THE REPRESENTATIVENESS OF OBSERVATIONS AND EMISSIONS FOR AIR QUALITY ANALYSIS ON REGIONAL SCALES

Workshop on Atmospheric Constituents Data Assimilation and Inverse Modeling

20 MARCH 2023 I ANNE CAROLINE LANGE

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and
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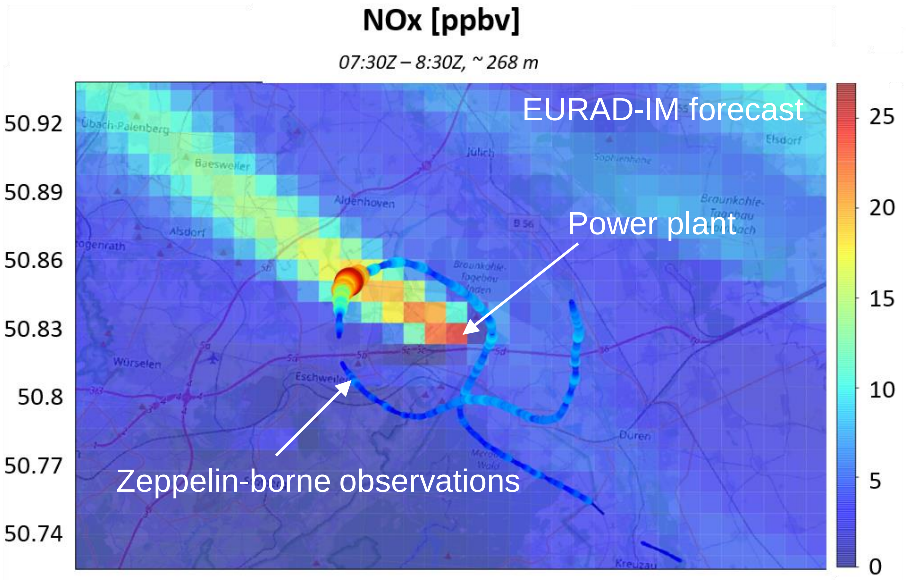
MOTIVATION – EMISSION OPTIMIZATION

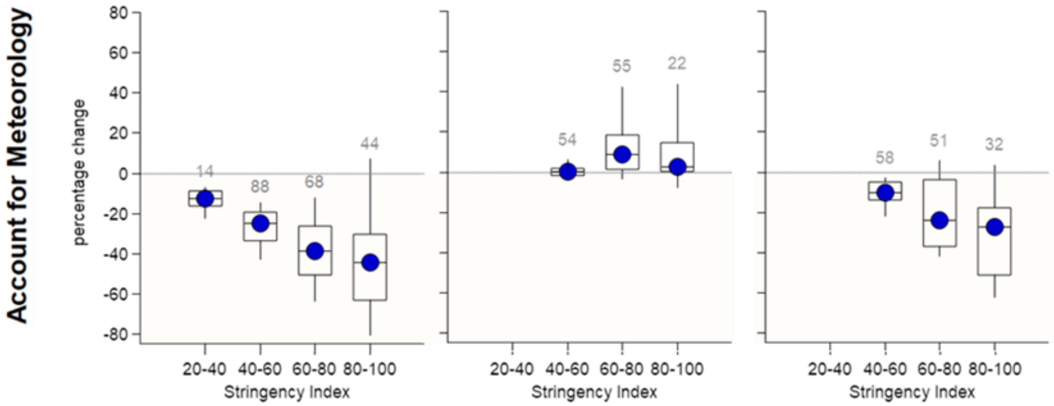
Renewable energies, electro mobility, working from home etc. increase the variability of emissions and thus the uncertainties in chemical weather forecasts.

How representative are annual emission inventory data for good air quality forecasting?



Comparison between modelled and observed NO_x concentrations at the Weisweiler power plant, 8 May 2020.

Tillmann et al., 2022, AMT



Pollutant changes during COVID-19 lockdowns, binned into intervals of the stringency index.

Gkatzelis et al., 2021, Elementa

4D-VARIATIONAL DATA ASSIMILATION

Cost function:

$$J(\mathbf{x}_0,\mathbf{e})=\frac{1}{2}\Bigg(\underbrace{(\mathbf{x}_0-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}_0-\mathbf{x}_b)}_{\text{optimal model state – first guess}}+\underbrace{\sum_{i=0}^{n}\Big((\mathbf{y}_i-\mathbf{H}[\mathbf{M}_i(\mathbf{x}_0)])^T\mathbf{R}_i^{-1}(\mathbf{y}_i-\mathbf{H}[\mathbf{M}_i(\mathbf{x}_0)])\Big)}_{\text{observations – optimal model state}}+\underbrace{(\mathbf{e}-\mathbf{e}_b)^T\mathbf{K}^{-1}(\mathbf{e}-\mathbf{e}_b)}_{\text{optimal emission factor – first guess emissions}}\Bigg)$$

$\mathbf{x}_0$: state vector of the chemistry transport model

$\mathbf{e}$: emission vector

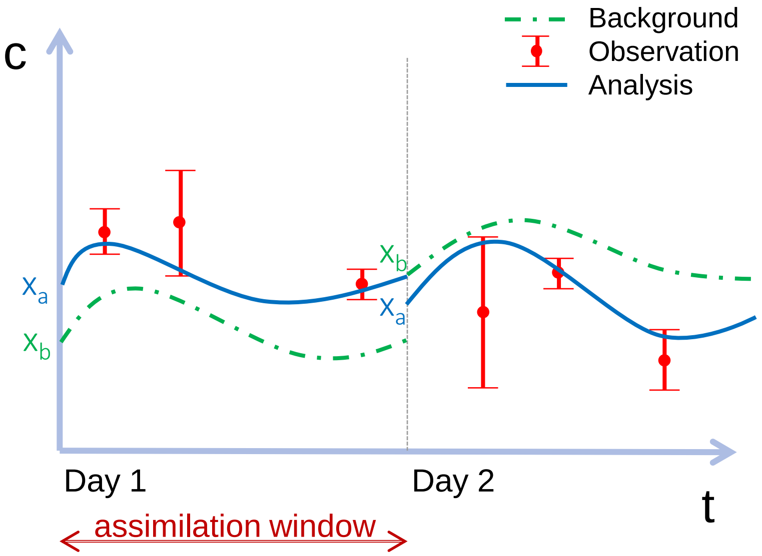
Elbern et al., 2007, ACP

Precondition

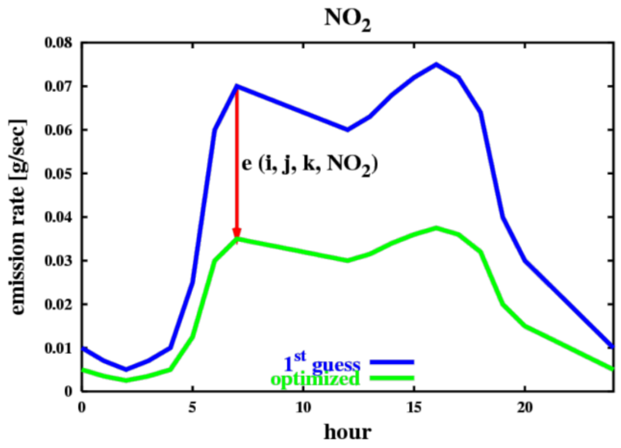
BLUE (Best Linear Unbiased Estimation)

- Unbiased errors
- Linearized model $\mathbf{M}$
- Linearized observation operator $\mathbf{H}$

Time series of species mixing ratio



Time series of NO2 emission rates



EURAD-IM

Copernicus
Europe's eyes on Earth

Atmosphere Monitoring Service

Part of the European Copernicus Atmospheric Monitoring Service regional Air Quality Ensemble

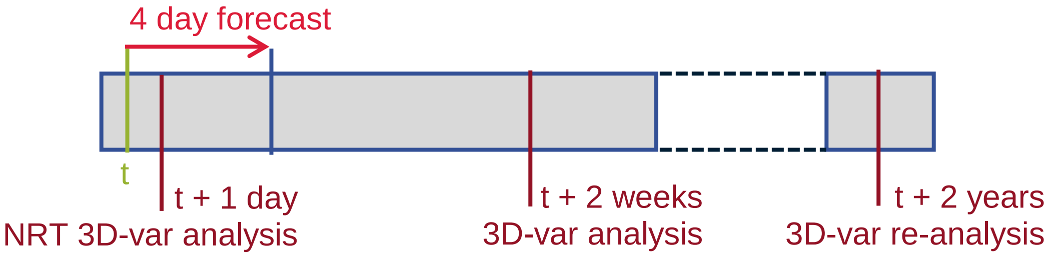
- CAMS is one of six services from the European Union's Earth observation programme focusing on:
  - Air quality and composition
  - Climate forcing
  - Ozone layer and UV
  - Solar radiation
  - Emissions and surface fluxes

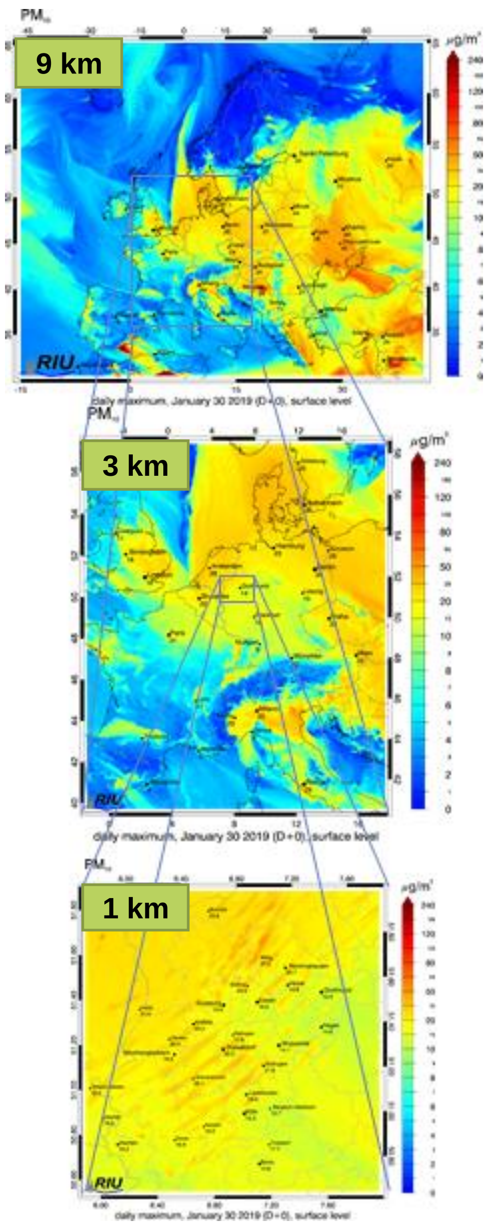
Main users:
Policy makers and public authorities

- We are one of eleven institutes contributing to the **operational regional multi-model ensemble for European air quality forecasts and analyses**

  (INERIS, Met Norway, FZ-Jülich, KNMI/TNO, SMHI, Meteo-France, FMI, Aarhus University, IEP-NRI, BSC, ENEA)

- Operational service includes:





EURAD IM System

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EVALUATION OF ANTHROPOGENIC EMISSIONS

Umwelt Bundesamt

Joint project with the German Environmental Agency

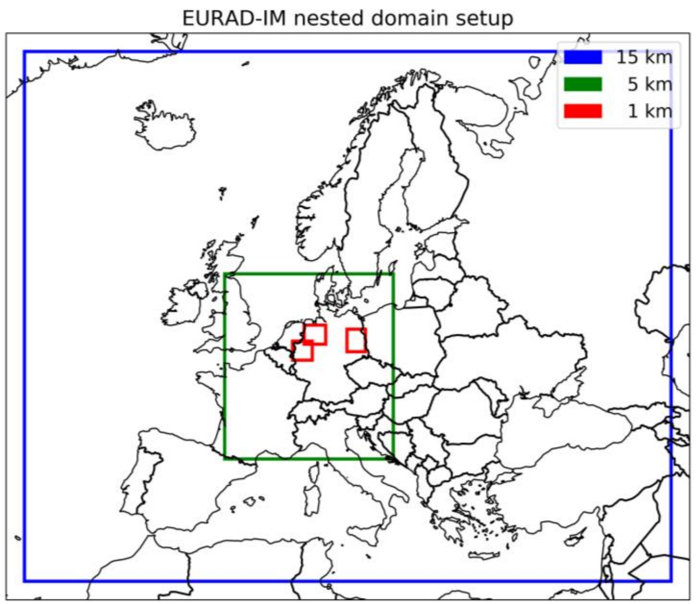
First comprehensive top-down investigation of anthropogenic emissions for gas-phase and aerosol species (CO, NO_x, NH_3, NMVOC, SO_x, PM_{10}, $PM_{2.5}$)

Aims

Improve:
- annual emissions,
- its spatial distribution,
- its seasonal cycle

Approach

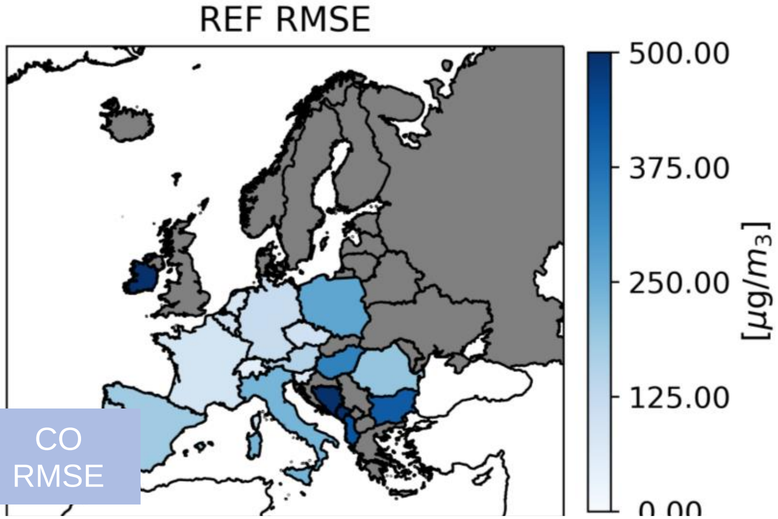
full year re-analysis of 2016 using 4D-var on 15 km, 5 km, and 1 km horizontal resolution assimilating ground-based, air- and space-borne observations



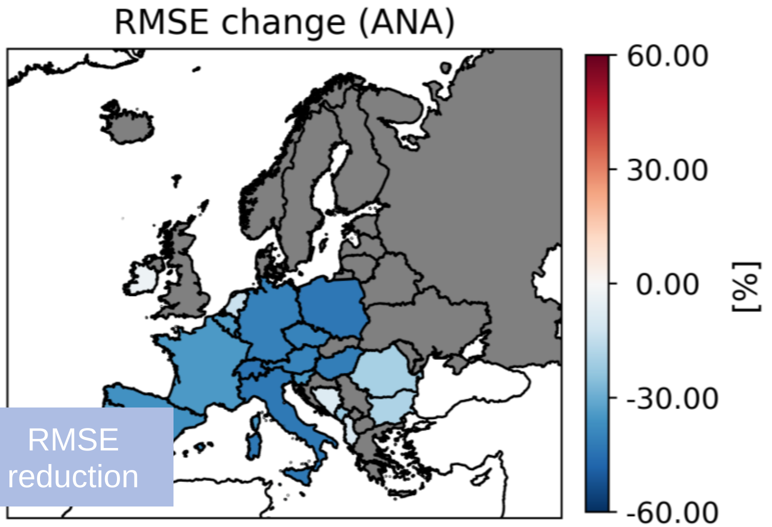
- Full adjoint transport, reactive gas-phase chemistry, and model for secondary inorganic aerosols
- Investigation allows insight into representativeness of observational networks, observability, influence of meteorological situation on assimilation
- Serve as reference of potential and limitations for current state of the art 4D-var analysis on air quality

CO EMISSION CORRECTIONS IN EUROPE

Validation stations

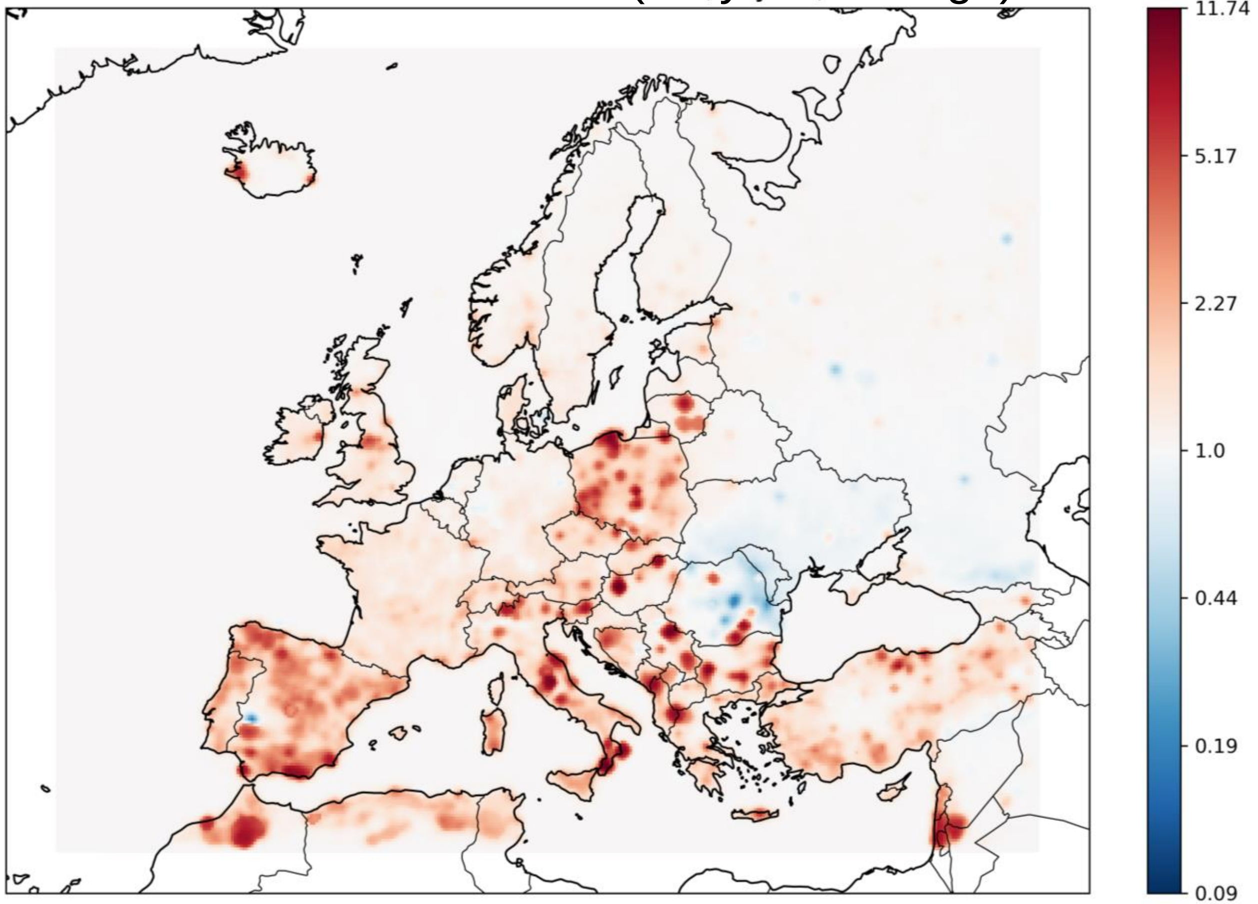


CO
RMSE



RMSE
reduction

CO emission corrections (full year average)



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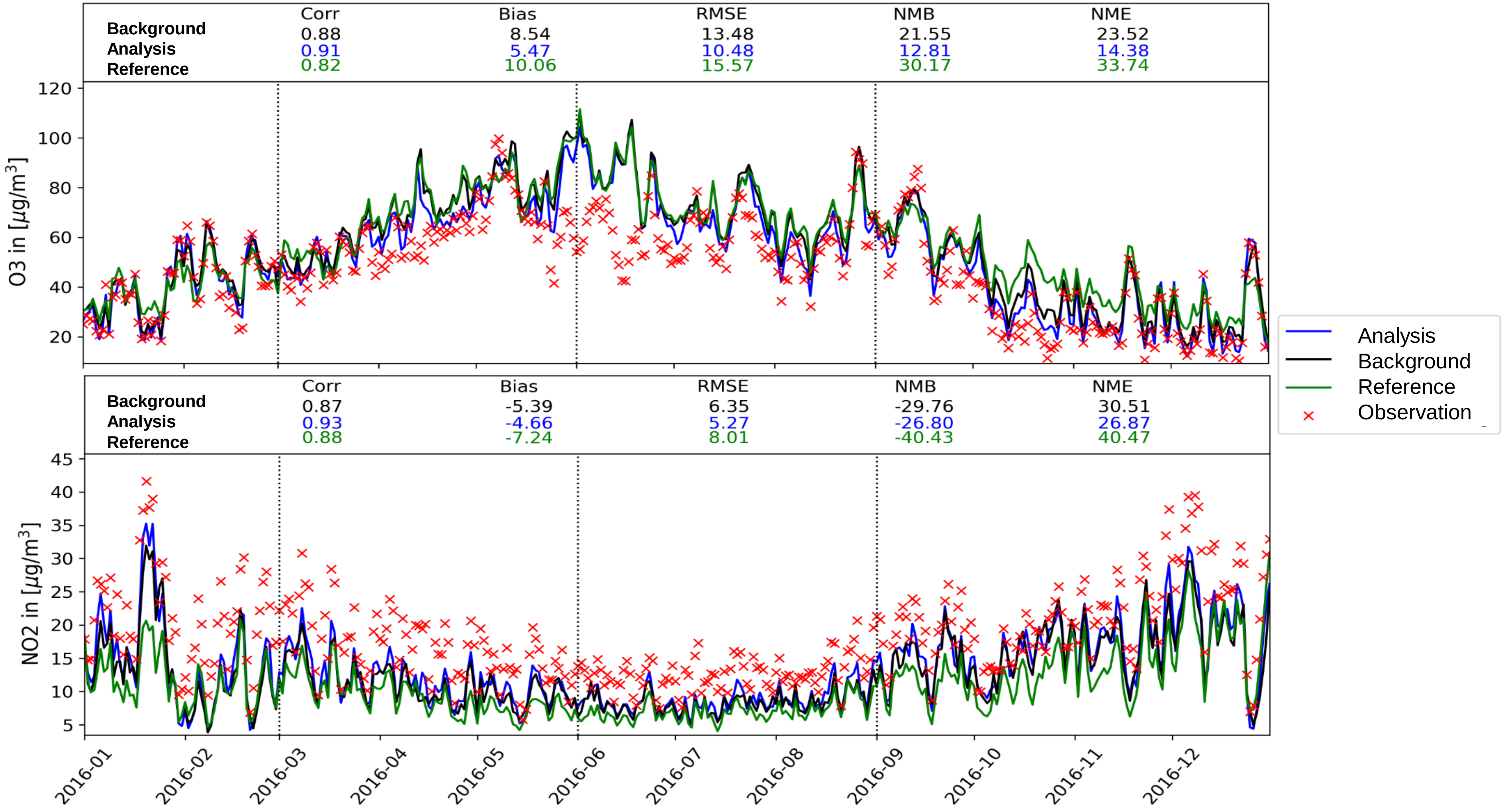
ANALYSIS EVALUATION

4D-var analysis allows for substantial improvement of the representation of atmospheric pollutants in the EURAD-IM simulations.

Illustrated is a mean over all validation stations in Germany (u05).



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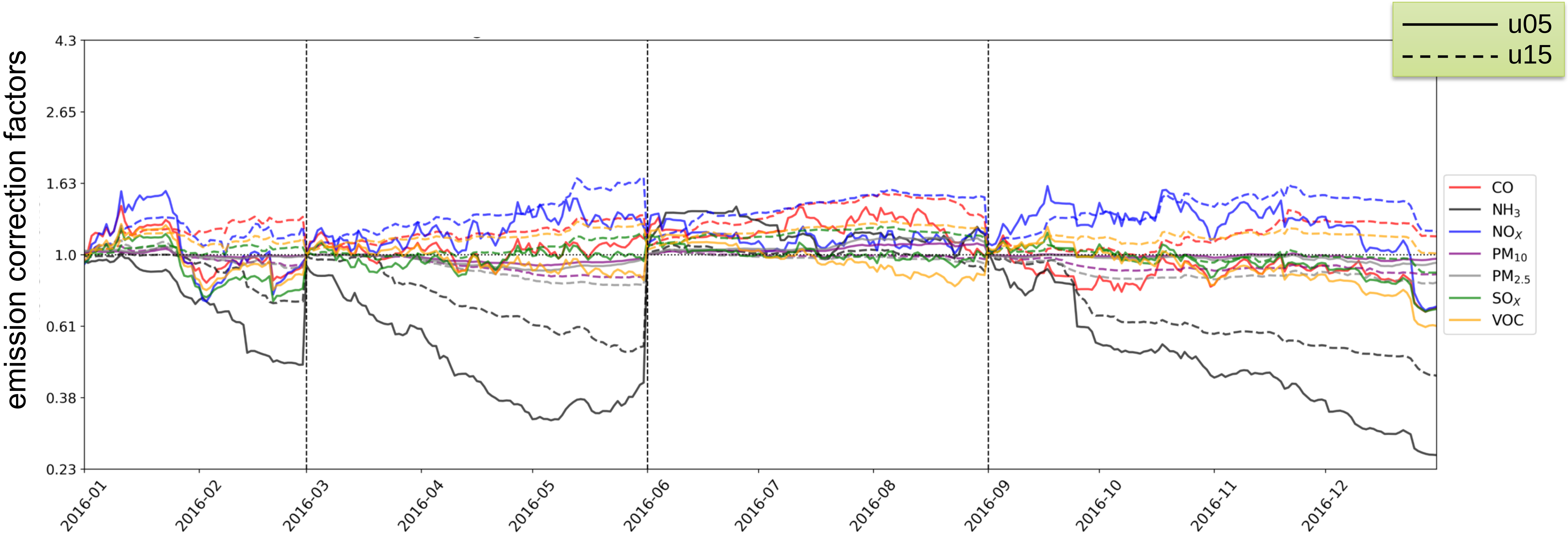
TEMPORAL EVOLUTION OF MEAN EMISSION FACTORS

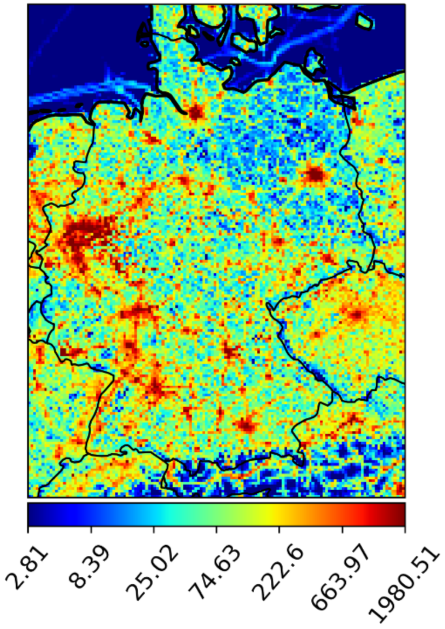
Germany (u05 & u15)



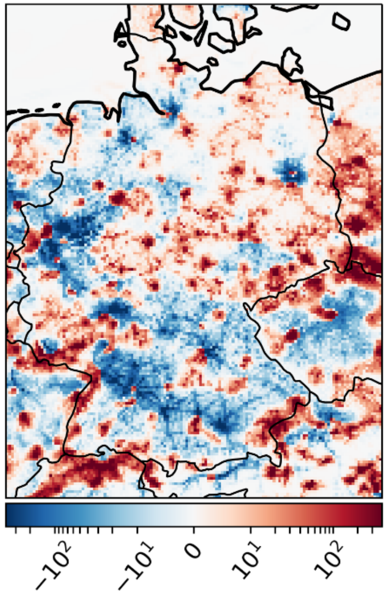
SPATIAL AND TOTAL EMISSION CORRECTIONS

National emission corrections are evaluated with respect to their horizontal distribution and national sum.

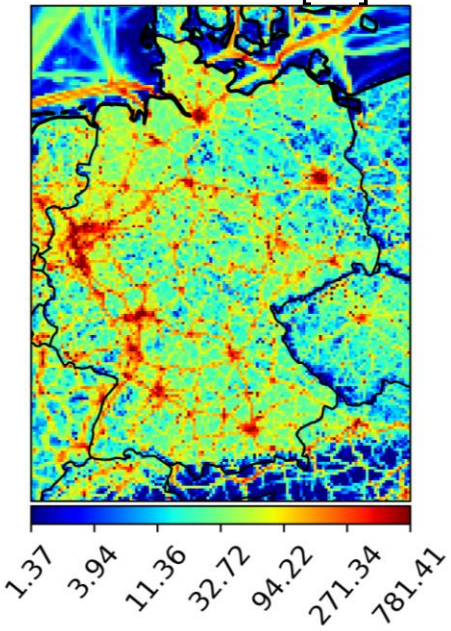
original CO emission [t/a]



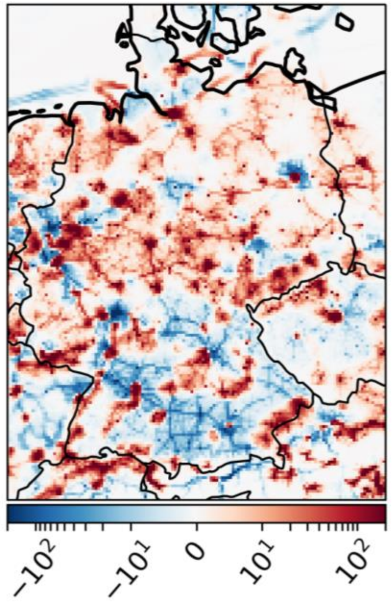
CO emission corrections [t/a]



original NO_x emission [t/a]



NO_x emission corrections [t/a]



	CO	NH_3	NO_x	PM_{10}	$PM_{2.5}$	SO_x	VOC
GRETA 2019 in [kt/a]	2869	682	1234	203	100	318	1050
	(100%)	(100 %)	(100 %)	(100 %)	(100 %)	(100 %)	(100 %)
Analysis in [kt/a]	2852	477	1421	203	102	238	1001
	(99 %)	(70 %)	(120 %)	(100 %)	(102 %)	(75 %)	(95 %)

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NO_X EMISSIONS

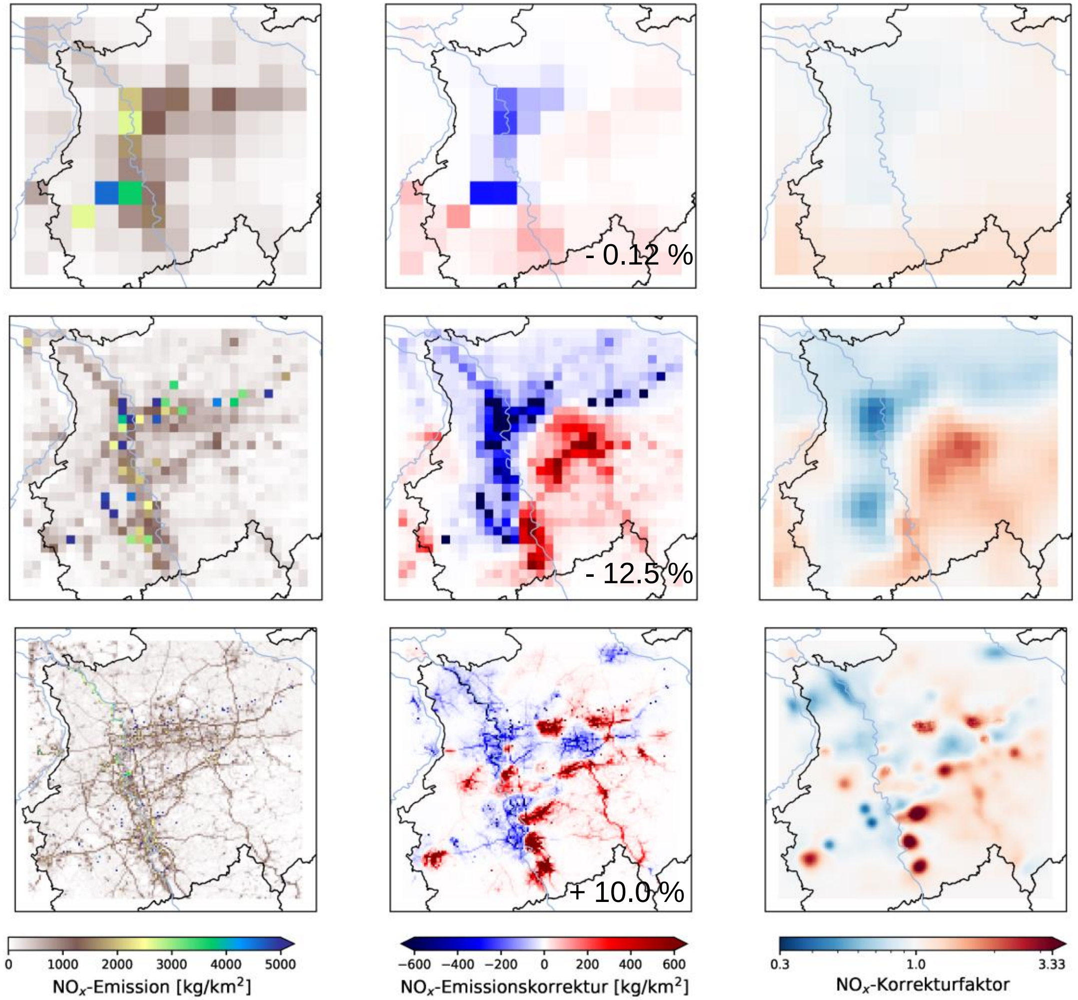
North-Rhine-Westphalia, 10-23 March 2016

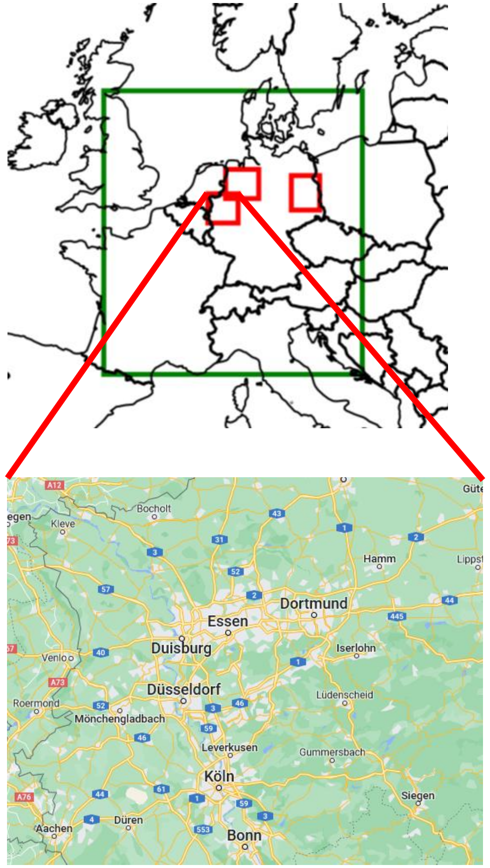
UBA emissions | analysed increments | correction factors

Coarse grid – u15
(15 km x 15 km)

Fine grid – u05
(5 km x 5 km)

Ultrafine grid – ub1
(1 km x 1 km)





google.com/maps

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POLLUTER GROUP SPECIFIC EMISSION CORRECTIONS

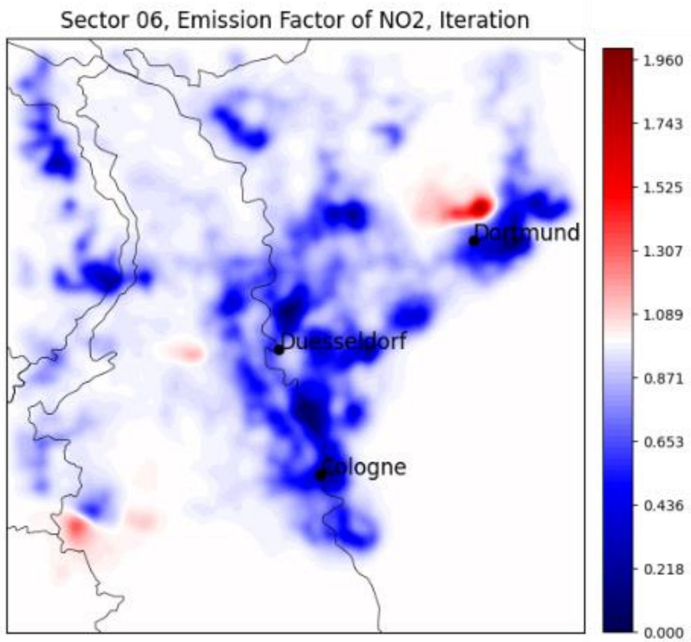
Technical implementation: augmented emission vector:

$$J(x_0,e) = J(x_0,e_1,e_2,\dots,e_{GNFR+1}) = \frac{1}{2}x^T B^{-1} x + \frac{1}{2}\sum_{i=1}^{N}(y_i - H_i M_i(x_0))^T R_i^{-1}(y_i - H_i M_i(x_0)) + \frac{1}{2}\sum_{s}^{GNFR+1} e_s^T K_s^{-1} e_s$$

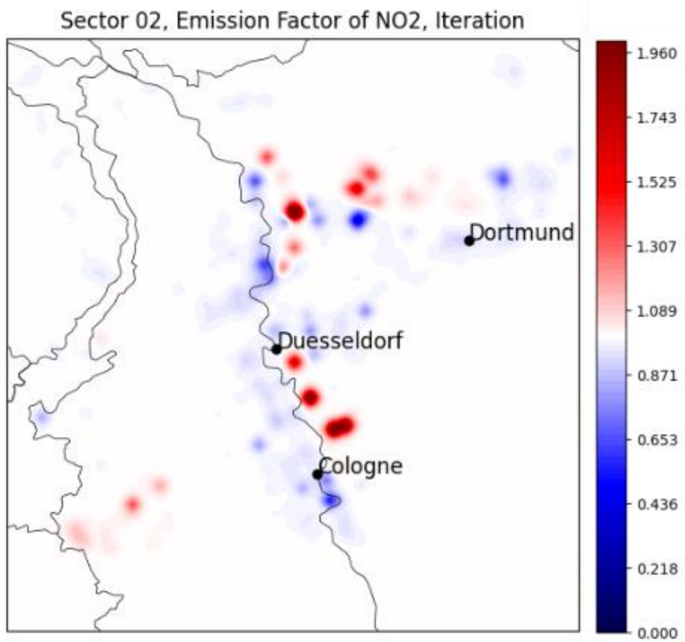
Assumption: chemical composition per polluter remains constant

→ Exploitation of spatial separation, different daily cycle, and diverse chemical composition of emissions

Road emission corrections



Industry emission corrections

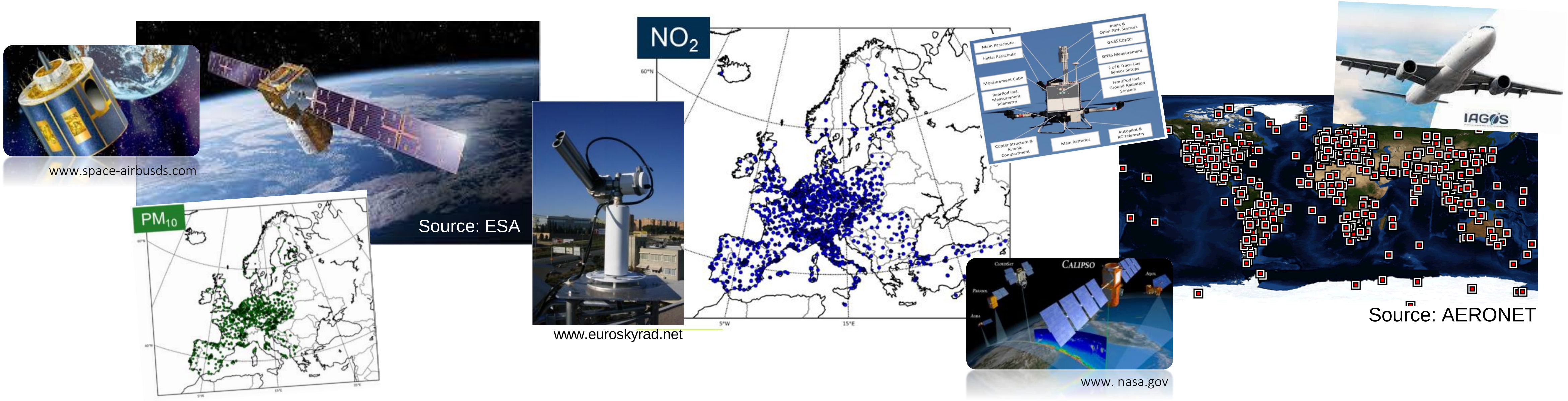


<u>Test setup</u>:
Identical twin experiment with 50% decrease of road emissions and 100 % increase of industry emissions

credit to Pascal Backes

MOTIVATION - OBSERVATION REPRESENTATIVENESS

The wealth of atmospheric constituents observation data increases constantly.
All observations have their own representativity error (mismatch between scales, observation operator error, pre-processing error).



What information gain is provided by the diverse observations?

How representative are the diverse observations for regional air quality analyses?

QUANTIFICATION OF THE GAIN AND LIMITS OF UAV OBSERVATIONS

Drone setup:

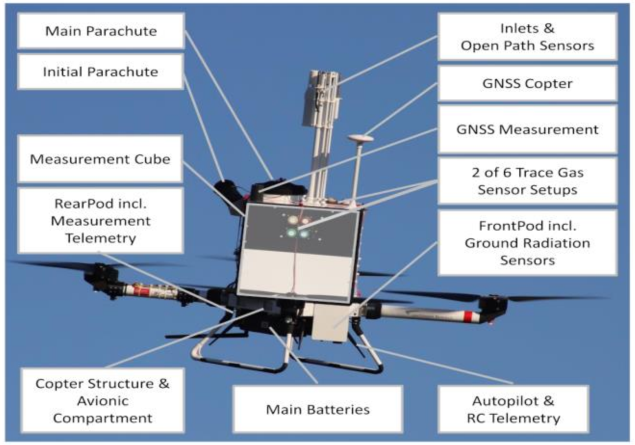


Image source : Bretschneider. L et al. Atmosphere (2022)

Two prototypes have been developed containing sensors for: Particulate matter, soot particle, NO_x, CO, and O_3, temperature, pressure, and humidity.

The advantages of UAVs:

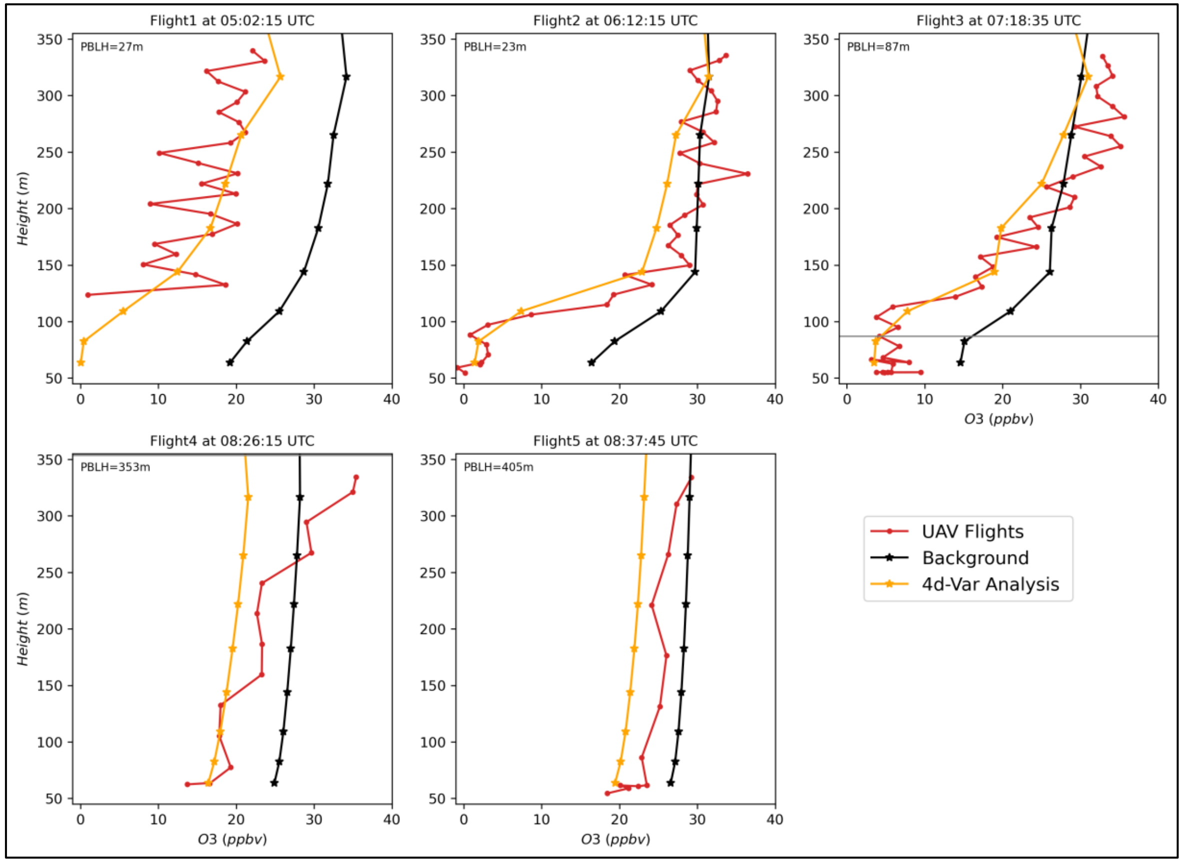
+ measure vertical profiles of atmospheric pollutants with high temporal resolution in the planetary boundary layer.

+ are flexible, inexpensive, and able to perform measurements close to emissions sources.

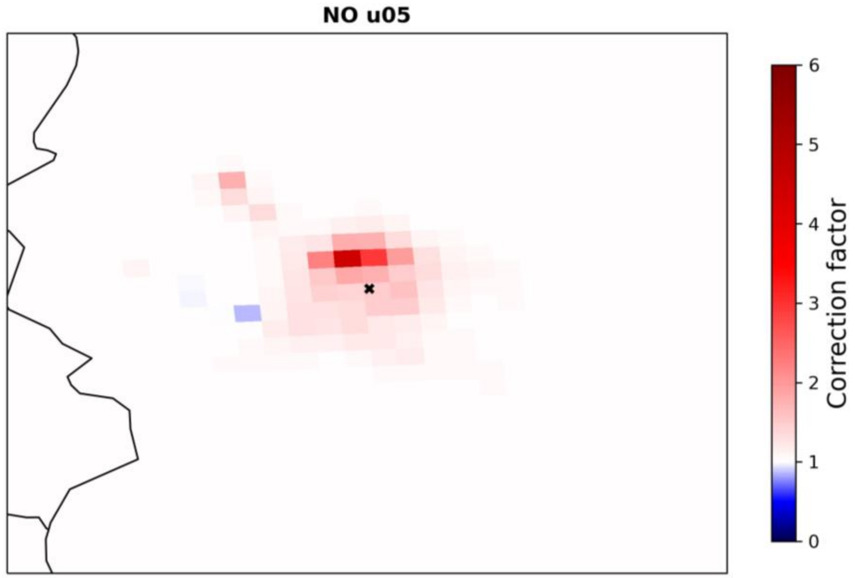
Do UAV observation data assimilation improve the representation of atmospheric constituents in the planetary boundary layer?

UAV DATA ASSIMILATION

Experiment: 4D-var Assimilation of Ozone (O_3) and Nitrogen monoxide (NO) vertical profiles.



Ozone vertical profiles measured by the drone system compared to the EURAD-IM background and 4D-var analysis in Wesseling for 23 September 2021.



Local impact: the analyzed emission factors for NO.

credit to Hassnae Erraji

HiTEC Graduate School for energy & climate

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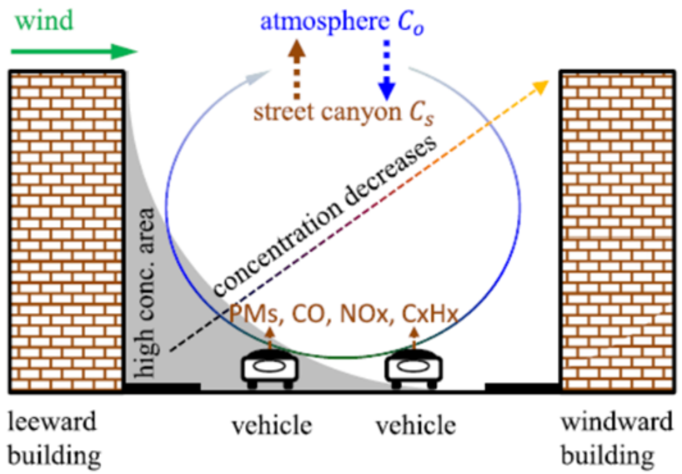
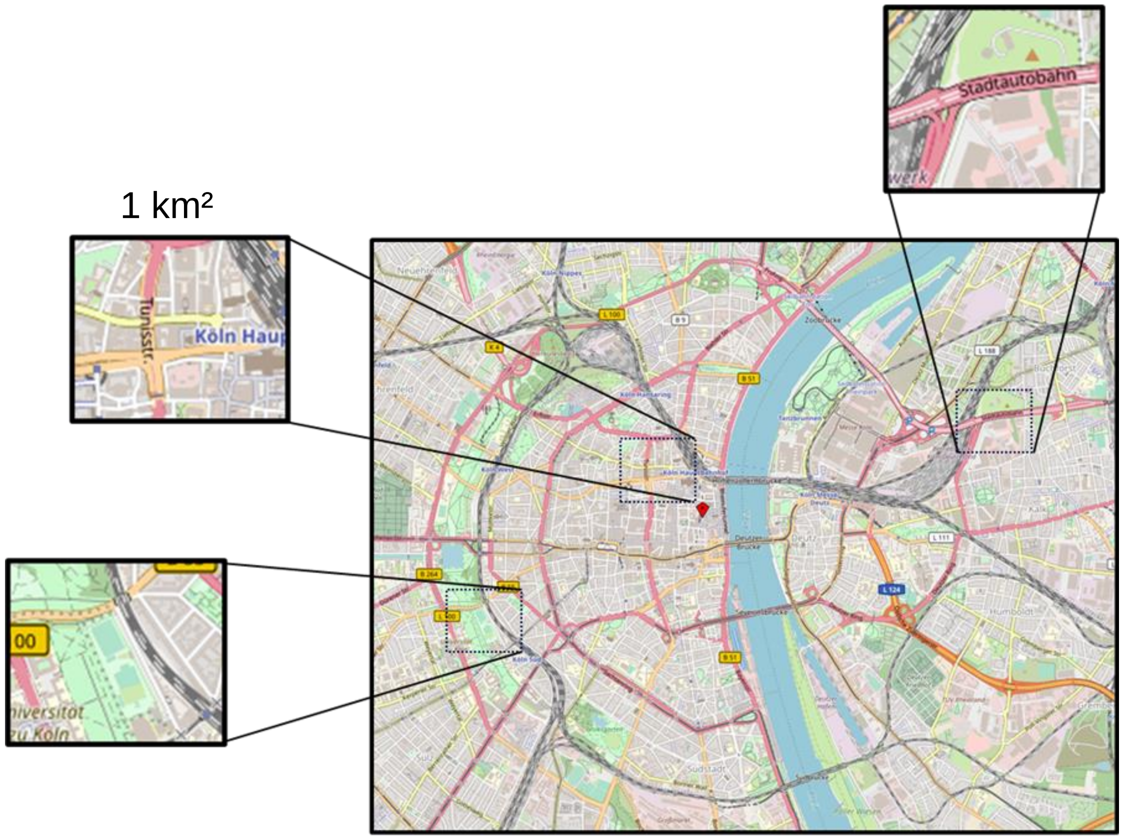
UPSCALING OF POLLUTANT CONCENTRATION FROM STREET CANYON TO REGIONAL SCALES

Inner-city observations:

- Pollutants representative for regions < 100 m
- High anthropogenic variability
- Highly depending on exact location
- In general, excluded from regional DA analyses

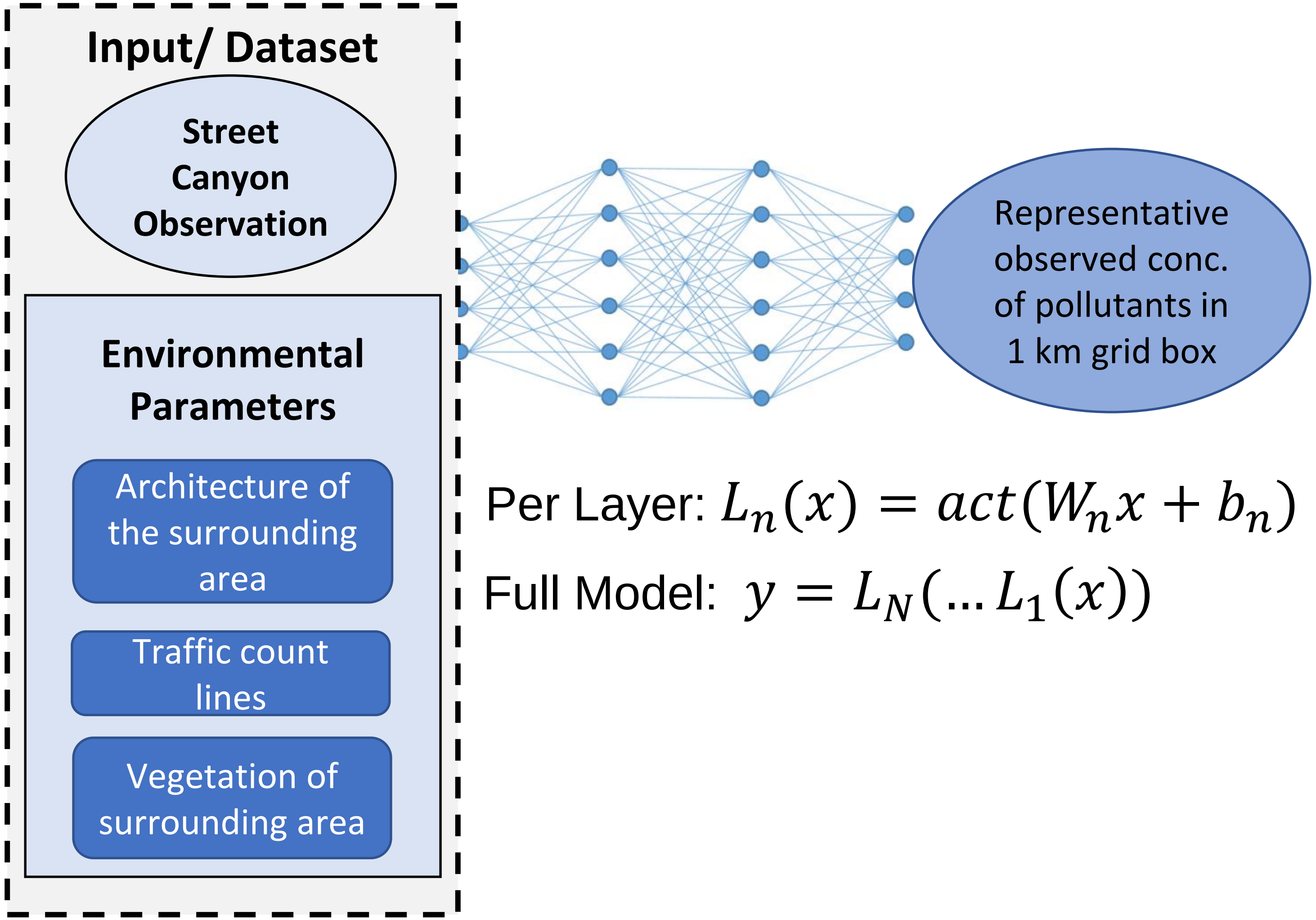


Scheme of Street Canyon
Ai, Z T, and C M Mak. "From street canyon microclimate to indoor environmental quality in naturally ventilated urban buildings: Issues and possibilities for improvement." *Building and environment* vol. 94 (2015): 489-503. doi:10.1016/j.buildenv.2015.10.008



Open street view

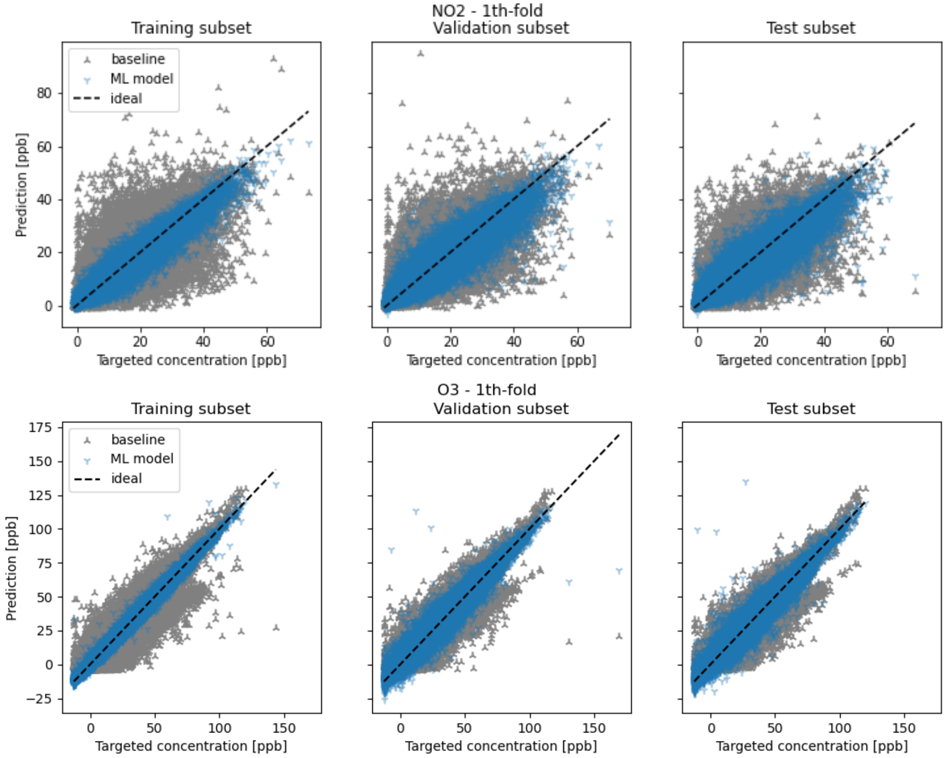
ENVIRONMENT INFORMED UPSCALING WITH NEURAL NETWORKS



Per Layer: $L_n(x) = act(W_n x + b_n)$

Full Model: $y = L_N(\dots L_1(x))$

First results in test environment, upscaling from 1 km to 3 km grid resolution



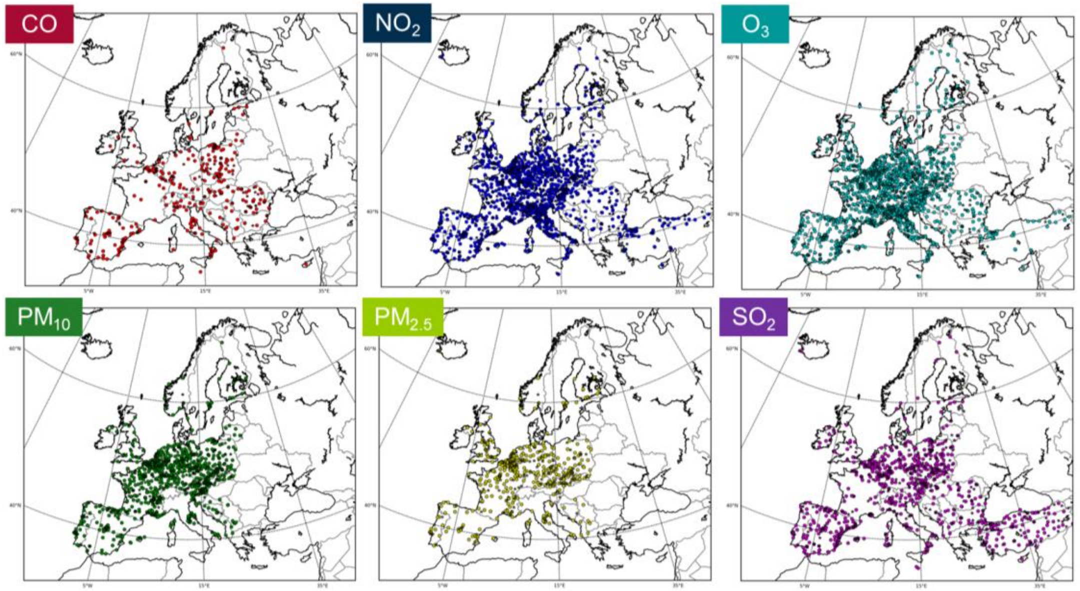
credit to Charlotte Neubacher

OPTIMAL DATA ACQUISITION FOR INITIAL VALUE AND EMISSION OPTIMIZATION

First challenge: To find the optimal split of observation data in assimilation and validation data sets

Method: Characterize observations based on intrinsic properties using clustering algorithms

- **CD:** K-means clustering based on mean and variance of annually averaged diurnal cycles
- **KSC:** K-means soft constraint clustering combining CD criteria with geographic location.

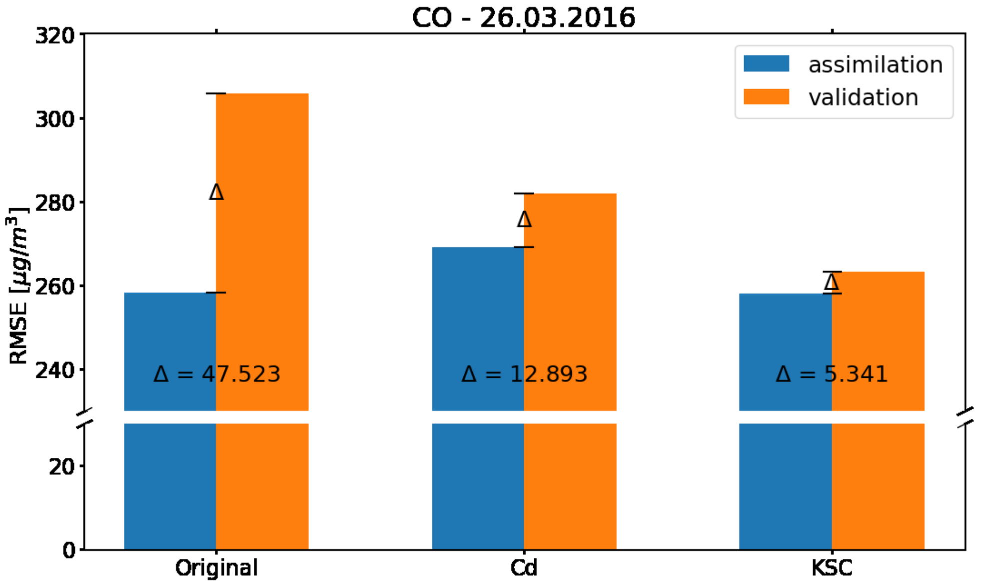


EEA ground-based observation stations

KSC cluster optimization function:

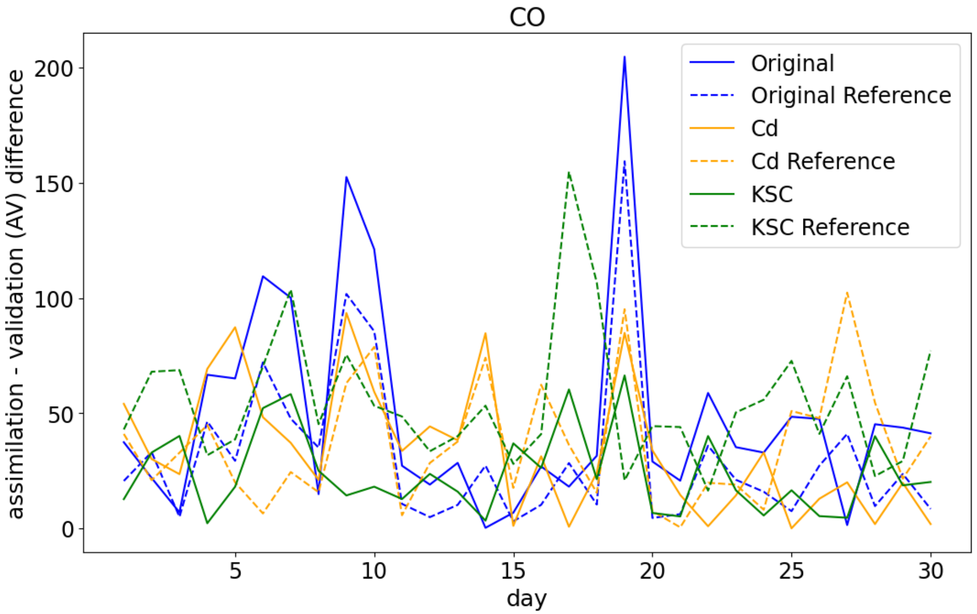
$$C := \operatorname{argmin}\left((1-\omega)\frac{\operatorname{dist}(d, C_i)^2}{V_{max}} + \omega\frac{CV_d}{CV_{max}}\right)$$

COMPARISON BETWEEN CD AND KSC SPLIT



4D-var assimiliation of all EEA ground-based stations for March 2016.

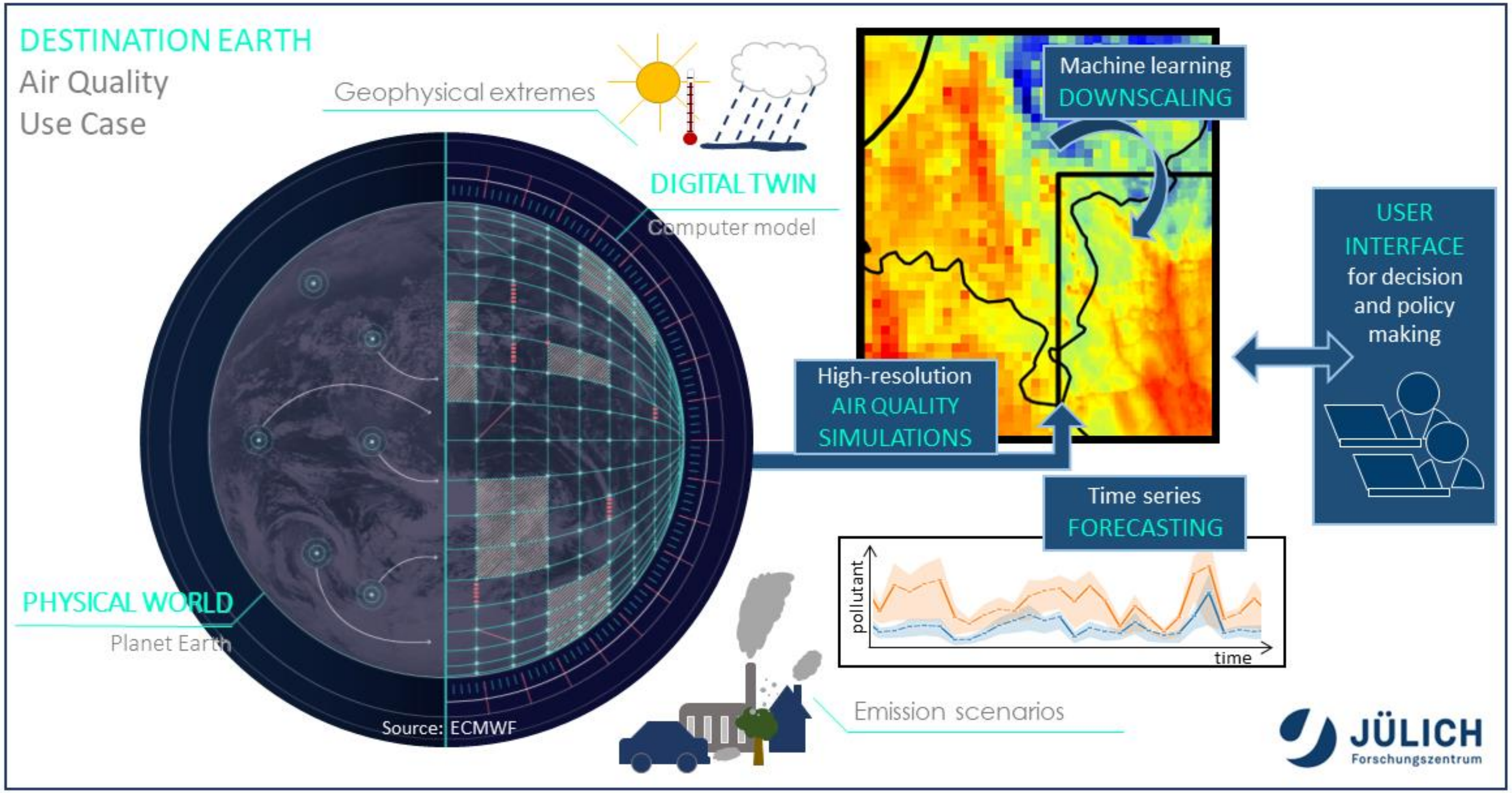
clustering method	mean AV diff
Original	48.80
CD	34.00
KSC	24.03



clustering method	var AV diff
Original	2087.22
CD	755.62
KSC	312.36

credit to Alexander Hermanns

DESTINATION EARTH USE CASE ON AIR QUALITY



Funded by the European Union Destination Earth implemented by ECMWF esa EUMETSAT

CONCLUSIONS

How representative are annual emission inventory data for good air quality forecasting?

- EURAD-IM 4D-var analysis with emission optimization allows for the assessment of uncertainties in the emission inventory data sets
- Emission optimization is performed assessing the spatial distribution of emissions – the temporal evolution partly constrained by the time profiles implemented in the model
- Emission correction factors can be obtained species-wise or for individual emission sectors
- The adjoint model enables the correction of unobserved atmospheric constituents

What information gain is provided by the diverse observations?
How representative are the diverse observations for regional air quality analyses?

- UAV observations provide valuable information to the assimilation system due to the detailed profiling of the planetary boundary layer
- Neural Networks can overcome the representativeness of different scales
- Data science can support the optimal acquisition of observational data for air quality analysis

THANKS TO

My co-authors and collaborators

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The audience for your attention!