equations* describing the behaviour of heat, air motion, and moisture

Lewis Fry Richardson (1916-1922): first numerical forecast by hand took 6 weeks of computing for a 6-hour forecast at 2 locations, and it was completely wrong

Causes: poor initial data and too large a time step

Svante Arrhenius (1896): first climate estimate, CO₂ doubling gives about +5 °C

Dynamics

Thermodynamics

Radiation

Chemistry

Numerical weather prediction in three steps

Observations: collect data from stations, satellites, radar, balloons and aircraft, increasingly including CO₂ measurements.

Data assimilation: combine observations with a short-range forecast to estimate the best initial state.

Traditional model integration: solve physical equations in time on a 3D grid to simulate how the atmosphere evolves.

AI-based forecasting: learn patterns from historical weather data to predict how the atmosphere will evolve.

Observations

Data assimilation

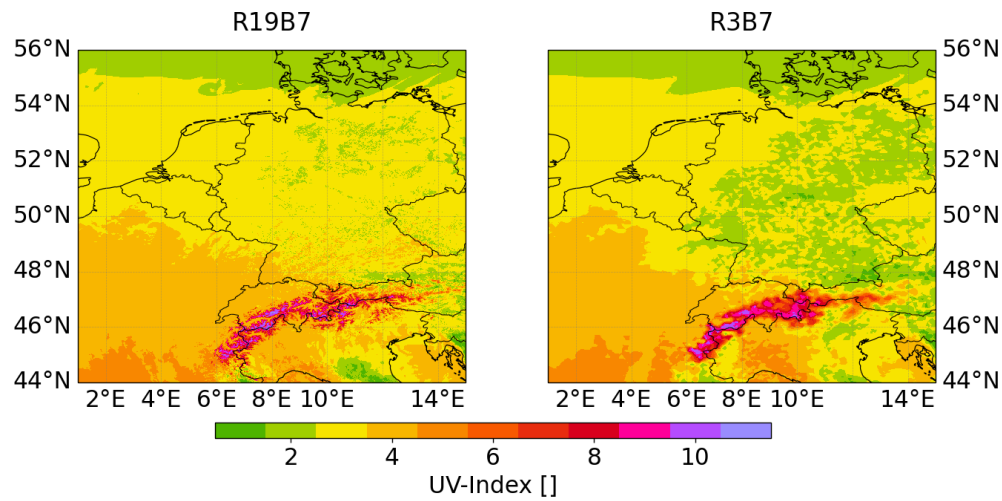
Model integration

Resolution costs computing time

Halving the grid spacing multiplies cost by about 8 ($2\times$ in x, $2\times$ in y, $2\times$ in time steps) assuming the time step is also halved (keep in mind diffusion)

DWD operational ICON: global 13 km, Europe 7 km, Germany 2 km

Our case study: 1 km local-area grid around Thessaloniki



UV index from ICON-ART:
2 km grid (R19B7, left)
and 13 km grid (R3B7,
right)

Resolution Δx
 $\div 2$

Cost
 $\times 8$

Picture: slide material Valentin HANFT (IMKASF)

2 ICON and ICON-ART

20 min

Where does ICON-ART come from?

ICON: the ICOSahedral Nonhydrostatic model, a joint development by DWD and MPI-M (supported by DKRZ)

Operational **forecasting** at DWD since early 2015, replacing the hydrostatic global model GME (Global Model Europe)

MPI-M uses ICON for **climate** projections

KIT adds ART (Aerosol and Reactive Trace gases)



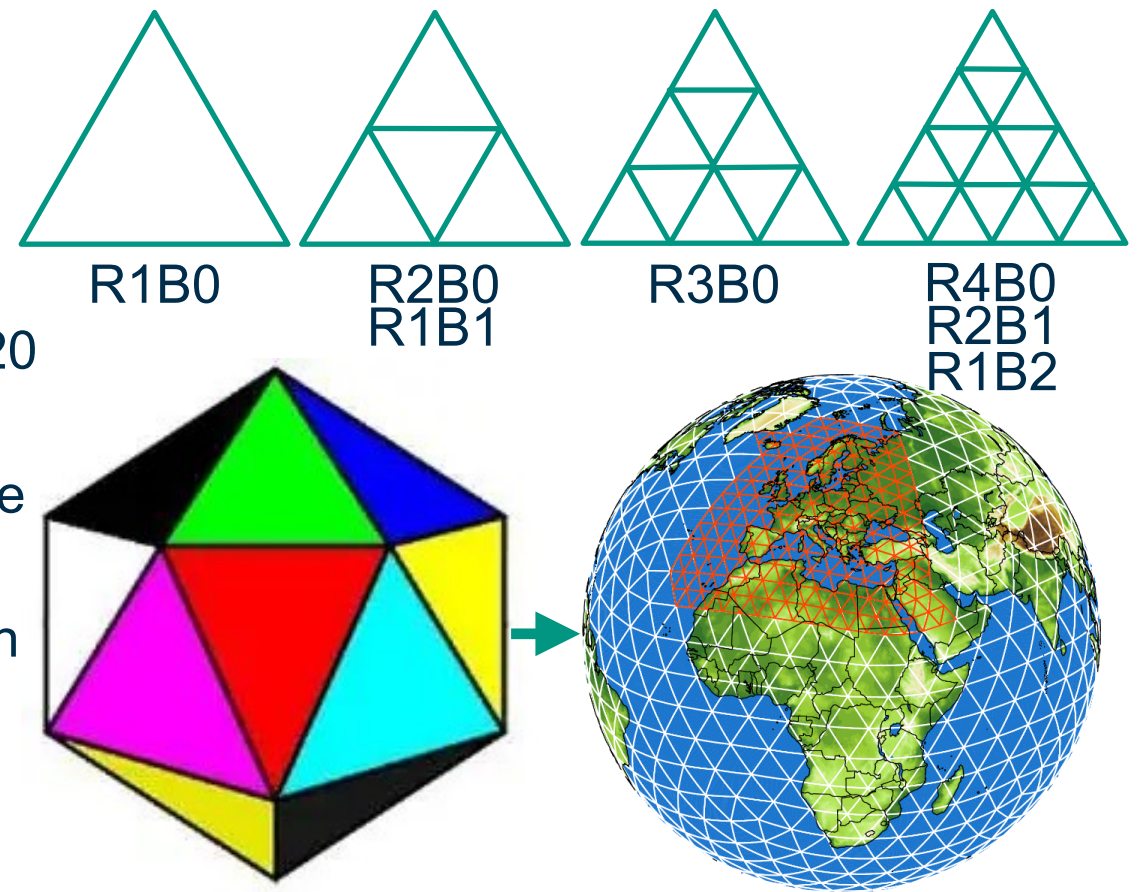
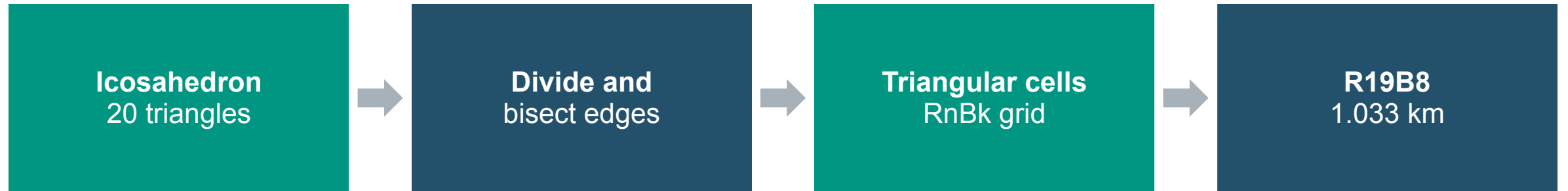
The icosahedral grid

Start from an icosahedron: 20-sided polyhedron with 20 triangular faces on the *sphere*

Refine by edge division and bisection, new vertices are projected radially onto the sphere: grid name RnBk

Near-uniform triangles: no pole singularity as on lat-lon grids

Resolution = square root of cell area: R19B7 $\approx$ 2 km, R19B8 $\approx$ 1 km



Sources: DWD; <https://personal.math.ubc.ca/~cass/courses/m308/projects/cchang/webpages/icosahedron.html>

$$N_{\text{cells}} = 20 n^2 4^k$$

$$N = n 2^k$$

$$\Delta x = R_{\text{Earth}} \sqrt[3]{(\pi/5) / (n 2^k)}$$

$$\approx 5050 / (n 2^k)$$

ICON: from global to 2 km

Two-in-one: operational weather model and climate model (core of an Earth System Model)

DWD operational:

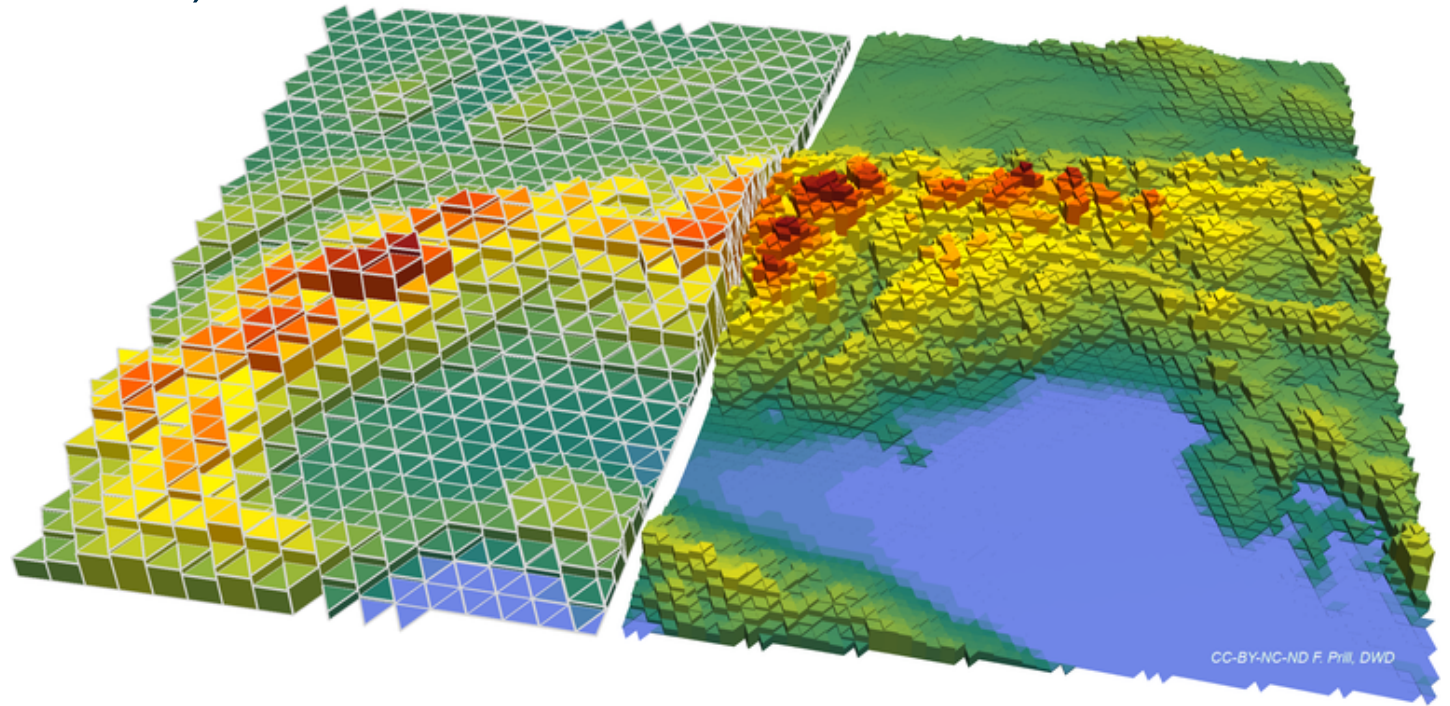
global ≈ 13 km, Grid: R3B7

Europe ≈ 7 km, Grid: R3B8

Local area model:

Germany ≈ 2 km, Grid: R19B7

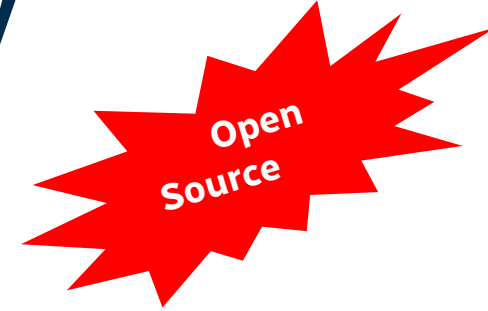
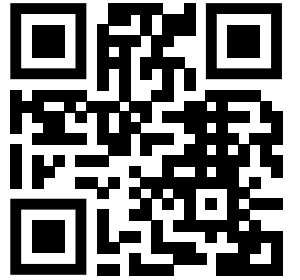
City scale ≈ 1 km, Grid: R19B8



The open source ICON model family

One dynamical core, several configurations

- Numerical weather prediction (DWD)
- climate (MPI-M)
- limited-area runs, and composition (KIT)



icon-model.org

Forecasts at opendata.dwd.de

Model code at icon-model.org

ICON-NWP

DWD operational
forecast, ICON-D2 2 km

ICON climate

MPI-M
climate projections

ICON-LAM

limited-area runs,
e.g. 1 km Thessaloniki

ICON-ART

KIT: aerosols and
reactive trace gases

ICON-ART: Aerosol and Reactive Trace gases

Prognostic treatment of atmospheric composition and its interactions

Online fully coupled for weather and climate simulations

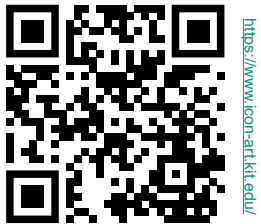
Global, nested and limited-area configurations

Fully modular

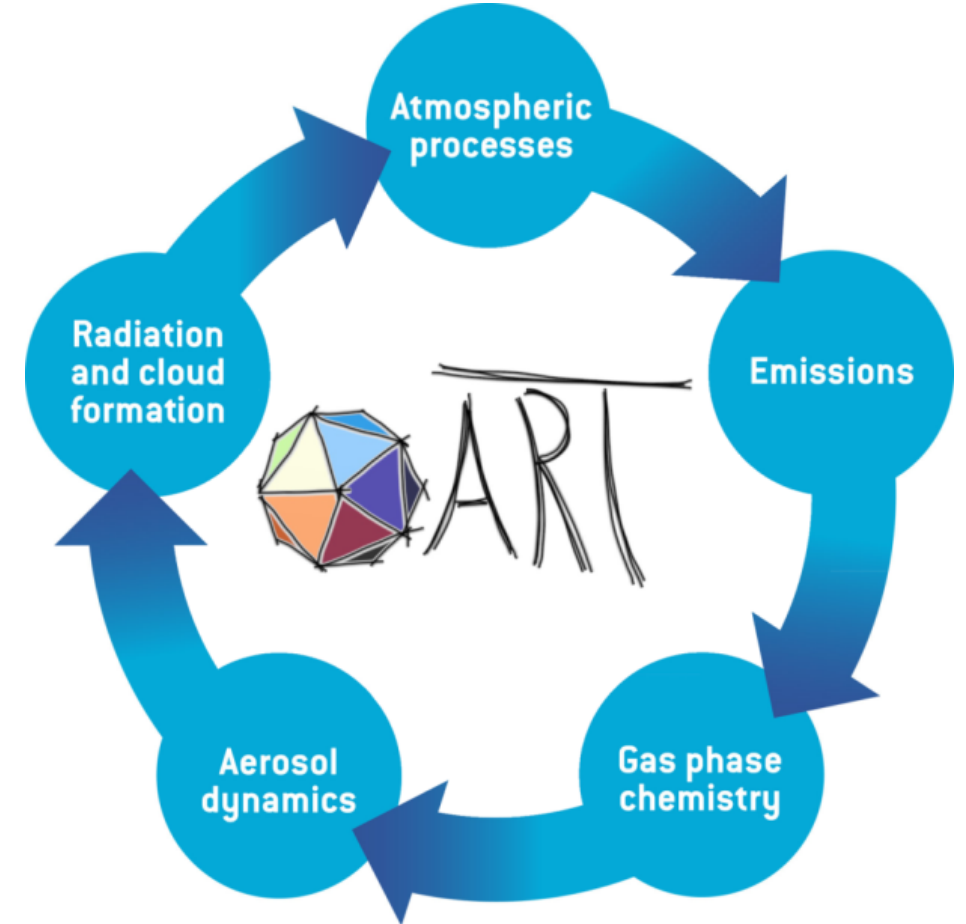
Flexible tracer, chemistry and aerosol structure

Rieger et al. 2015, Weimer et al. 2017, Schröter et al. 2018

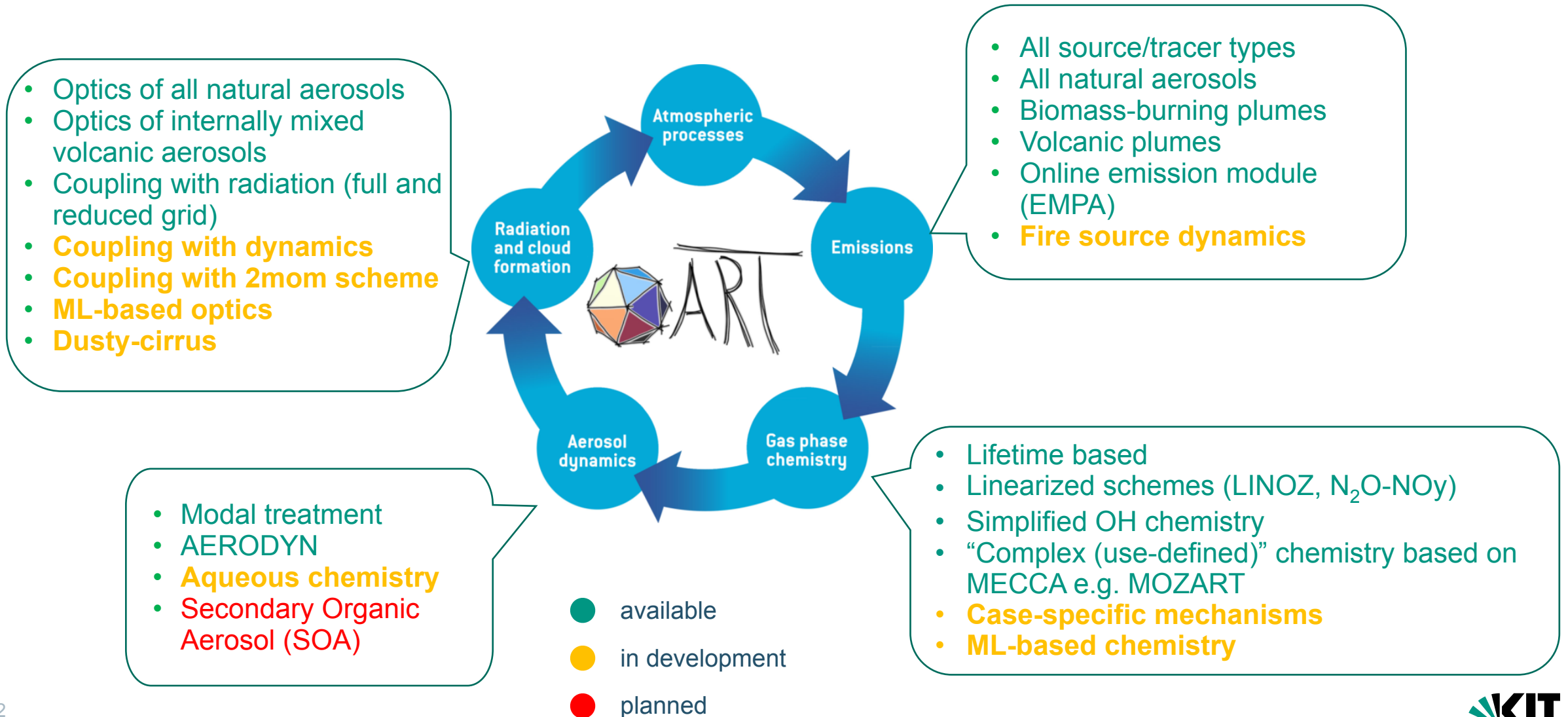
[Hoshyaripour et al. \(2026\), GMD 19, 1645–1681, 2026](https://doi.org/10.5194/gmd-19-1645-2026)



Picture: ICON-ART process wheel, slide material Valentin HANFT (IMKASF)



ICON-ART : what is available, what is planned



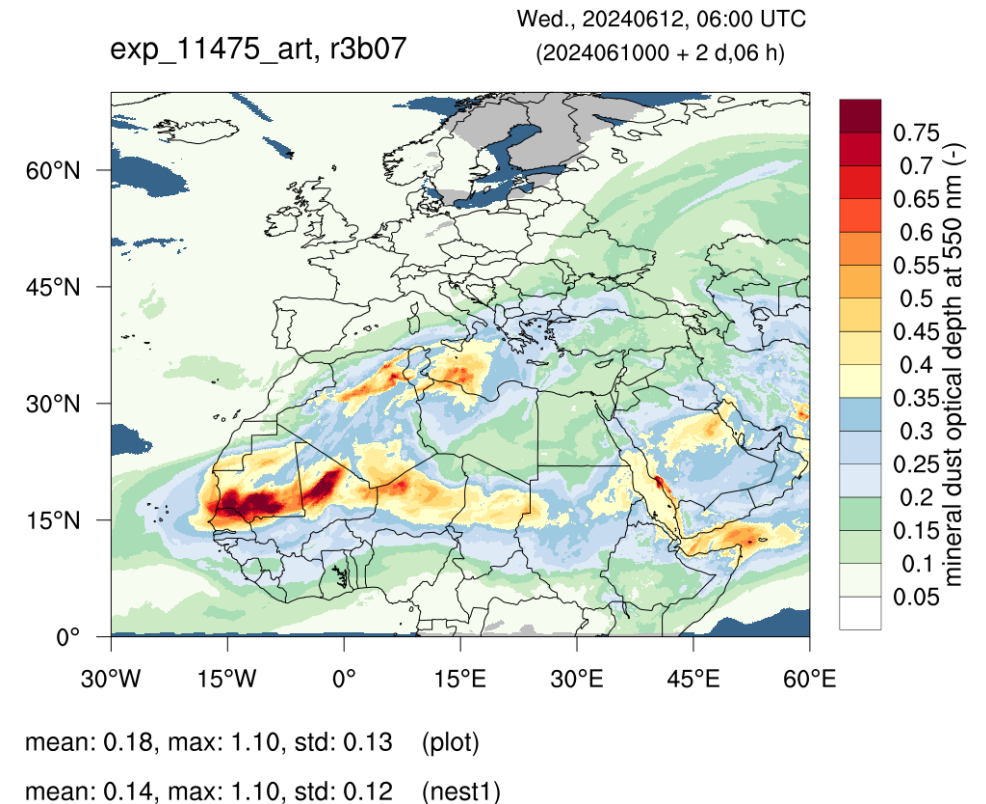
What -ART can simulate

Emergency: radionuclides, volcanic eruptions, vegetation fires, chemical accidents

Quasi-operational: sea salt, vegetation fires, passive CH₄ and CO₂

Operational at DWD: pollen and mineral dust

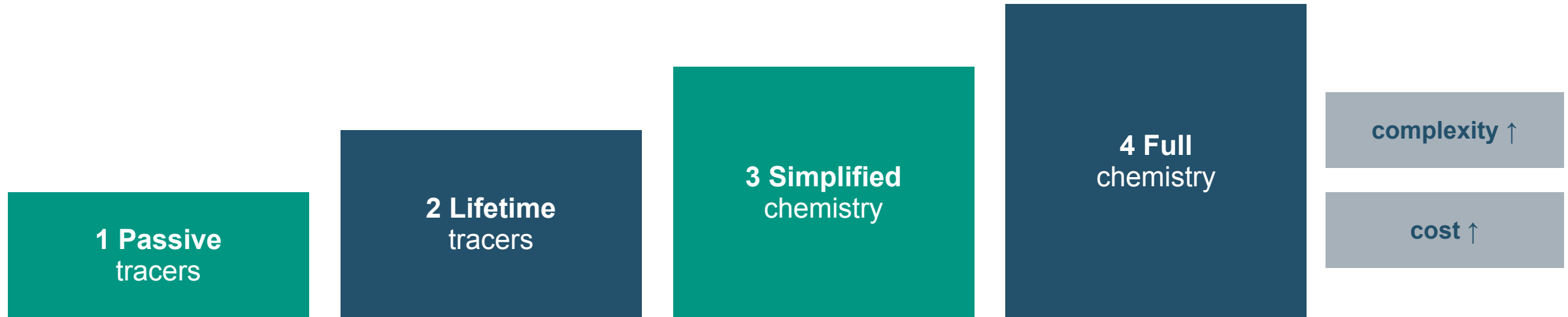
Applications from tracers to full chemistry



From passive tracers to full chemistry

Choose the chemistry that fits the question and the (time) budget

1. **Passive** and 2. **lifetime tracers**: CO_2 , CH_4 , air-mass origin
3. **Simplified chemistry**: LINOZ ozone, N_2O - NO_y , simple OH
4. **Full chemistry**: MECCA/KPP mechanisms, e.g. MOZART



Ozone chemistry options in ICON-ART

LINOZ v2: linearised ozone chemistry (Taylor expansion in temperature, ozone column, mixing ratio)

Look-up tables with climatological coefficients

Cold tracer for polar ozone loss ($T < 195$ K)

MECCA gas-phase chemistry: O_3 , CH_4 , HO_x , NO_x , halogens, sulfur

KineticPreProcessor (KPP) generates the code;
Rosenbrock solvers handle stiff ODEs

CloudJ gives photolysis rates

+7 %
runtime with LINOZ

195 K
cold-tracer threshold

x10
runtime with MECCA

UV-index forecasts: ozone for the German Weather Service (DWD)

Forecast ozone and UV index in an operational, fast setting

Classify the influence of atmospheric quantities on the UV index

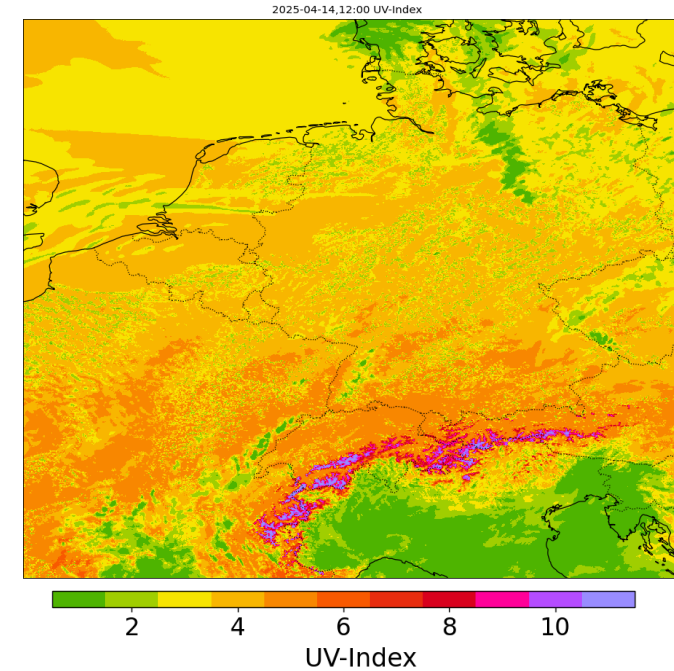
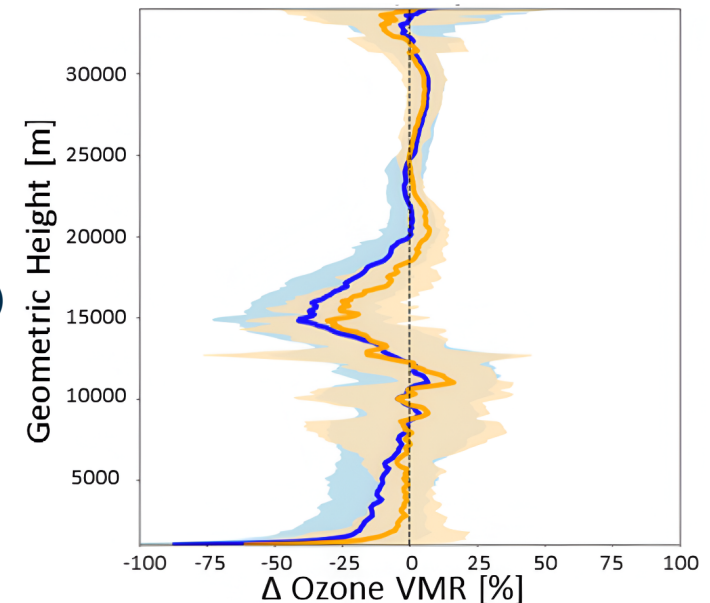
UV radiation is harmful: forecasts help to reduce health risks

Mean (Sonde - ICON-ART)

— : Feb. to June 2022

— : Feb. to Nov. 2022

Pictures: slide material Valentin HANFT, IMKASF (UV-index maps; ozone profile comparison)



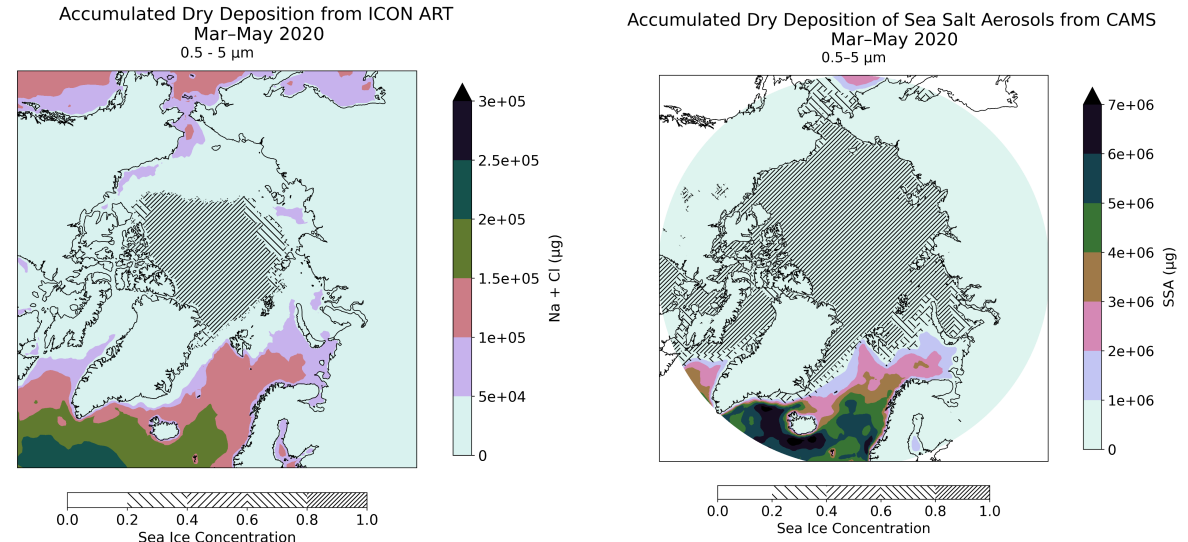
Polar ozone depletion and bromine explosions

Tropospheric ozone in the Arctic spring often drops below 5 ppb: **tropospheric** ozone depletion events

Plumes of enhanced BrO in satellite data: bromine explosions

Question: how much bromide in Arctic snow comes from gas-phase deposition?

ICON-ART simulates the accumulated dry deposition



Snow
sampling,
Ny-Ålesund,
April 2024

Pictures: Stefanie FALK, Arianne LE CARDINAL (IMKASF); photo Lucas REISSIG 2024

Modelling at IMKASF: more ICON-ART topics

mloz: machine-learning ozone for climate runs

ICON-SmART: seamless ICON with ART, with IMKTRO and SCC

Regional tracers for **flight planning**

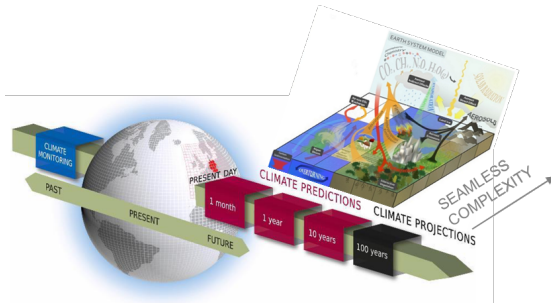
Black carbon in Himalayan glacier valleys

Solar activity and the mesosphere / lower thermosphere

[QBO](#) in ICON

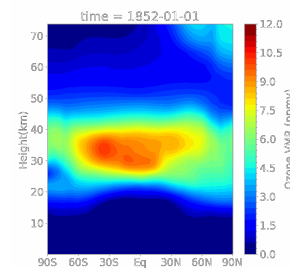
Radiation and ozone feedback

[Training course online \(natESM\)](#)

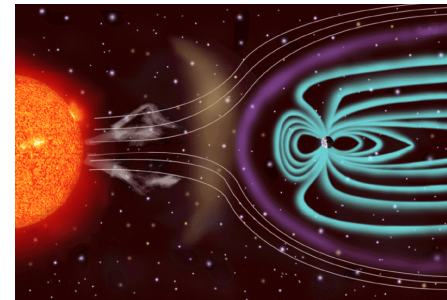


ICON-SmART

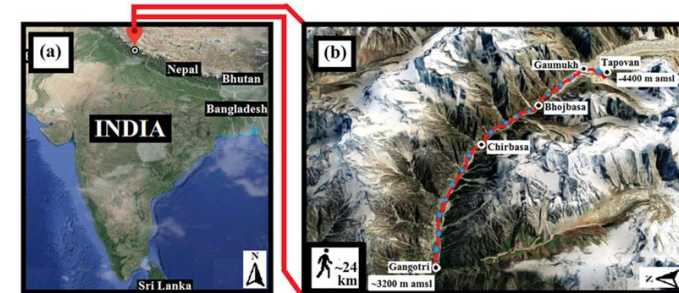
Pictures: slide material Valentin HANFT (IMKASF)



mloz: machine-learning ozone



Solar activity and the mesosphere / lower thermosphere



Black carbon in Himalayan glacier valleys

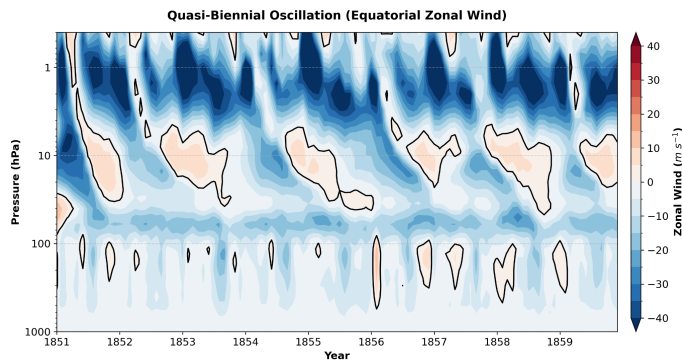
QBO in ICON: model versus observation

[ATMOHub](#) hosts the observed QBO winds (monthly, since 1953); we use them to evaluate ICON

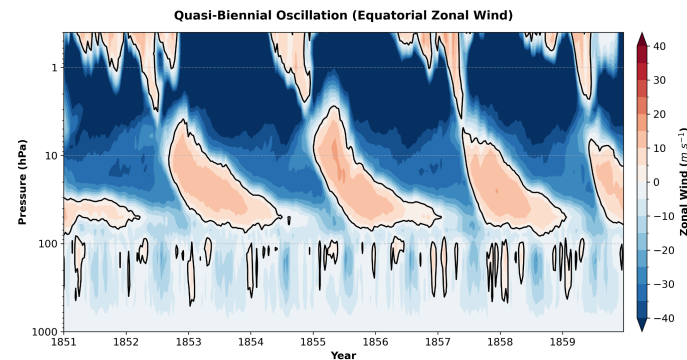
Climate models underestimate QBO amplitudes; ozone feedbacks are missing

Baseline ICON: weak amplitudes, unrealistic period

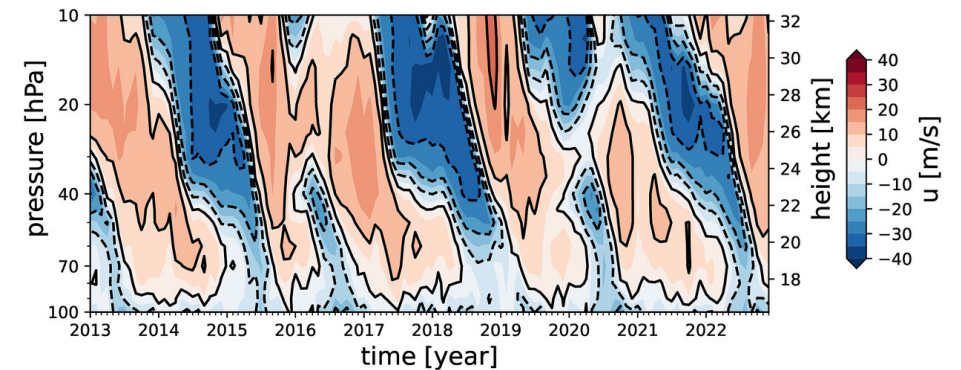
After tuning: period, amplitude and structure are much improved



Baseline ICON QBO



Improved setup



Observed QBO, 2013-2022

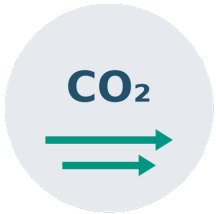
Figures: Stefan VERSICK (IMKASF); observations: ATMOHub QBO series

model shown for a historical decade; observations for 2013–2022”

Modelling at IMKASF: current projects

Selected projects of the modelling and data groups

CATRINE
2024-2027



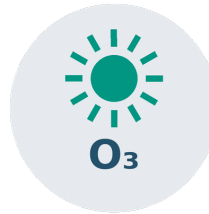
Better transport simulation; metrics and test beds for CO₂ and CH₄ fluxes

ITMS
2022-2026



Integrated greenhouse gas monitoring system for Germany (observations)

POF
2020-2025



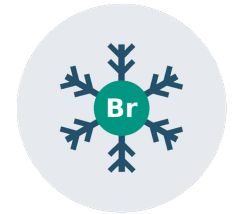
Prognostic ozone for ICON: enabling UV forecasts

UA-ICON
2024-2027



DFG project: ICON extended to the upper atmosphere

BromoPole
2023-2026



Bromine chemistry in the polar atmosphere and its deposition

3 Case study: Thessaloniki, Greece



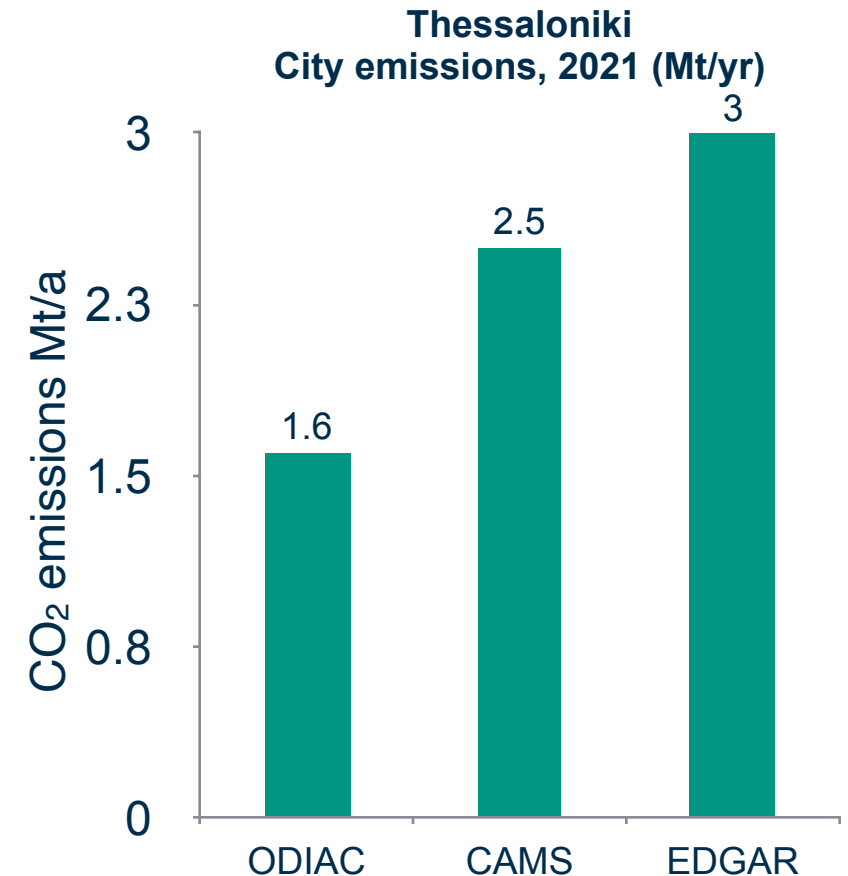
Cities are hard to constrain with emission inventories

Emission inventories are bottom-up (reported activity × emission factor, gridded in space and time): a model of emissions

Urban areas: about one third of global anthropogenic greenhouse gases (2015)

Thessaloniki (1.09 million inhabitants): three inventories that disagree

Question: can a short campaign plus a km-scale model test them?



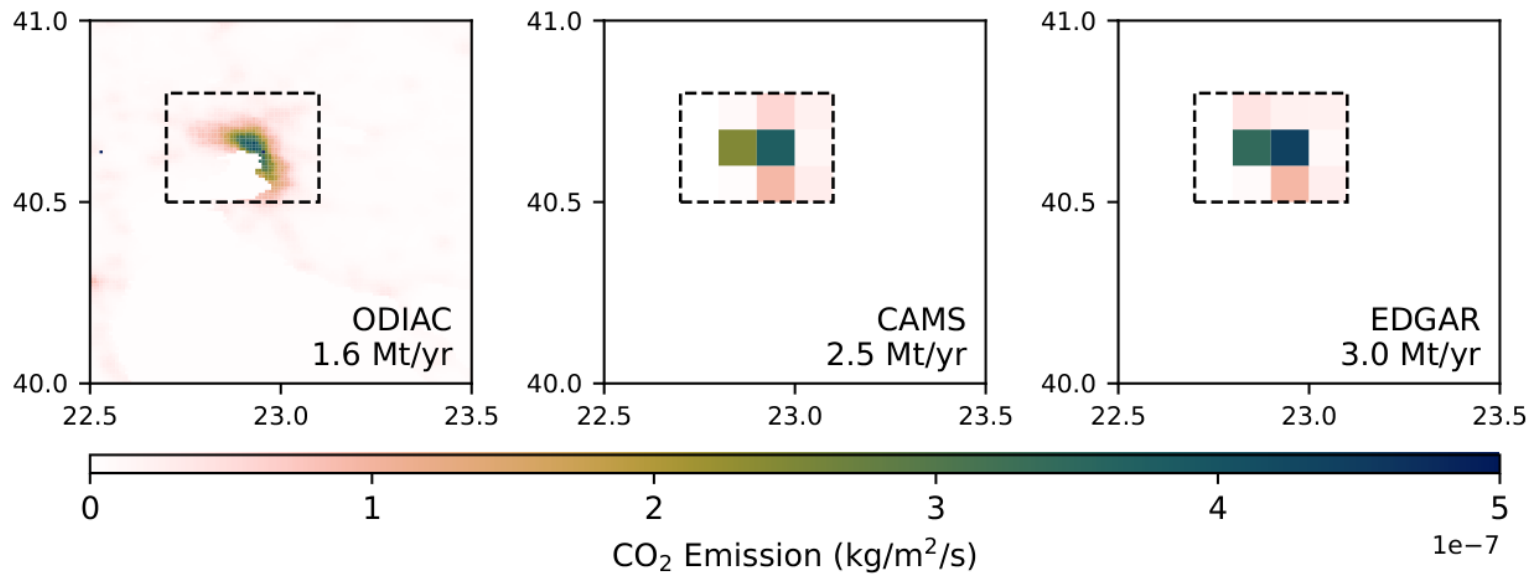
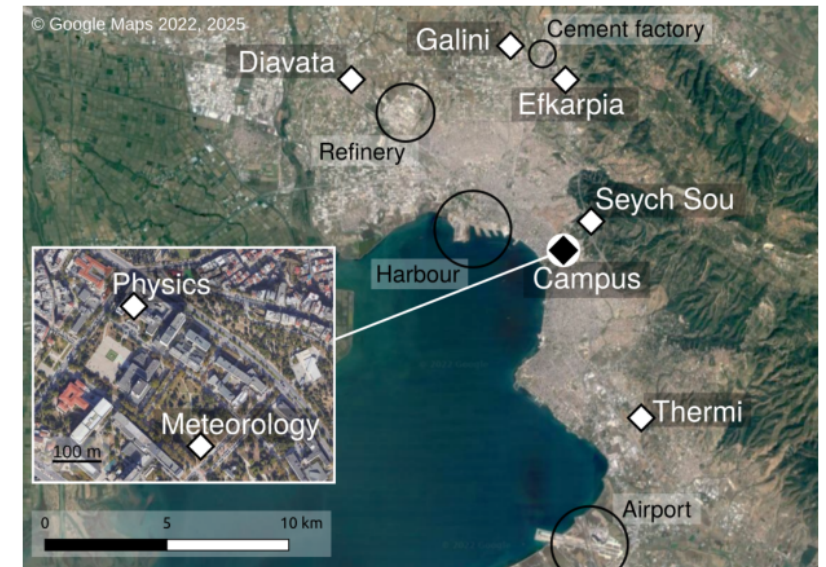
Three inventories 2021

ODIAC (Open-Data Inventory for Anthropogenic Carbon dioxide) 1.6 Mt/yr

CAMS (Copernicus Atmosphere Monitoring Service) 2.5 Mt/yr

EDGAR (Emissions Database for Global Atmospheric Research) 3.0 Mt/yr

ODIAC resolves the city at 1 km, CAMS and EDGAR at a few 0.1° pixels (≈ 10 km)



Figures: Lena FELD et al. (2025), Fig. 1 and Fig. 2; satellite image © Google Maps

Measurements: portable FTIR spectrometers

EM27/SUN solar absorption spectrometers
(Bruker / KIT)

COCCON network standards, ESA-supported



Two instruments: one stationary on campus, one mobile with solar power

30 days: October 2021 and May-July 2022

221 h of data; **21 days (170 h)** used in the analysis

2
EM27/SUN

30
campaign days

221 h
measured

0.22 ppmv
calibration

What does the instrument measure? XCO_2

Output: XCO_2 , column-averaged dry-air mole fraction, 0.13 ppmv precision

$$\text{XCO}_2 = \text{VC}(\text{CO}_2) / \text{VC}(\text{air})$$

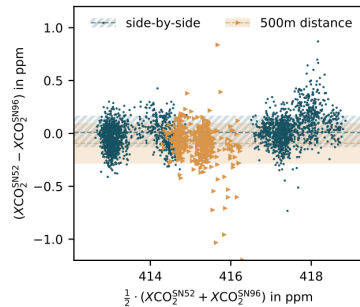
$$= \text{VC}(\text{CO}_2) / \text{VC}(\text{O}_2) \cdot 0.2095$$

where 0.2095 is the fraction of O_2 in air

Calibration by side-by-side runs: 0.22 ppmv uncertainty

City signals are small: variations of about 1 ppmv

PROFFAST retrieves columns of CO_2 along with O_2 , H_2O , CH_4 , and CO .



Two spectrometers measuring side by side (blue) and 500 m apart (orange) differ by 0.15 and 0.19 ppm (standard deviation). Lena FELD et al. (2025),

0.13 ppmv
precision

0.22 ppmv
calibration uncertainty

≈ 1 ppmv
city signal

0.2095
 O_2 fraction of dry air

Why do we need a high-resolution transport model?

Daily XCO₂ variations: median 1.33 ppmv but the gradient between sites only 0.17 ppmv

For comparison: Tokyo campaign saw gradients up to 9.5 ppmv

Complex orography and land-sea wind system

Box models do not work: the plume and wind change during the day

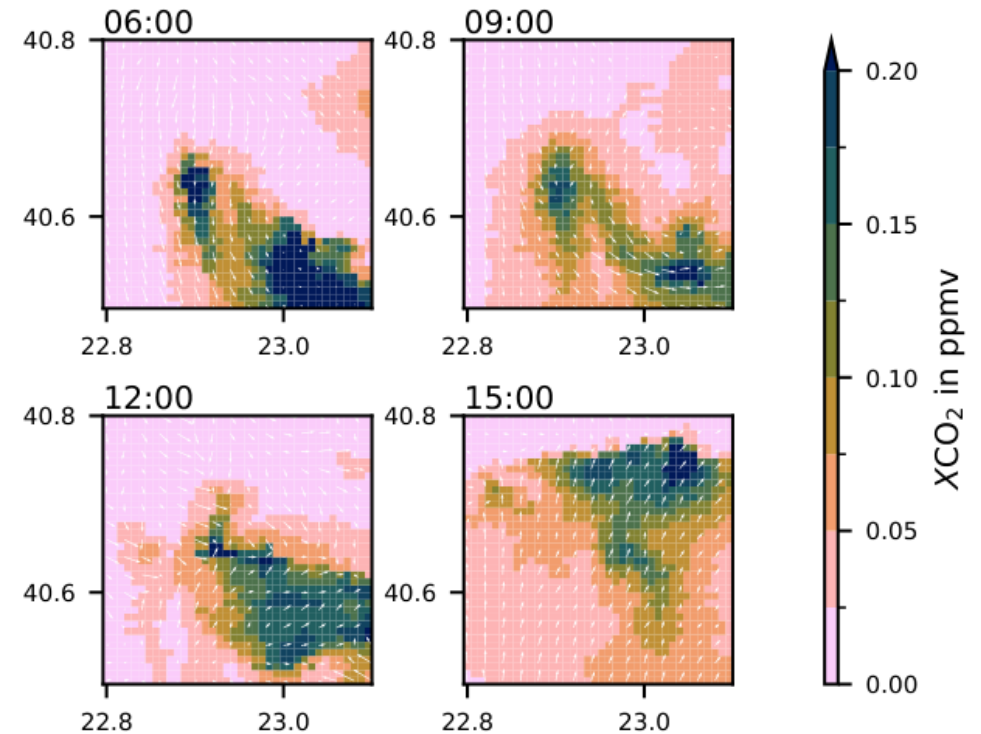


Figure: Lena FELD et al. (2025), Fig. B1: simulated XCO₂ enhancement and 10 m wind, 15 June 2022

Simulation setup

ICON-ART 2025.04, R19B8 grid, 1 km (Domain 1, about 170×180 km)

Domain 2: 6.5 km, about 500×420 km, for far-field influence

Initial and boundary data from DWD; background CO_2 set to 0, passive tracers

Anthropogenic: ODIAC 1 km remapped with emiproc; biogenic Net Ecosystem Exchange (NEE) from MODIS, SMAP, FLUXCOM



1 km

ICON-ART grid

6.5 km

outer domain

≈ 0.8 km

ODIAC grid

21 days

analysed

Figure: Lena FELD et al. (2025), Fig. 4; map © Google Maps

Does the model get the weather right?

Wind roses at two sites only 5 km apart differ, and the model reproduces this

Wind correlation up to $r = 0.83$; wind speed has a bias

Water vapour column: $r > 0.96$, bias below 3 %

But the correlation of the water vapour gradient between the two sites is weak ($r = 0.28$): small-scale transport is imperfect.

The CO_2 signal we invert is itself a small gradient (~ 0.17 ppm), so transport is a main uncertainty.

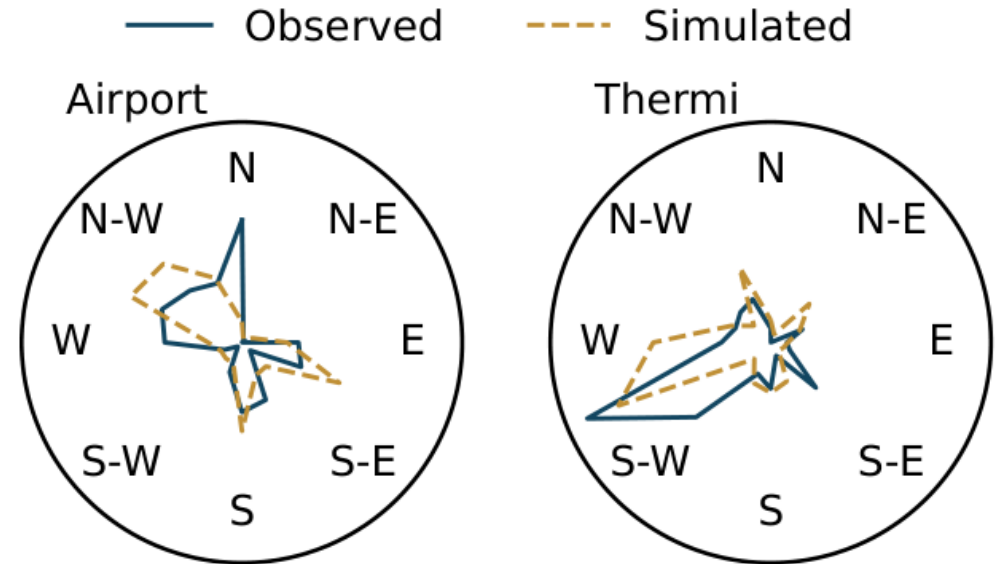


Figure: Lena FELD et al. (2025), Fig. 9

Comparing model and observation

Derive XCO_2 from model pressure, temperature and mixing ratio

Average observations to 10 min (wind travels about 0.9 km, close to the grid size)

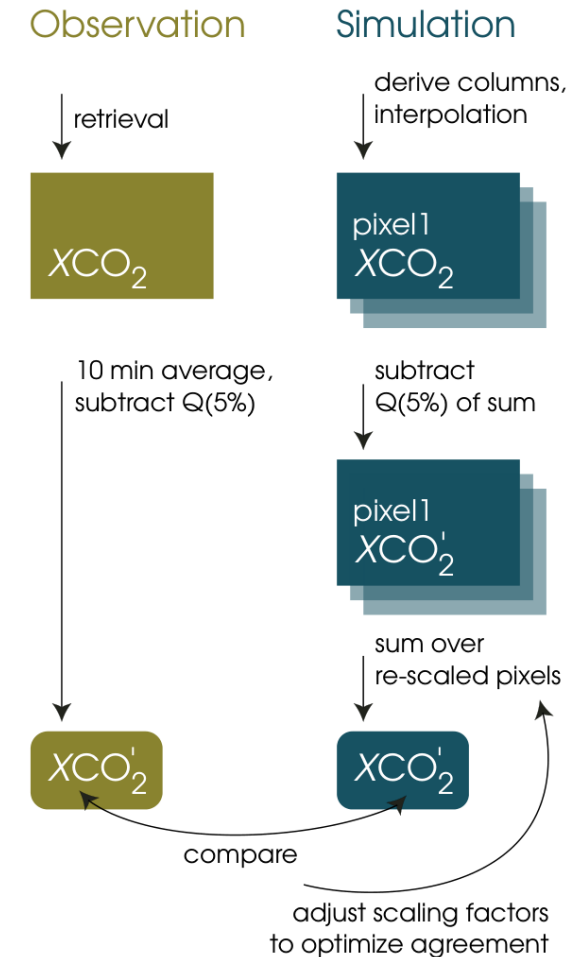
Subtract the daily 5 % quantile from both series: XCO_2' is the enhancement

Compare, then adjust the scaling factors above daily baseline

$Q(5\%)$ = daily 5th percentile of XCO_2 , used as the background baseline.

$$XCO_2' = XCO_2 - Q(5\%).$$

Figure: Lena FELD et al. (2025), Fig. 7



Inversion by pixel-wise rescaling

Cost function: $c = \frac{1}{2} \| \sum x_i a_i - b \|^2$,

a_i = simulated contribution of pixel i ,

b = observations

Bounded least squares (scipy lsq_linear), factors limited to 1/6 ... 6

City scaling (one factor) or pixel scaling (one per pixel)

No prior uncertainty needed, unlike Bayesian inversion

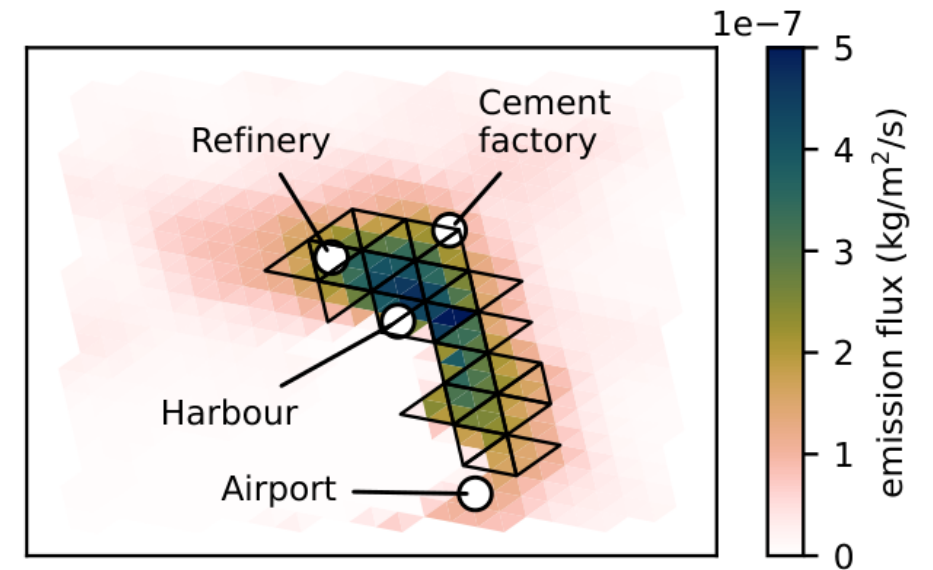
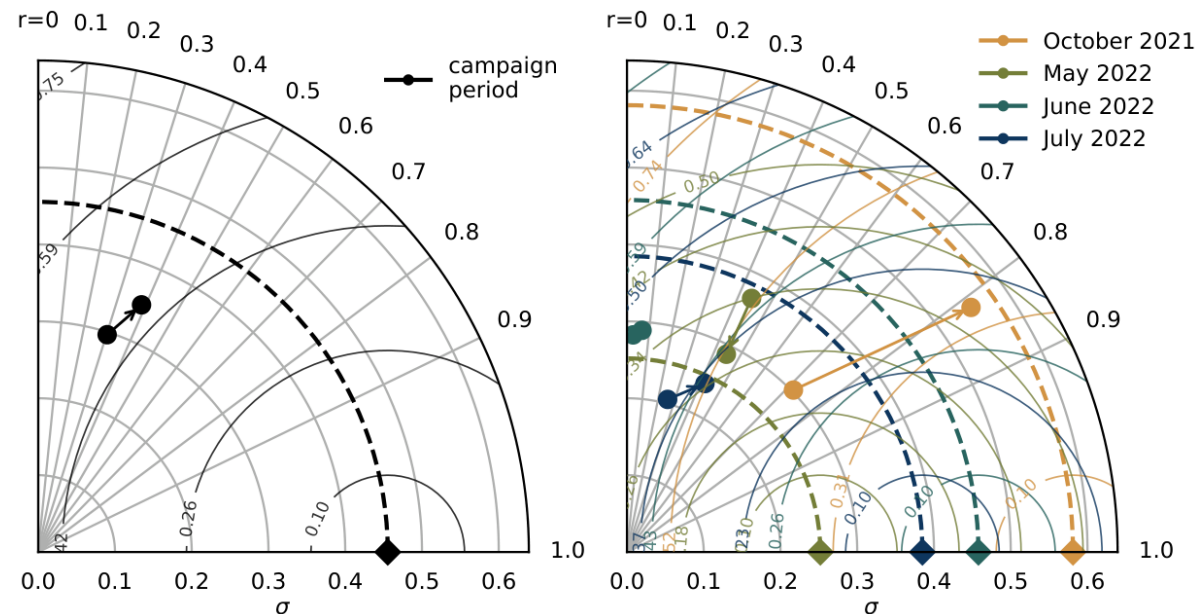


Figure: Lena FELD et al. (2025), Fig. 6: ODIAC on the ICON grid, hot-spot candidates

Agreement improves, most clearly in October 2021

Prior correlation in October 2021: $r = 0.72$; after pixel scaling 0.82 and gradient between spectrometers improves with pixel scaling from -0.26 to 0.60

Campaign period overall: r from 0.30 to 0.39



Taylor diagram:
variability (standard deviation), pattern agreement (correlation) and the distance from the diamond combines them into RMSD

Figure: Lena FELD et al. (2025), Fig. 12

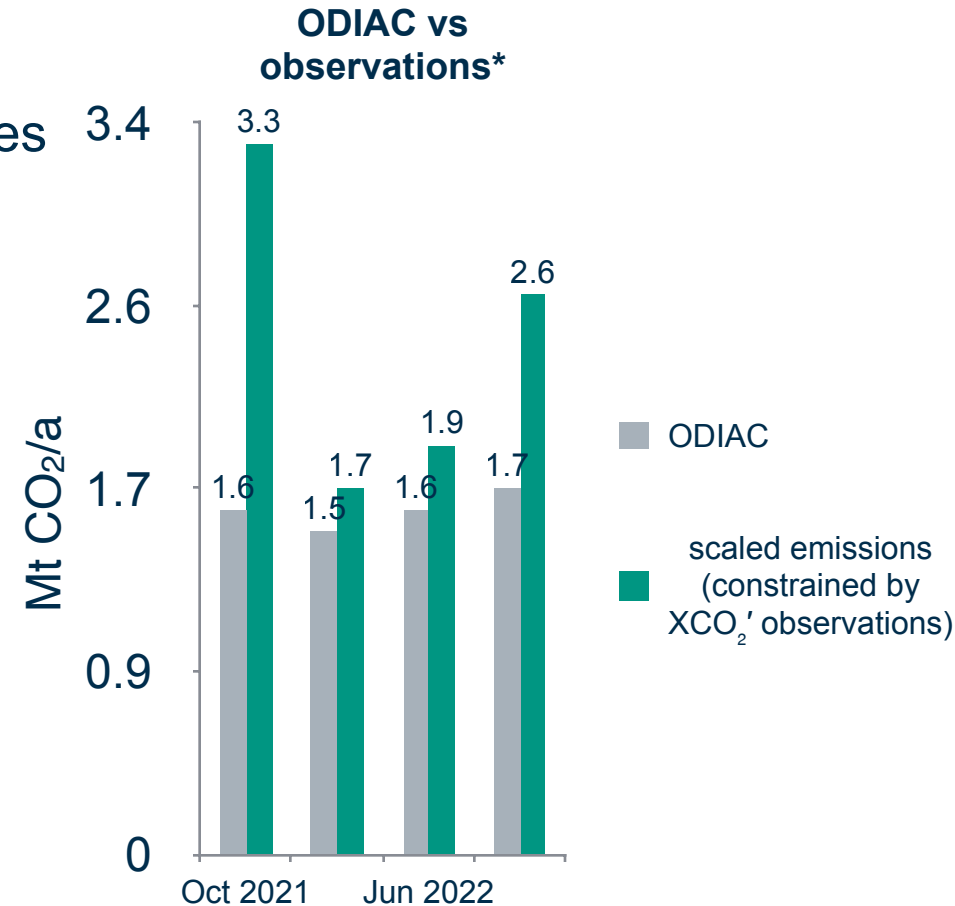
Results: ODIAC-based enhancements are too low

October 2021: 3.1-3.7 Mt/yr versus ODIAC 1.6 Mt/yr

Summer 2022: 1.5-2.6 Mt/yr, weaker improvement; biogenic fluxes matter

Whole campaign: 1.9-2.2 Mt/yr

Robust against domain size and initialization



*Total emissions derived by scaling ODIAC city emissions to match observed XCO₂' enhancements using ICON-ART. Bars show the prior (ODIAC) and posterior (scaled) estimates

Where are the sources? Harbour and refinery

Harbour pixels are scaled up consistently across all configurations.

Near the refinery, a pixel is also scaled up — but not exactly at the refinery location.

Likely explanation: ODIAC has no stack-height information, so all emissions are released at the surface; the optimisation compensates with a horizontal displacement.

Caveat: only some pixels are robust across configurations. The spatial pattern is plausible, not proven.

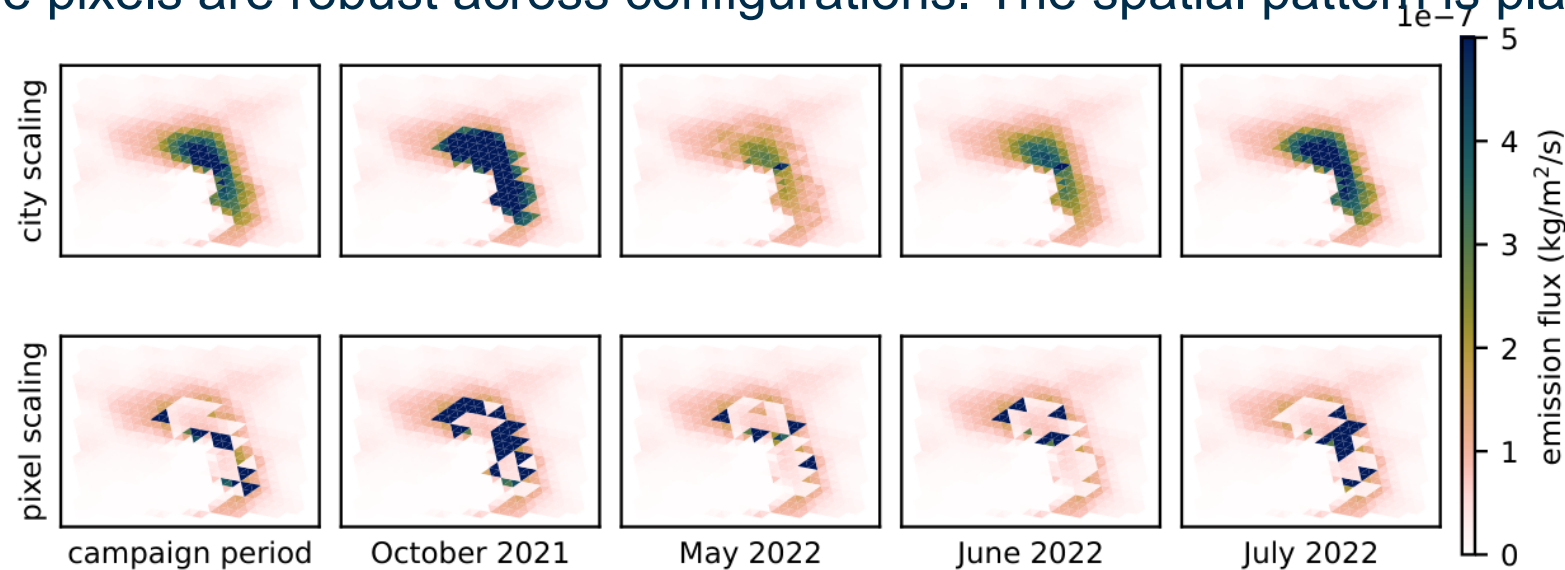


Figure: Lena FELD et al. (2025), Fig. 13

Limitations and lessons

Transport: wind speeds and between-site XH_2O gradients imperfect

Inventory: no diurnal/weekly time profiles; no emission heights

Biosphere: NEE uncertain, Mediterranean stomatal closure not represented (relevant for summer months)

Observations: calibration uncertainty 0.22 ppmv; only 21 days, two sites

Message: campaign data plus km-scale modelling can provide conditional evidence to test inventories of medium-size cities

Transport

Inventory

Biosphere

Calibration

4 COCCON and data management



ATMOHub: research data infrastructure at KIT

Part of the Helmholtz DataHub, Research Field Earth and Environment

Research data, services and data management of KIT's atmospheric research

Partners: IMK institutes, KIT Computer Center (SCC), KIT Library

Funded by the **Helmholtz Association**; running since 2019

IMK institutes

KIT SCC

KIT Library

Logo: DataHub / ATMO Hub (from Peter BRAESICKE's slides)

DataHub



Research Field Earth & Environment



NFDI4Earth

The data world at IMK



Many instruments, models and campaigns, many repositories
Published in RADAR4KIT, Zenodo, WDCC, TCCON/EVDC and more

Collected in the [ATMOHub catalogue](#)

IMKASF

MIPAS, GLORIA, IAGOS-CARIBIC,
NDACC/MUSICA, TCCON,
COCCON,
QBO winds, model results

IMKAAF

AIDA aerosol chamber,
ice-nucleating particles (PINE),
analysis software (PIA)

IMKTRO

ICON model releases,
KITCube,
Swabian MOSES campaign,
dust and weather extremes

IMKIFU

TERENO,
regional climate and
hydro-meteorological data

COCCON and TCCON: greenhouse gases at KIT

EM27/SUN spectrometers developed by Bruker and KIT

COCCON enabled by ESA

Standards for instruments and data analysis

PROFFAST retrieval

Calibration against the Karlsruhe TCCON station

Karlsruhe time series show the rise of CO₂ and CH₄

Open data with DOIs (COCCON Karlsruhe, TCCON Karlsruhe)

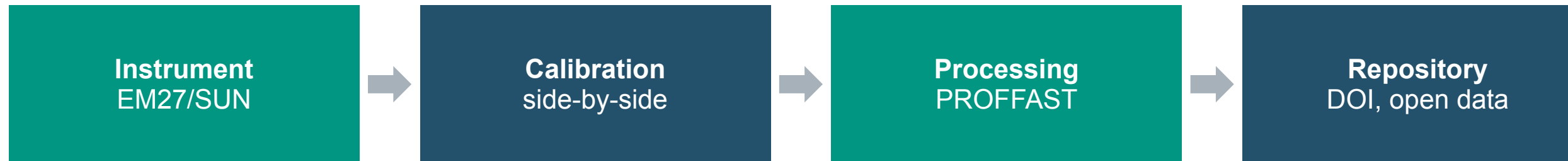
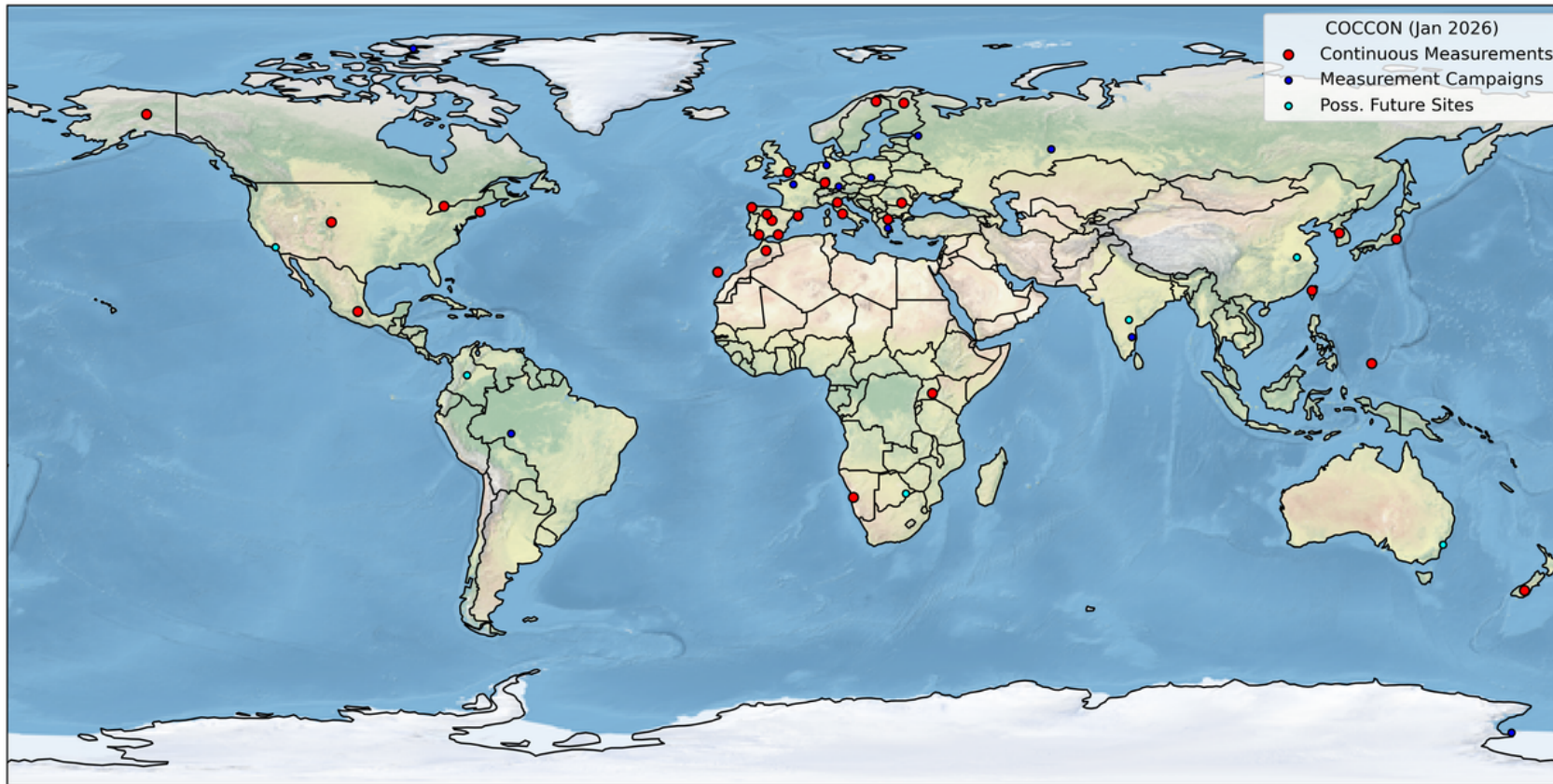


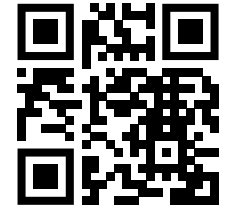
Photo: EM27/SUN spectrometers on a roof, COCCON (www.coccon.kit.edu)

COCCON: a worldwide EM27/SUN network



Map (Jan 2026) and photo: COCCON (www.coccon.kit.edu)

COCCON: www.coccon.kit.edu

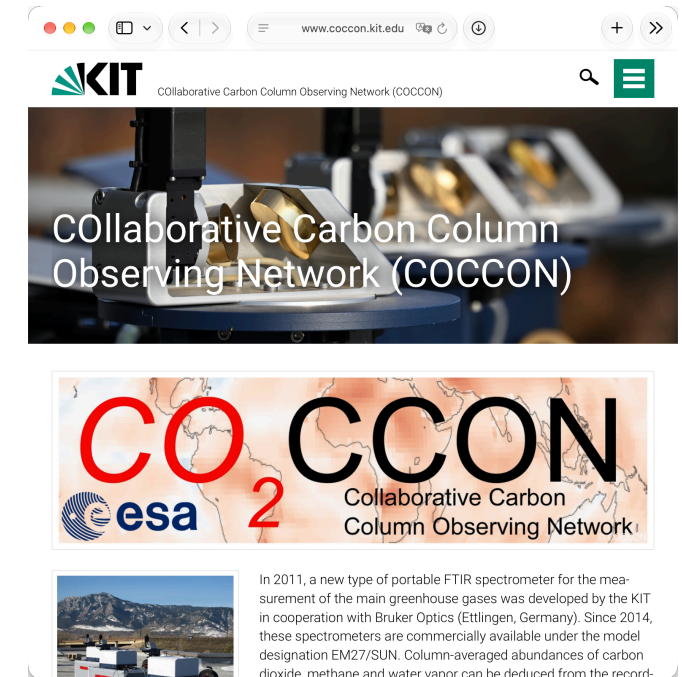


Central COCCON activities are hosted by KIT (IMKASF)

Instrument: standards, calibration, shelter solutions, Q & A

Data: repository, PROFFAST processing, PROFFASTpylot documentation

Operational sites, membership, publications, telephone conferences



2011

EM27/SUN developed at KIT with Bruker

2014

commercially available

>40

instruments worldwide

CO₂ CH₄ H₂O
optional CO channel

COCCON data pool at ESA's EVDC: evdc.esa.int



EVDC: ESA Validation Data Center, long-term repository for validation data of satellite atmospheric composition products

COCCON datasets: GEOMS-compliant HDF files with DOIs, e.g. Karlsruhe, Rome, Arrival Heights, Thessaloniki

Licence CC-BY 4.0 plus the COCCON data use agreement

COCCON membership means publishing EM27/SUN XGas data

XGas = column-averaged dry-air mole fraction of a gas

(e.g. 1 ppm Gas = 1 Gas molecule per 10^6 dry-air molecules)



1.5 M

correlative products at EVDC

20+

data networks

1000+

ground stations

CC-BY 4.0

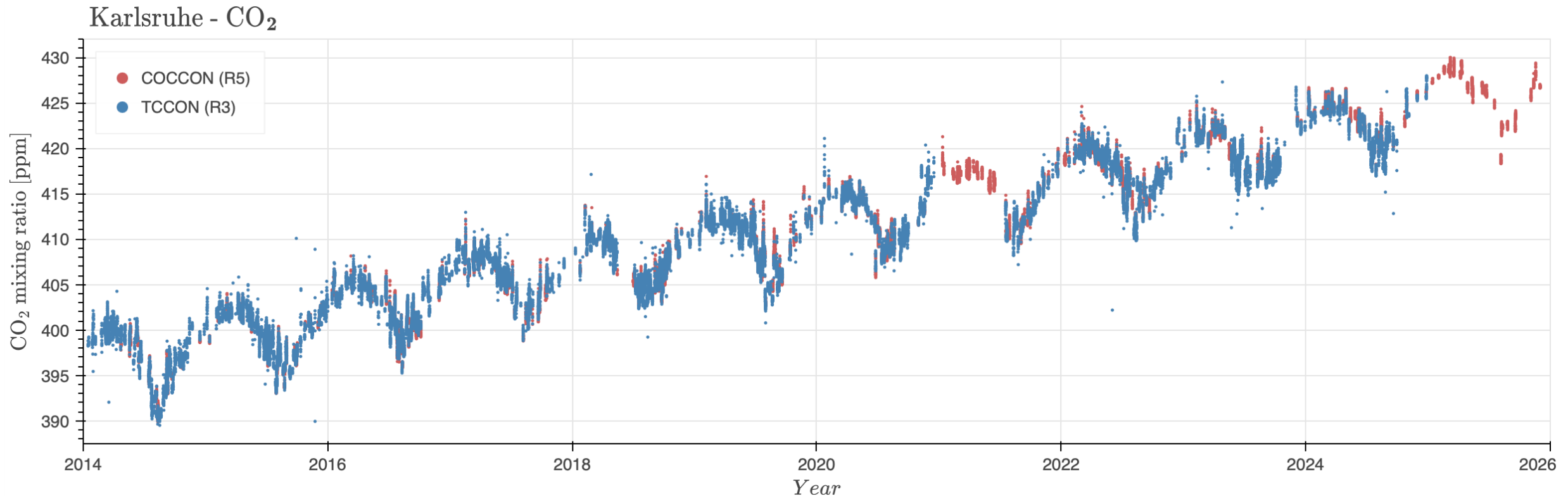
COCCON data policy

Karlsruhe CO₂ (ATMOHub)



FTIR column measurements at KIT (TCCON and COCCON)

Time series show the rise of CO₂ (and CH₄)



5 Outlook

3 min

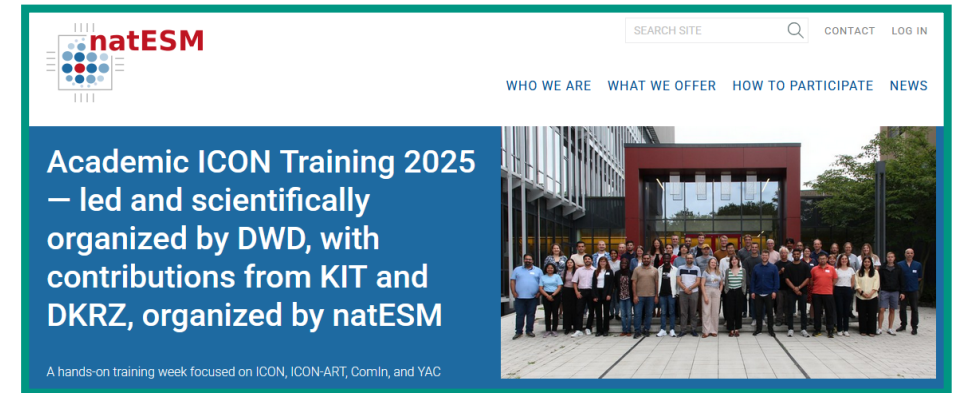
Outlook: greenhouse gas monitoring, teaching

CATRINE: better transport simulation, metrics and test beds

ITMS: integrated greenhouse gas monitoring for Germany

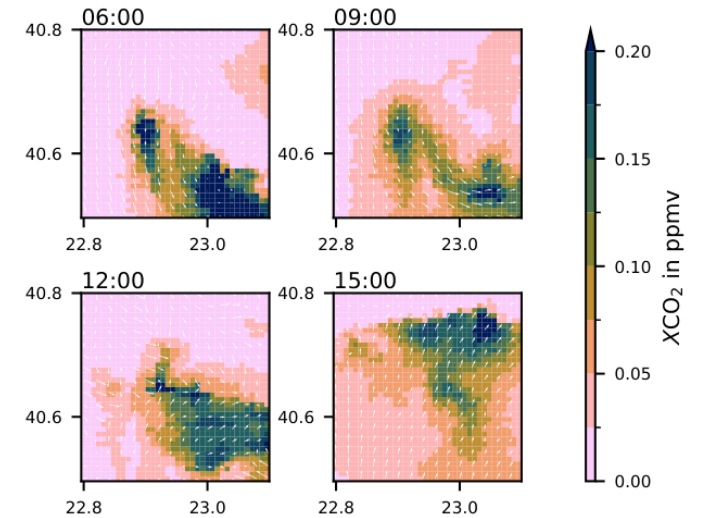
Time profiles and stack heights for emissions

[Open training: Academic ICON Training 2025 \(natESM\), videos are online](#)



Picture: natESM Academic ICON Training 2025 (slide material Valentin HANFT)

A 1 km atmospheric model plus portable column sensors can test city CO₂ inventories



Lena FELD et al. (2025), KIT / AUTH

Thank you – questions and discussion



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