Co-assimilation of NH_3 and NO_2 satellite observations

with the LETKF methodology in the LOTOS-EUROS model

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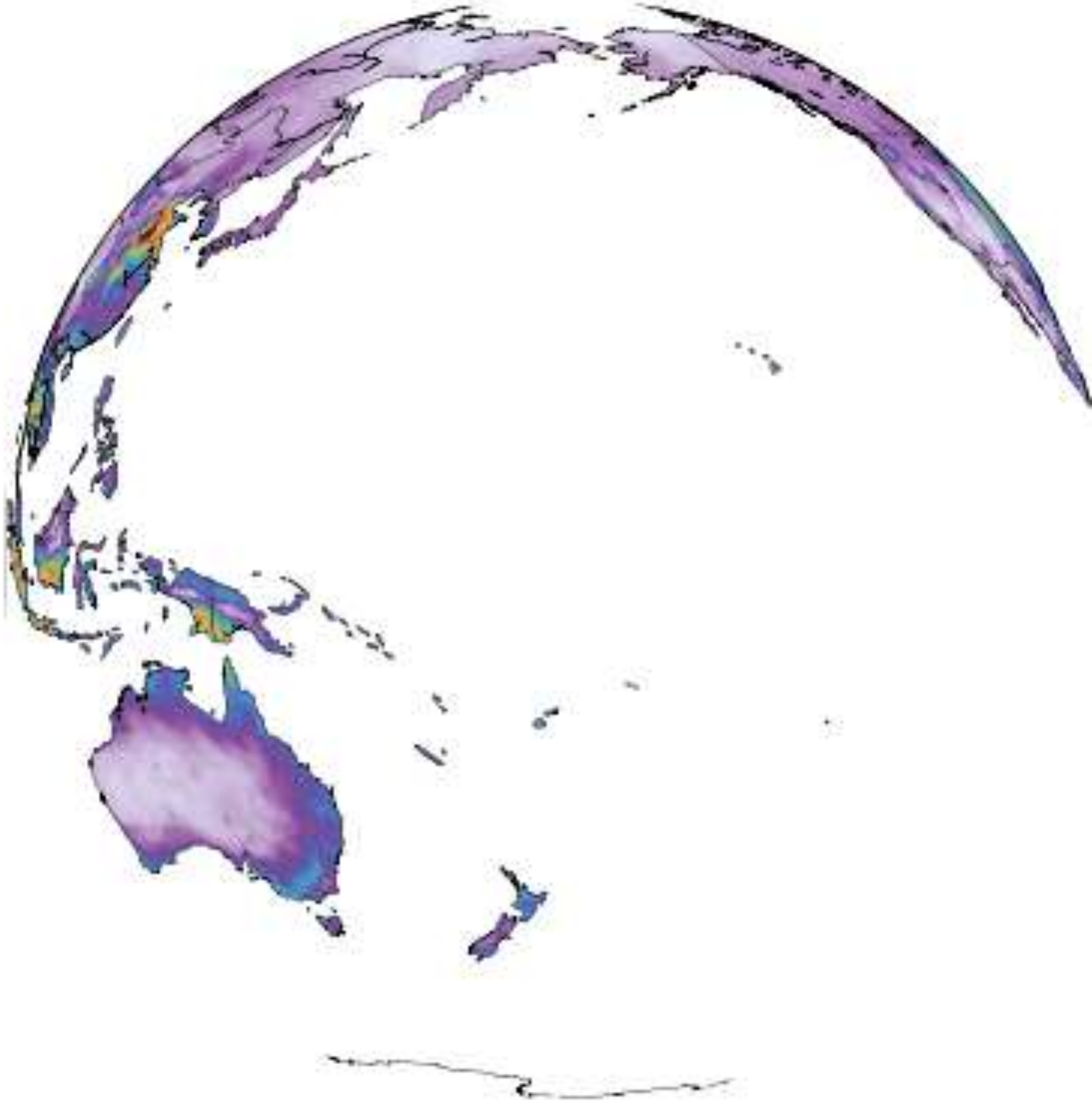
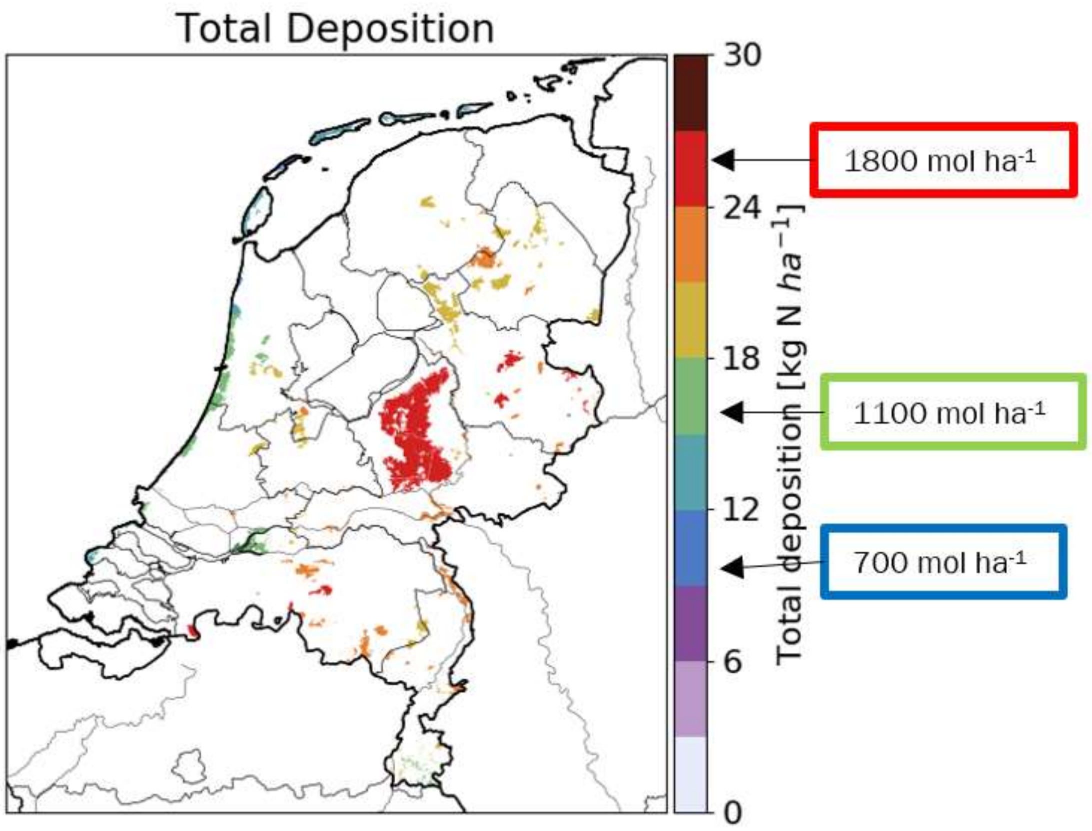
H. Eskes | KNMI

And many more

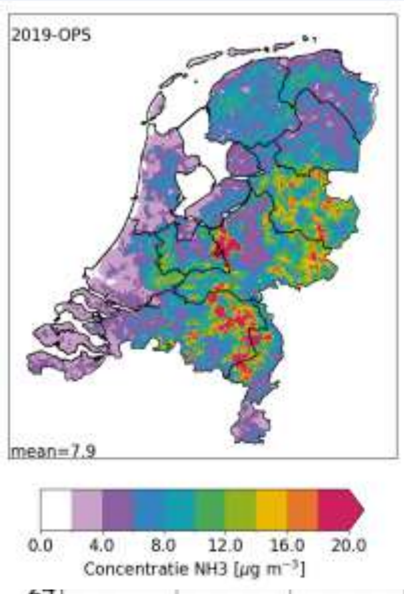


Introduction – The Nitrogen Problem

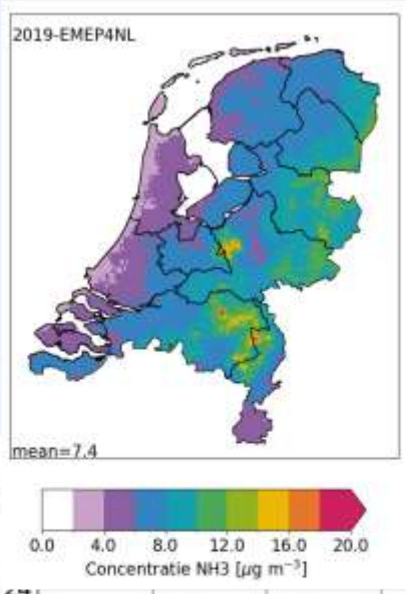


Introduction – Modelling Nitrogen Deposition

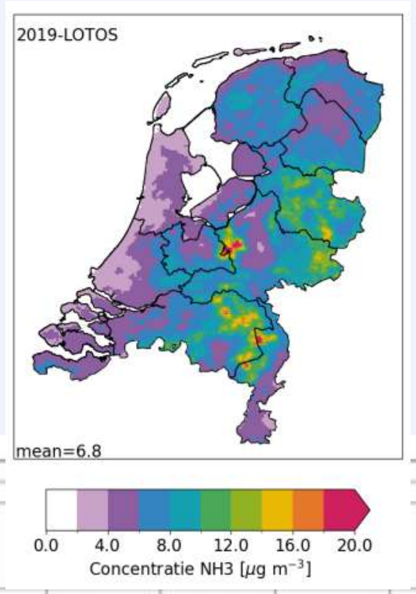
WIP



All three models show an overestimation in the east

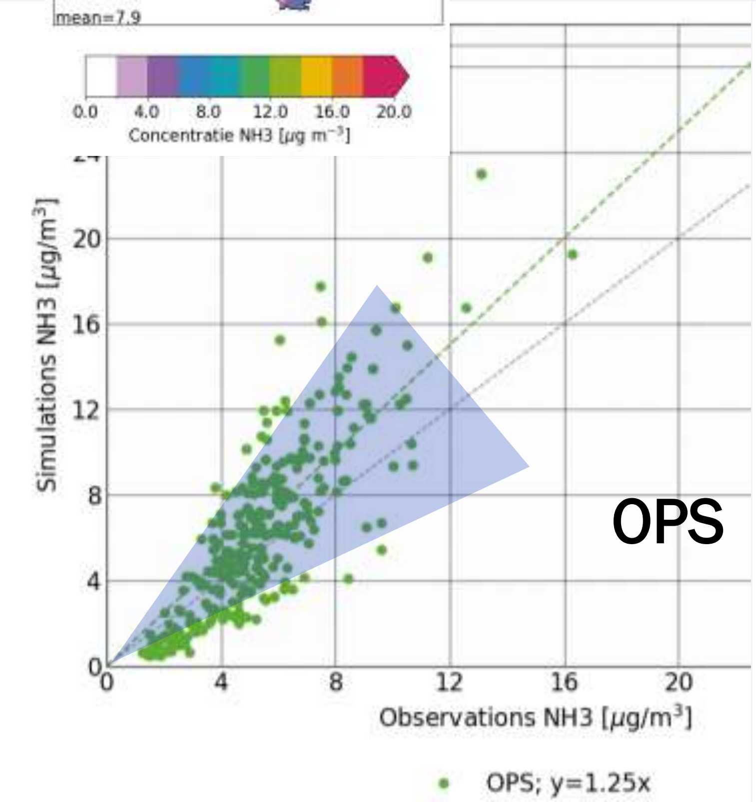


At the same time give an underestimation in the west

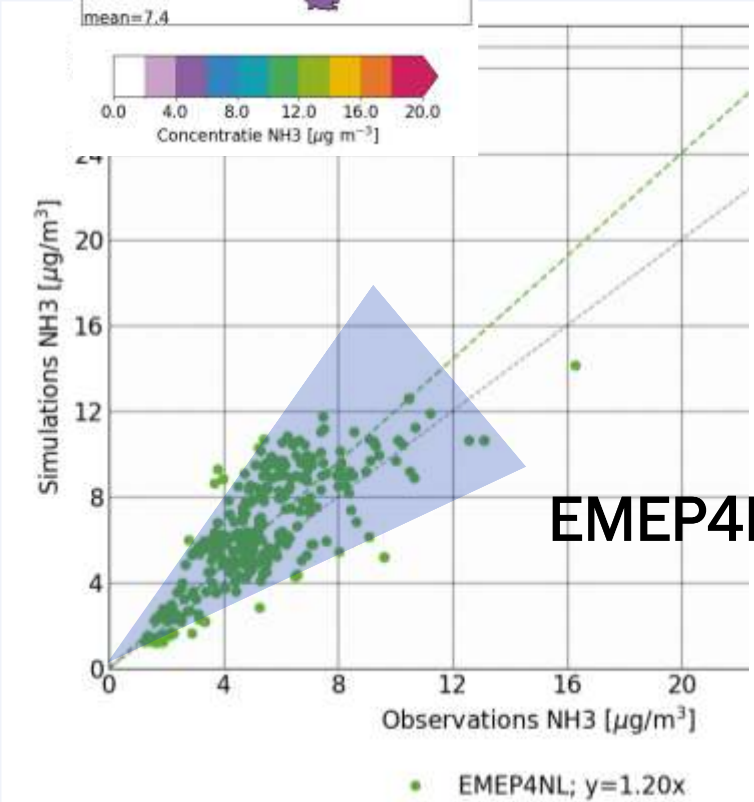


Note that most of the MAN locations are within Natura 2000 zones, away from the hotspots

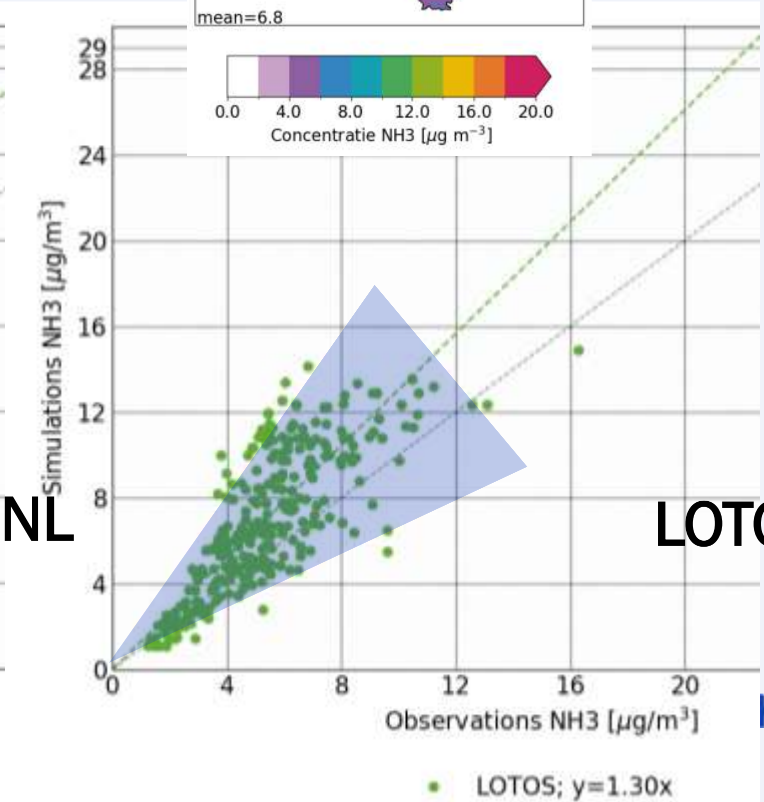
NKS



OPS



EMEP4NL

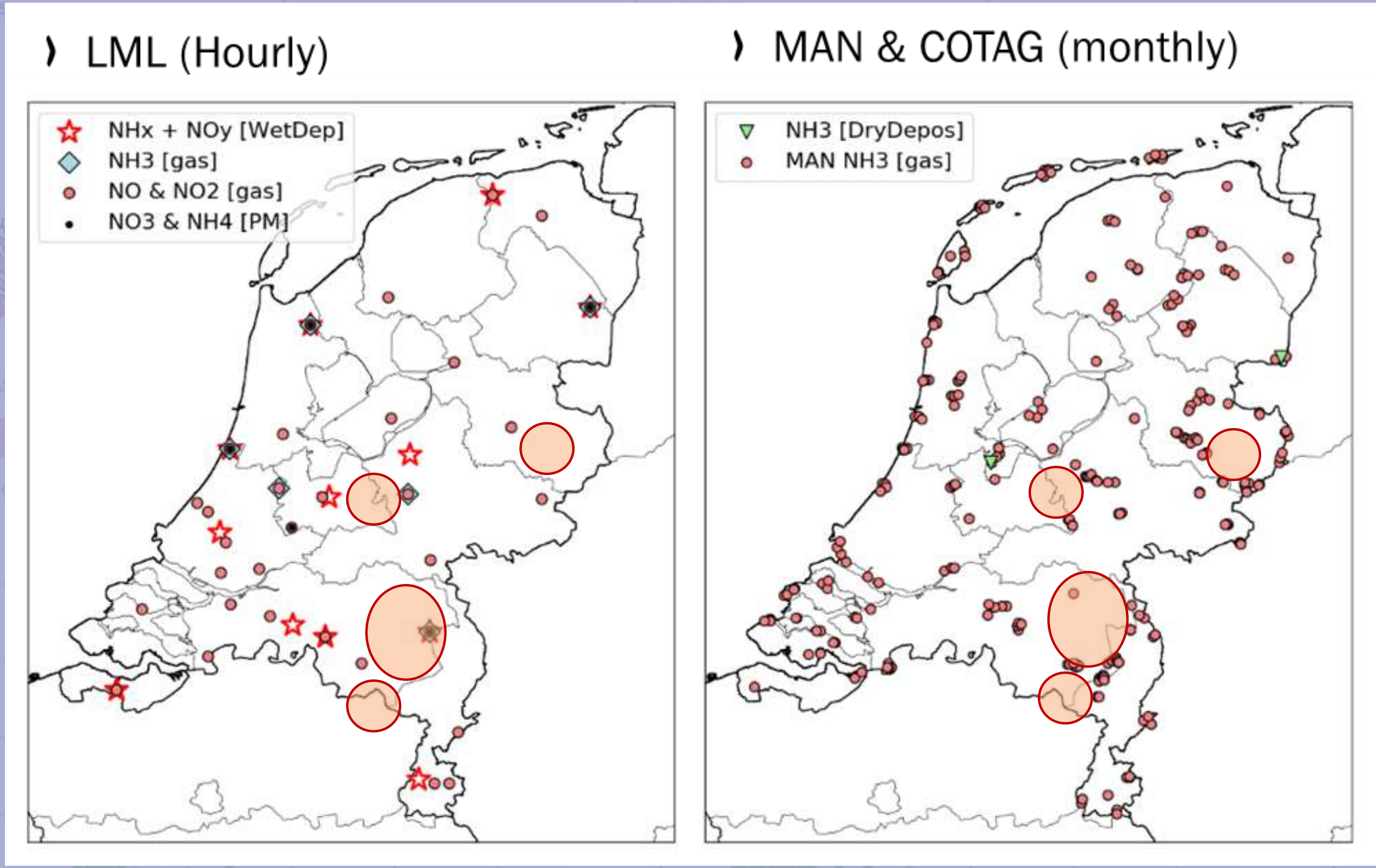


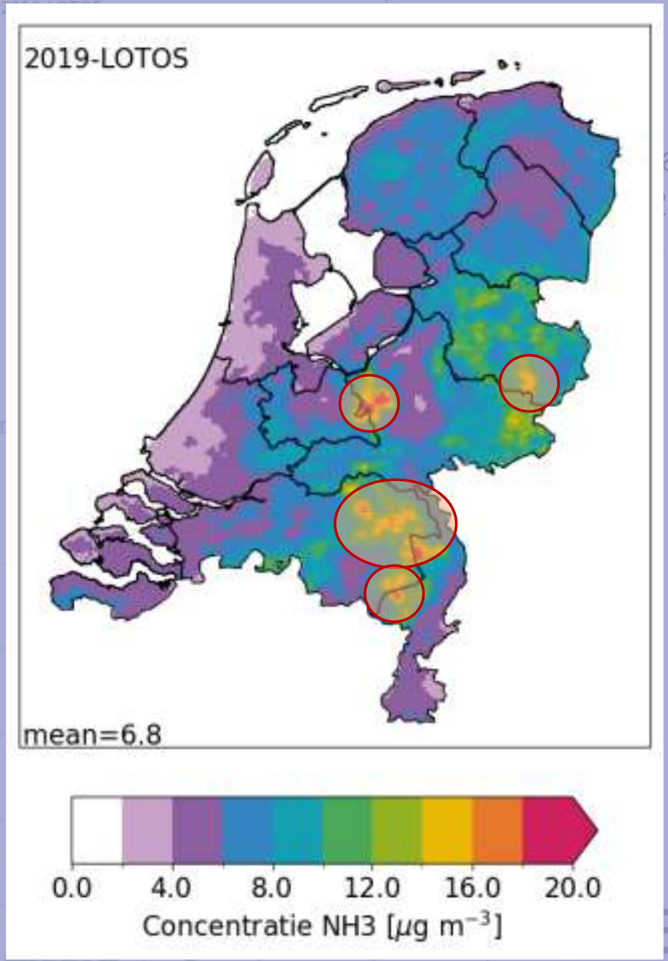
LOTOS-EUROS

innovation for life

Introduction – Modelling Nitrogen Deposition

WIP





Observations NH3 [μg/m³]

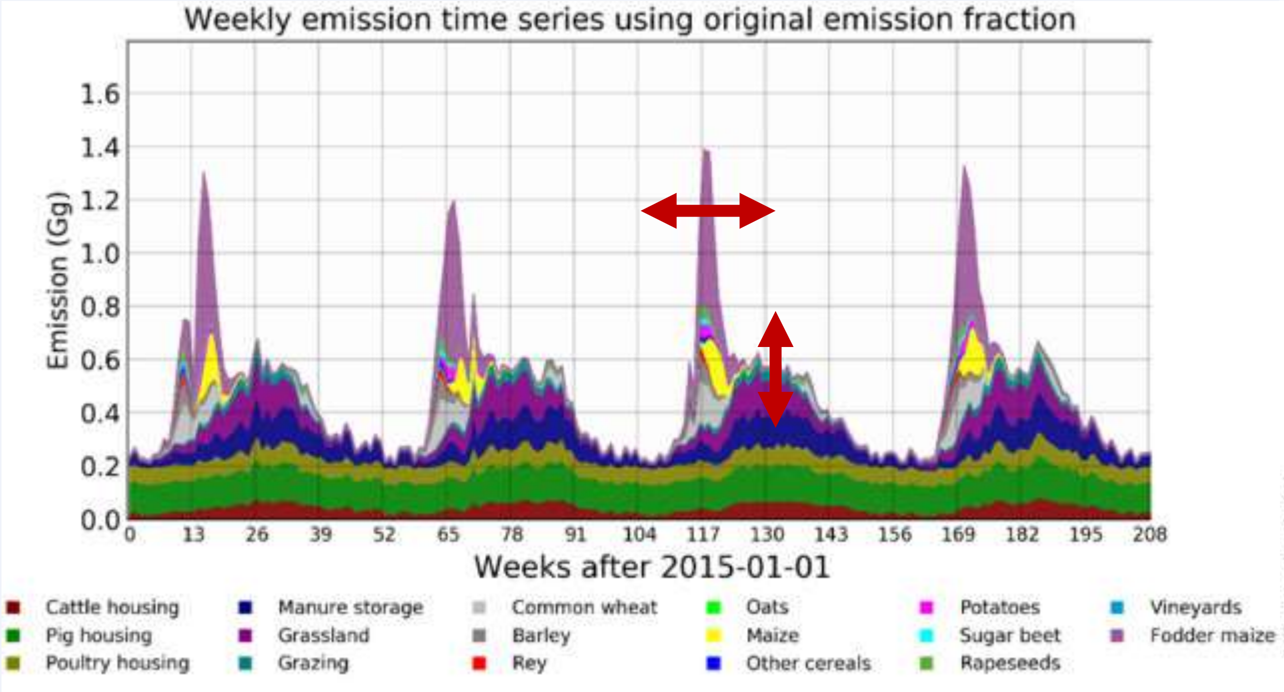
OPS; y=1.25x

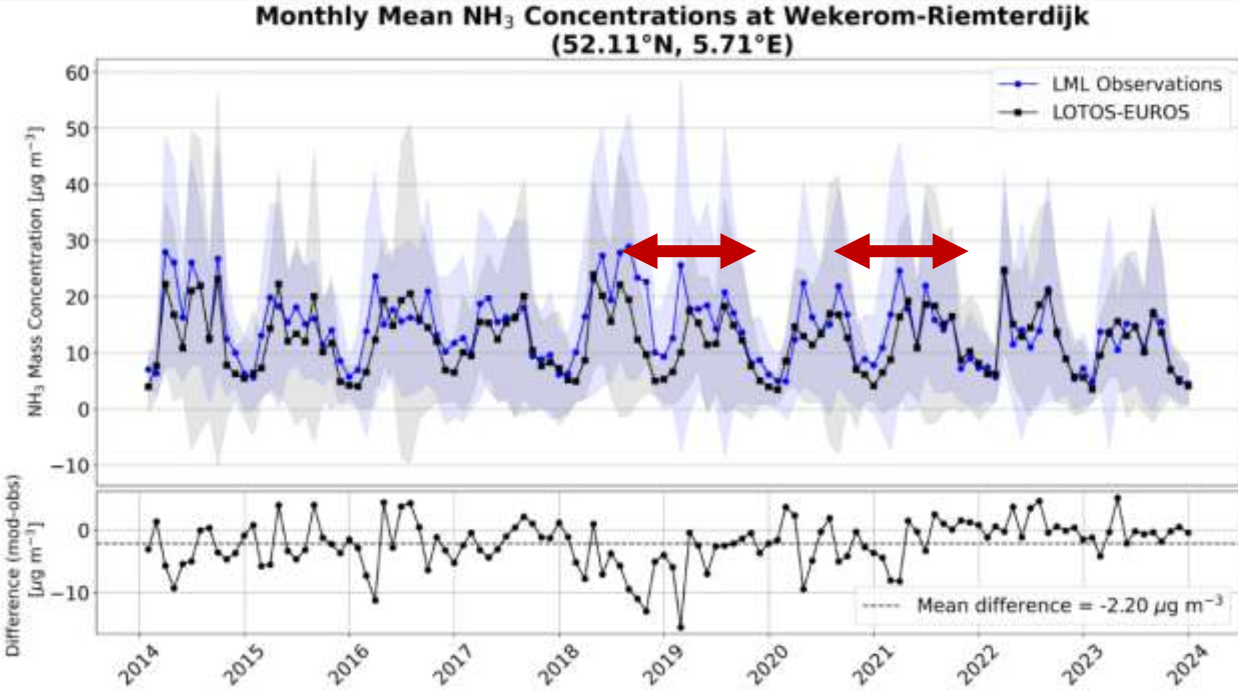
EMEP4NL; y=1.20x

LOTOS; y=1.30x

Introduction – Modelling Nitrogen Deposition

WIP





So what role can satellites play?

Introduction – NKS

Project NKS/SAGEN

Project ministry LNV: 4 years

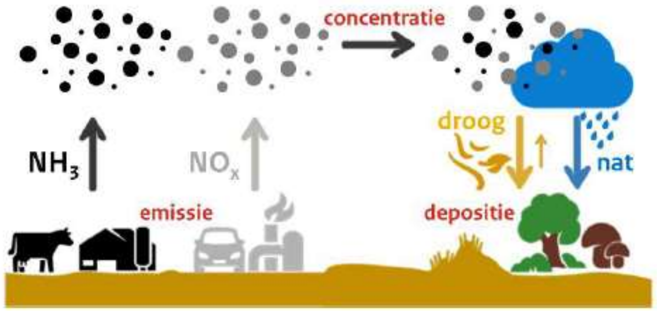
Goal

- Investigation of the possibilities of the use of **satellite data** and **ensemble modelling** for improving models for nitrogen deposition

Over arching goals

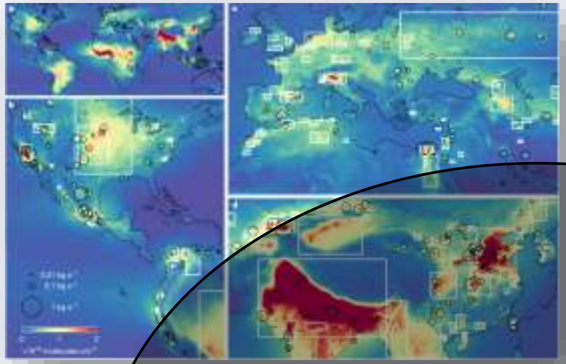
- Improve knowledge nitrogen deposition and modelling
- Collaboration in NL
- Sharing knowledge
- Improve transparency and support base

Scientific research: AIO, postdocs, publications

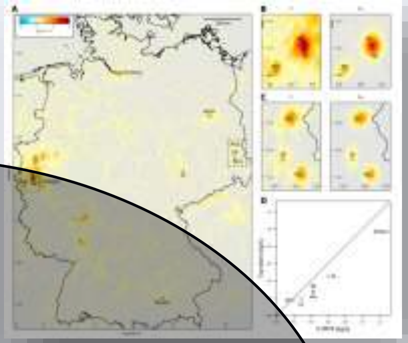


Introduction – Methods for emission estimates

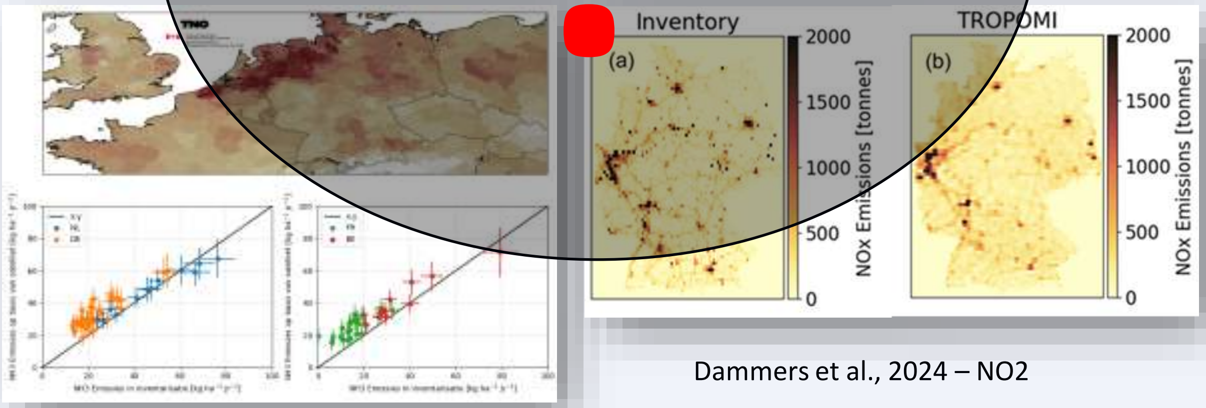
Mass-balance & plume-based methods



Van Damme et al., 2018 – NH3

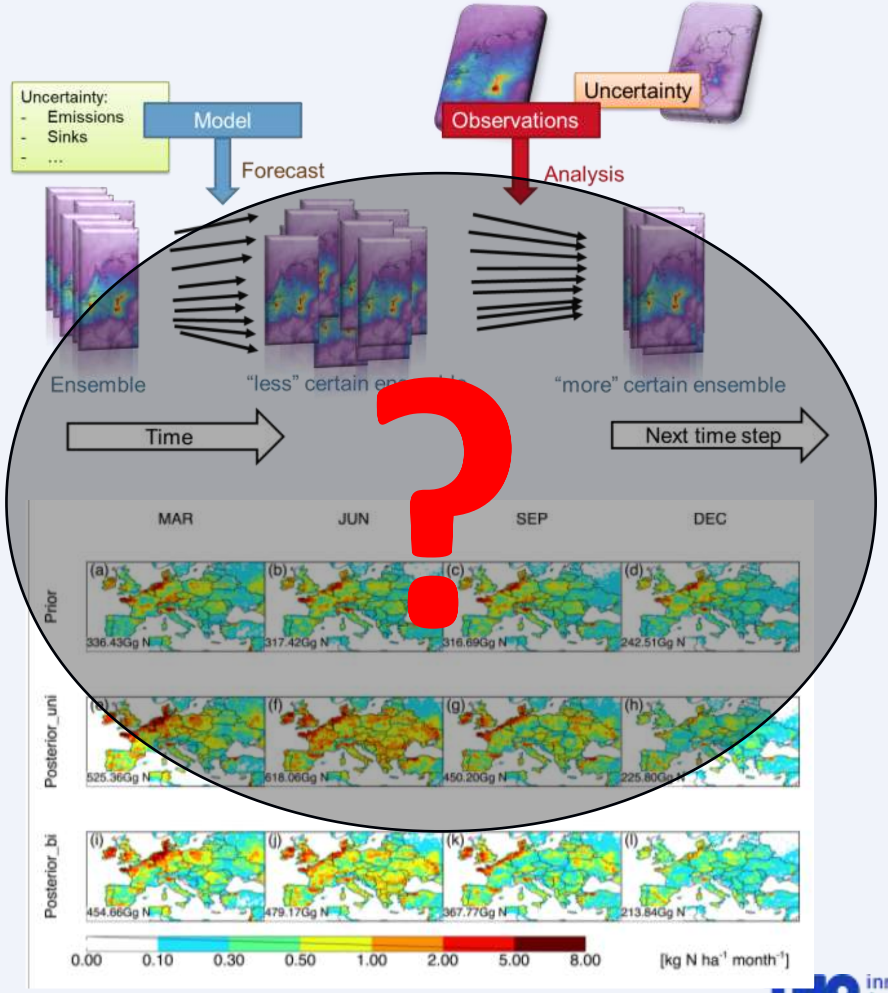


Beirle et al., 2019 – NO2



Dammers et al., 2024 – NO2

LETKF / 4D-EnVar etc methods



Cao et al., 2022 – NH3

Introduction – Local Ensemble Transform Kalman Filter

Important parameters (current "*optimum*" for system):

Temporal correlation

NH_3: *3 days*

NOx: *1 day*

Spatial correlation (gaussian)

NH_3: 15 km – IASI A+B+C (~9:30) + CrIS1+2 (~13:30)
NO_2: 5 km – TROPOMI (~13:30)

Amount of variation allowed on emissions:

Mean at *1.0* + standard deviation *0.5*

Other:

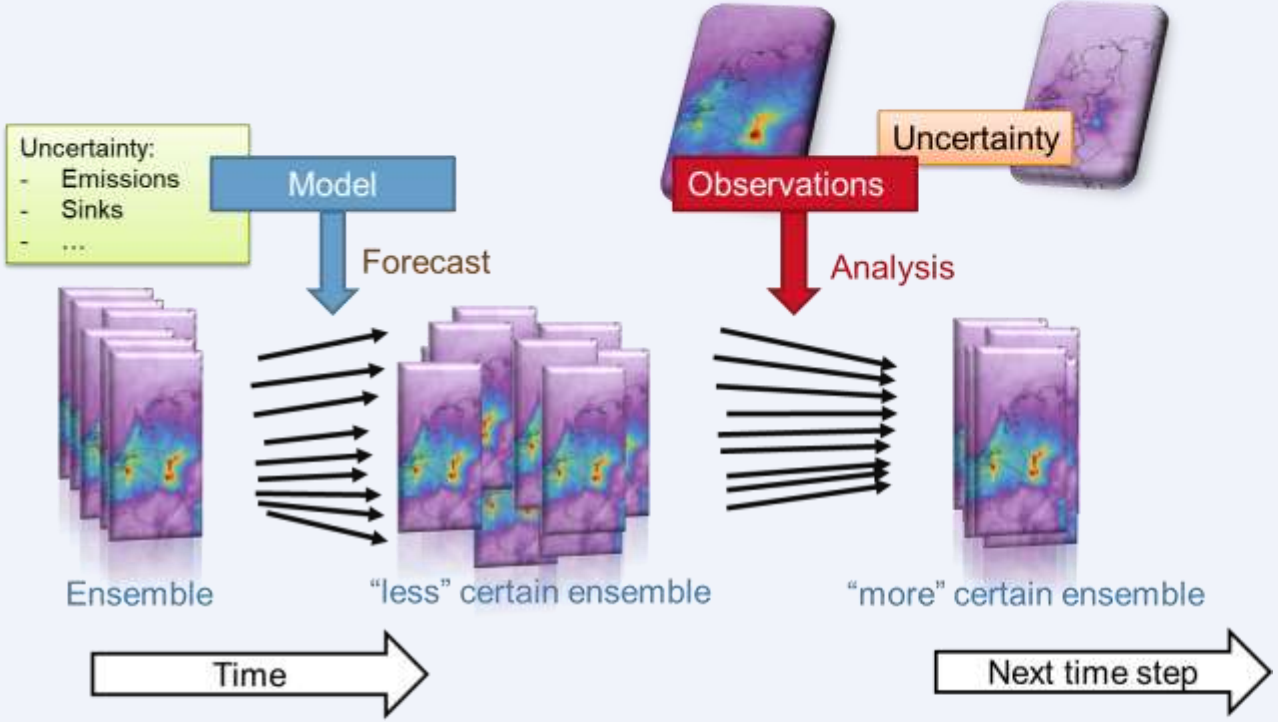
LOTOS-EUROS v2.2.003

NW Europe + Iberian Peninsula 7x7km2

Emissions: CAMS-REGv5.1 + ER (NL) + GrETa (Germany)

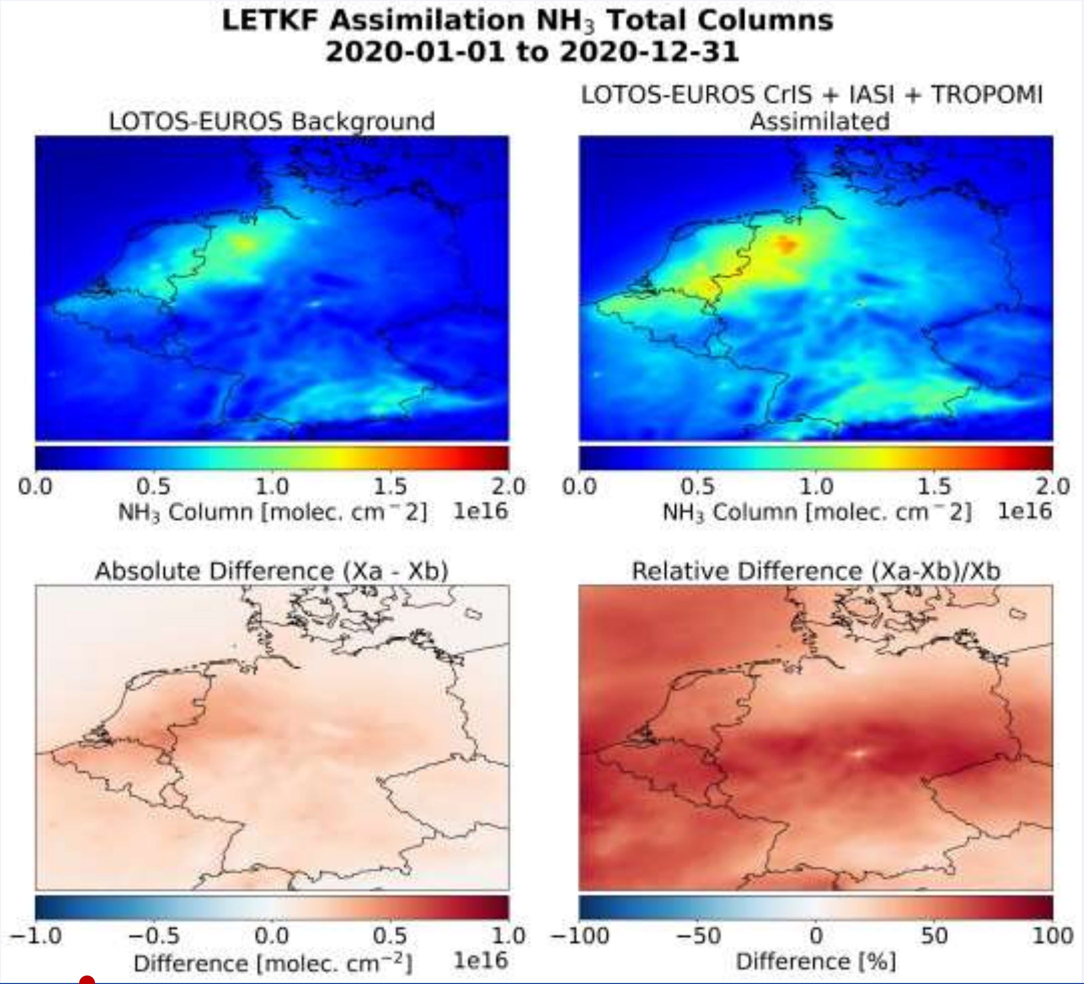
Timing: TEMPO + further detailing NH_3 temporal allocation

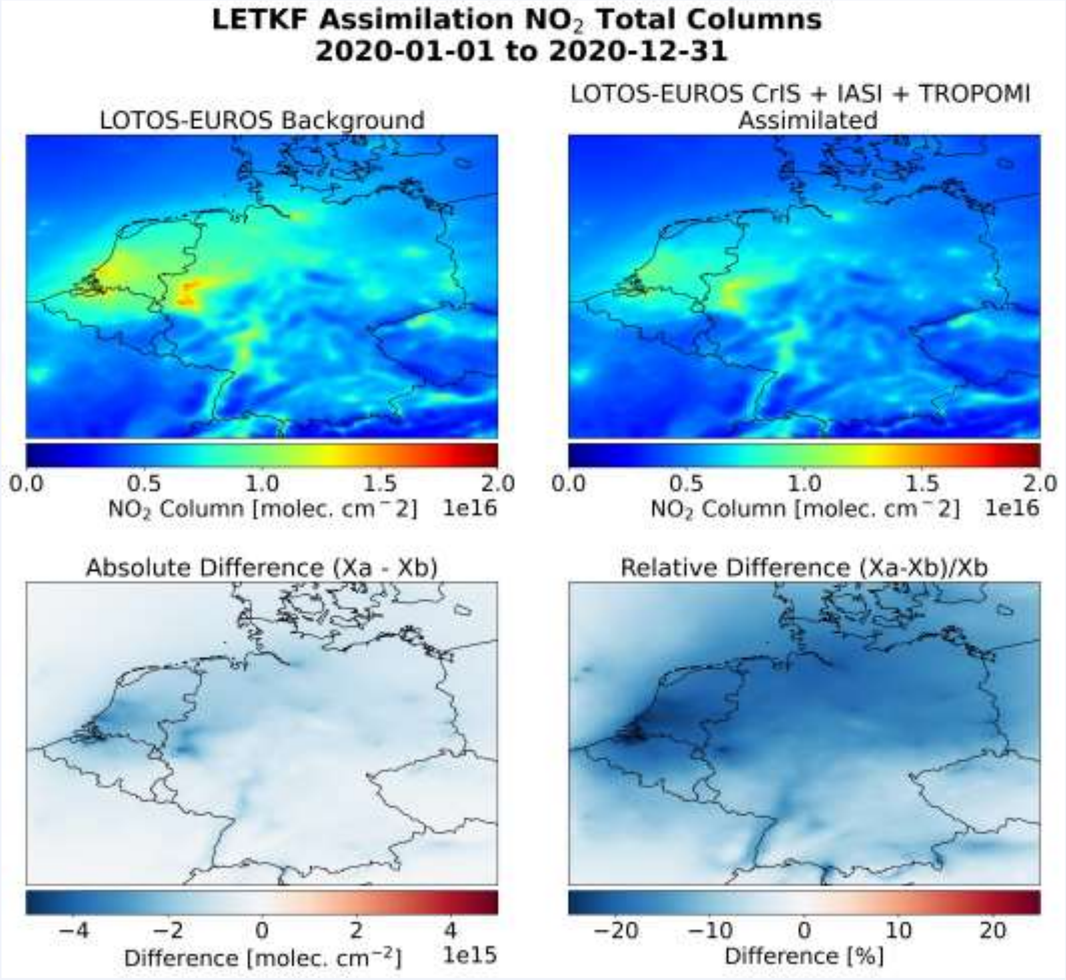
BC: CAMS IFS



Results – Column level changes + emission totals

	NL-base	NL-LETKF	GER-base	GER-LETKF
NH_3	124kt	150kt	574kt	695kt
NOx	258kt	187kt	1216kt	1046kt

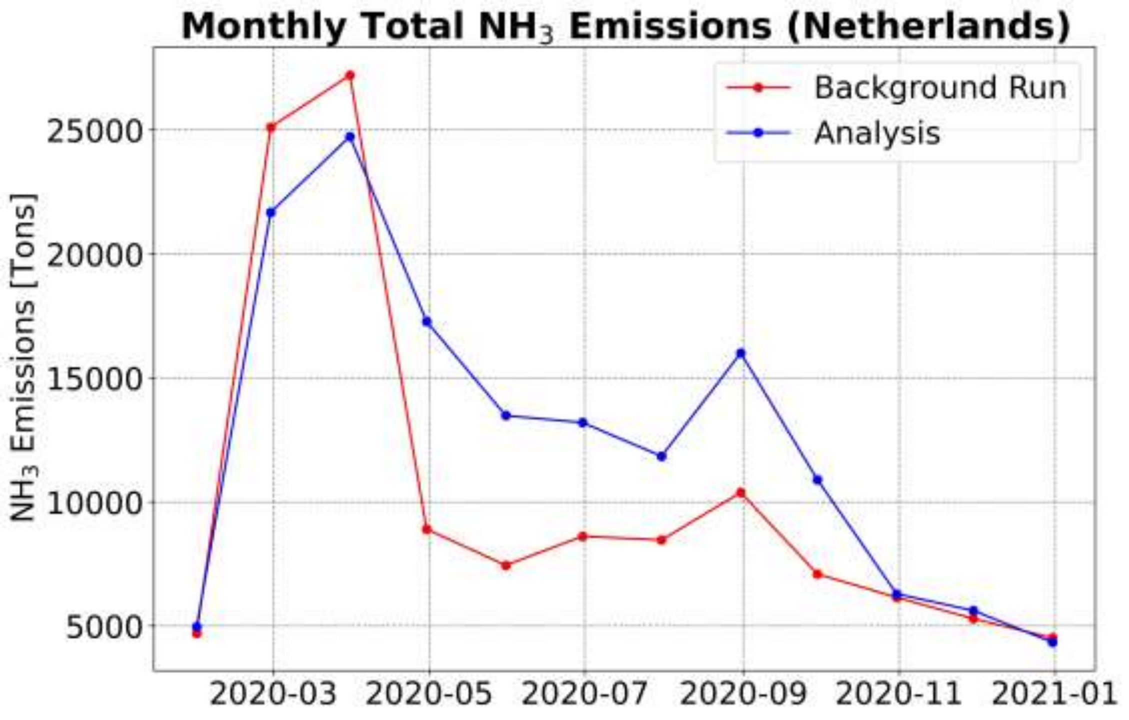


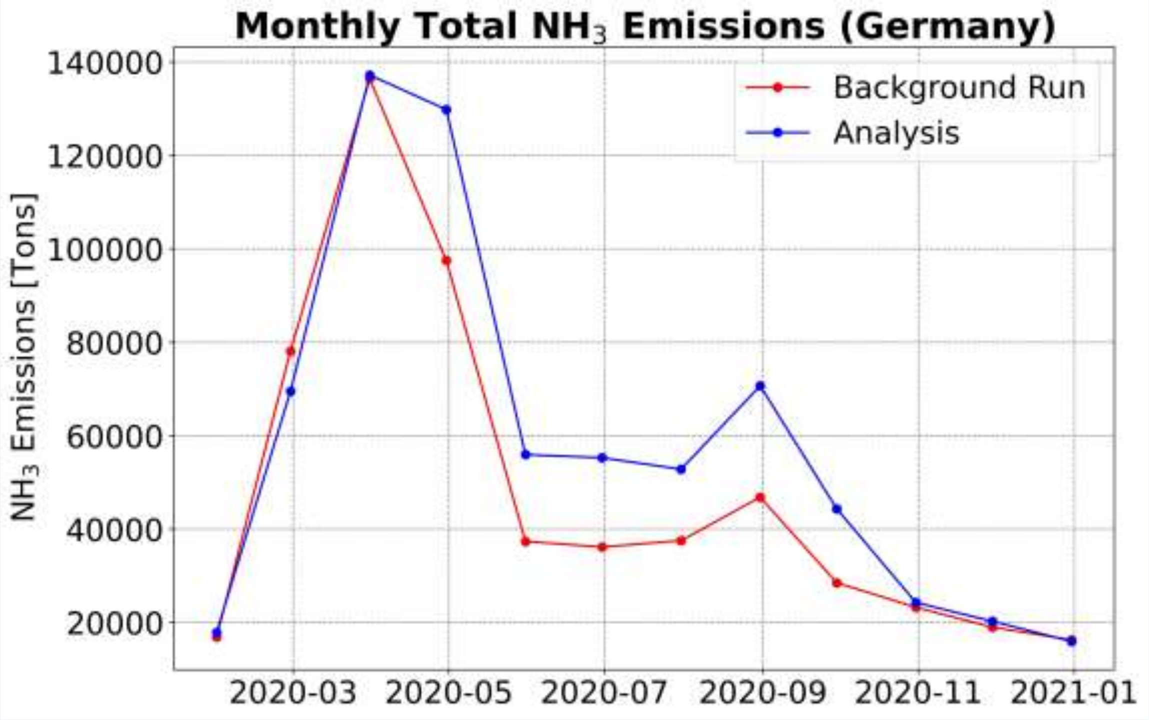


2020 NOx: COVID restrictions + overall decreasing in NOx over last decade – Lower emissions

2020 NH3: Higher than average temperatures, exceptional sunny Spring + longer lifetimes decreasing NOx/HNO3

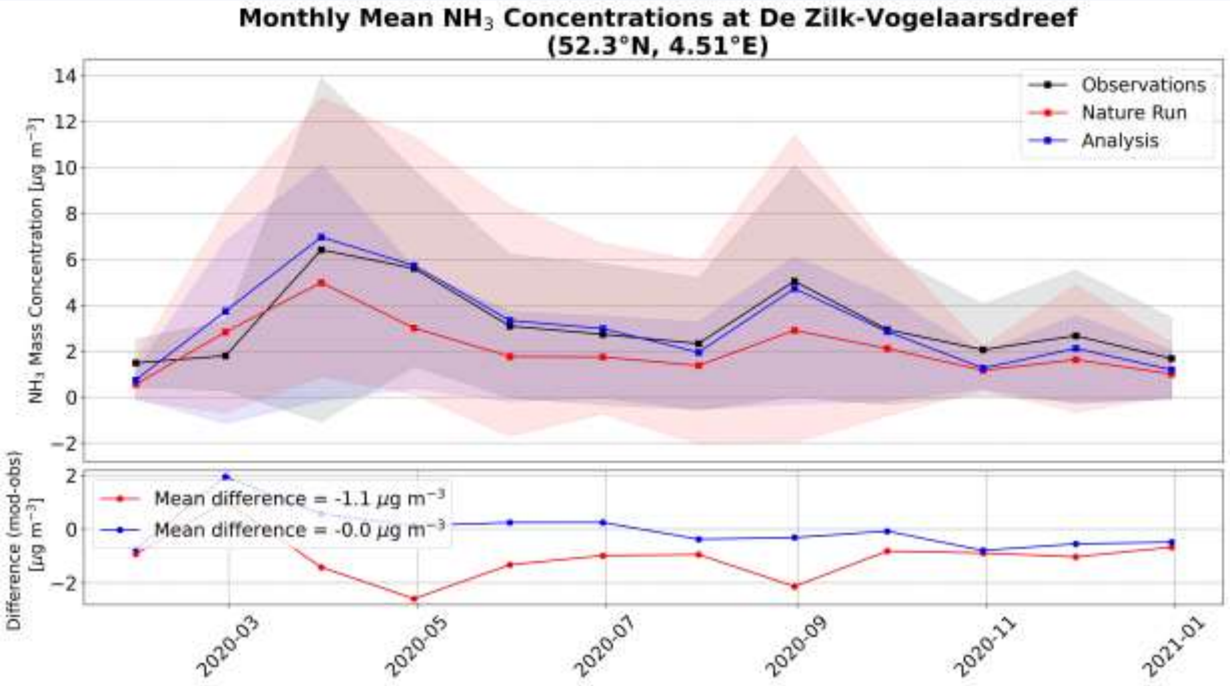
Results – Monthly emission totals



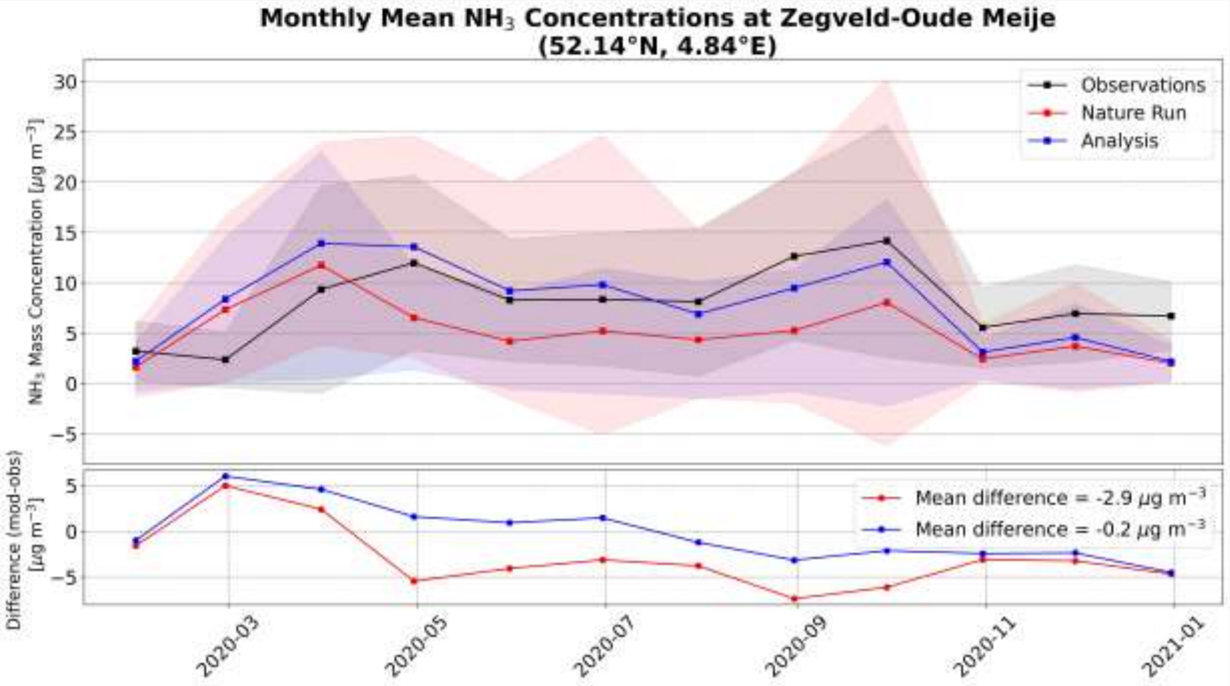


Shift from spring emissions to summer. Higher total emissions, as expected from increased temperatures, increasing volatilization of NH_3

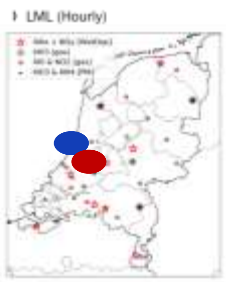
Results – Surface Concentrations - Temporal



Coastal



Inland



Large improvement in Mean Bias
Seasonal cycle generally well captured
Differences in winter months / early spring (Zegveld)

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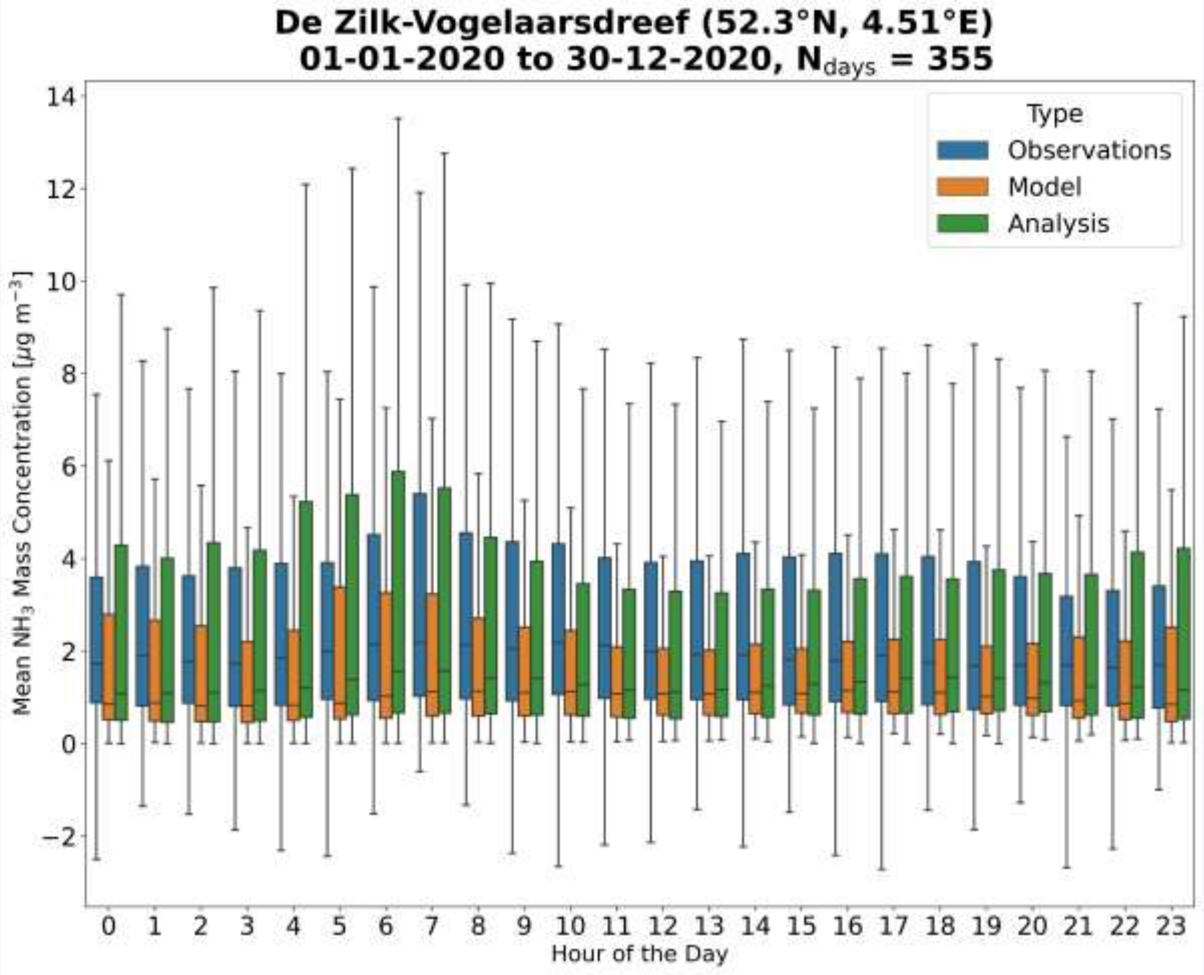
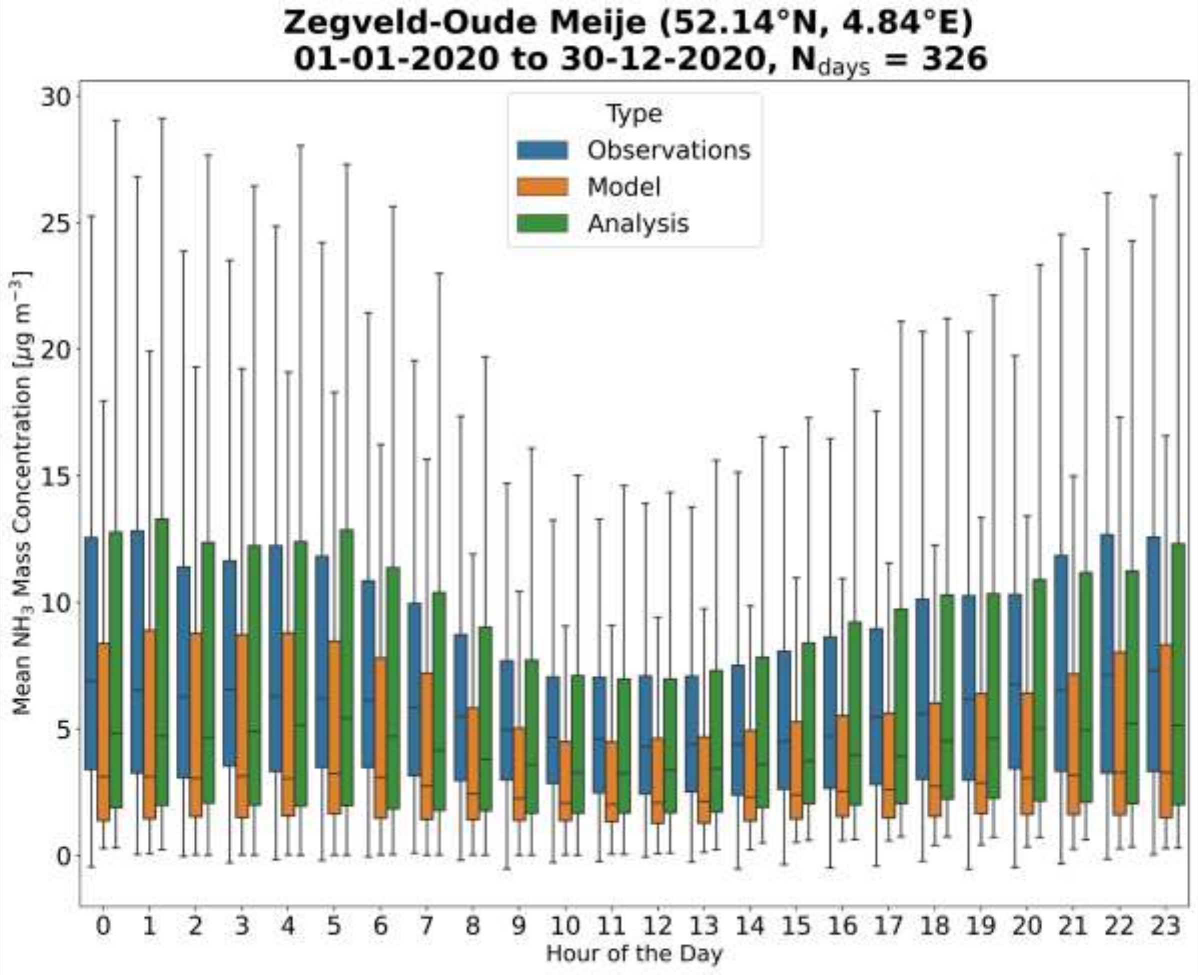
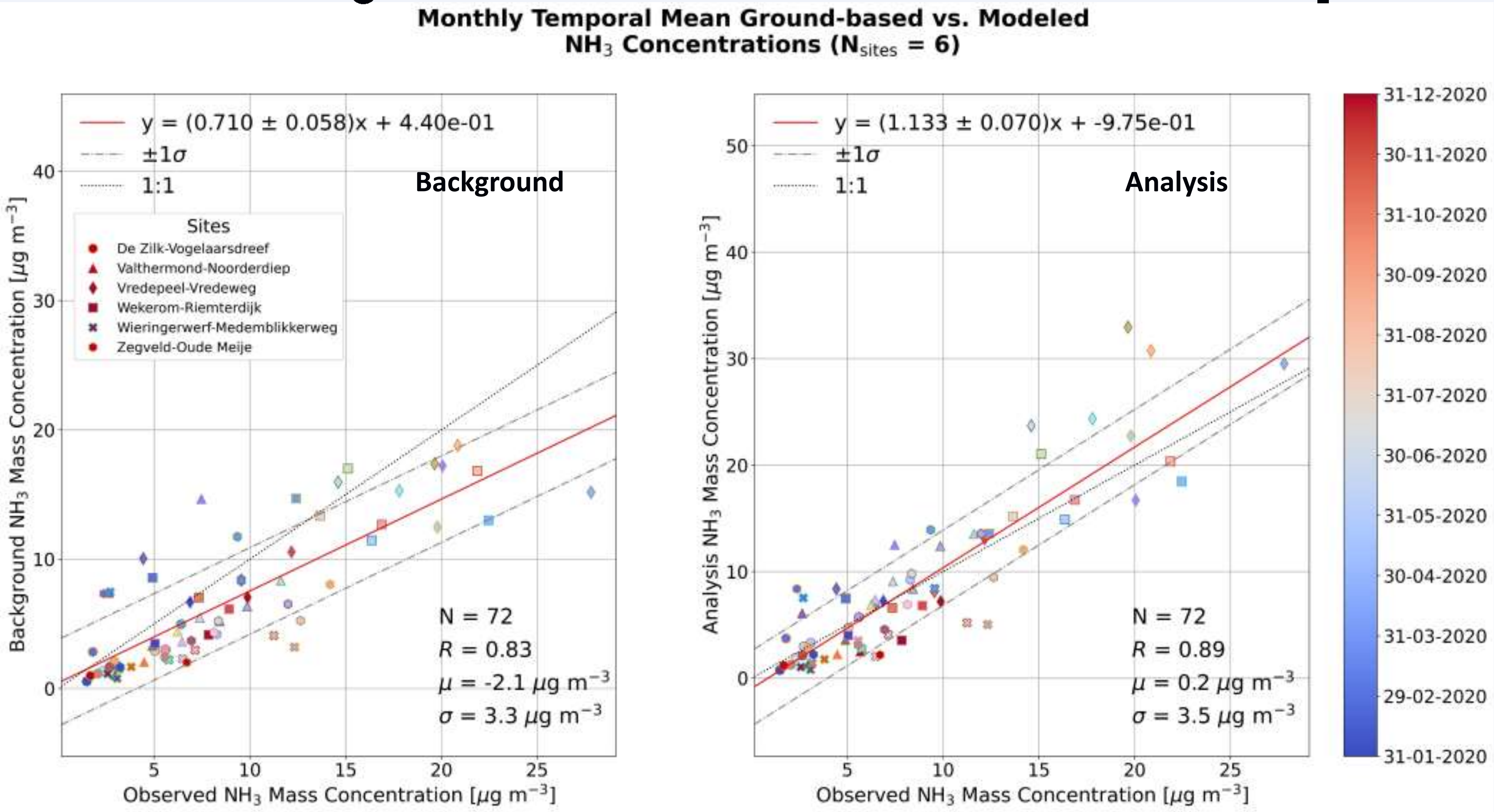
Results – Surface Concentrations - Diurnal





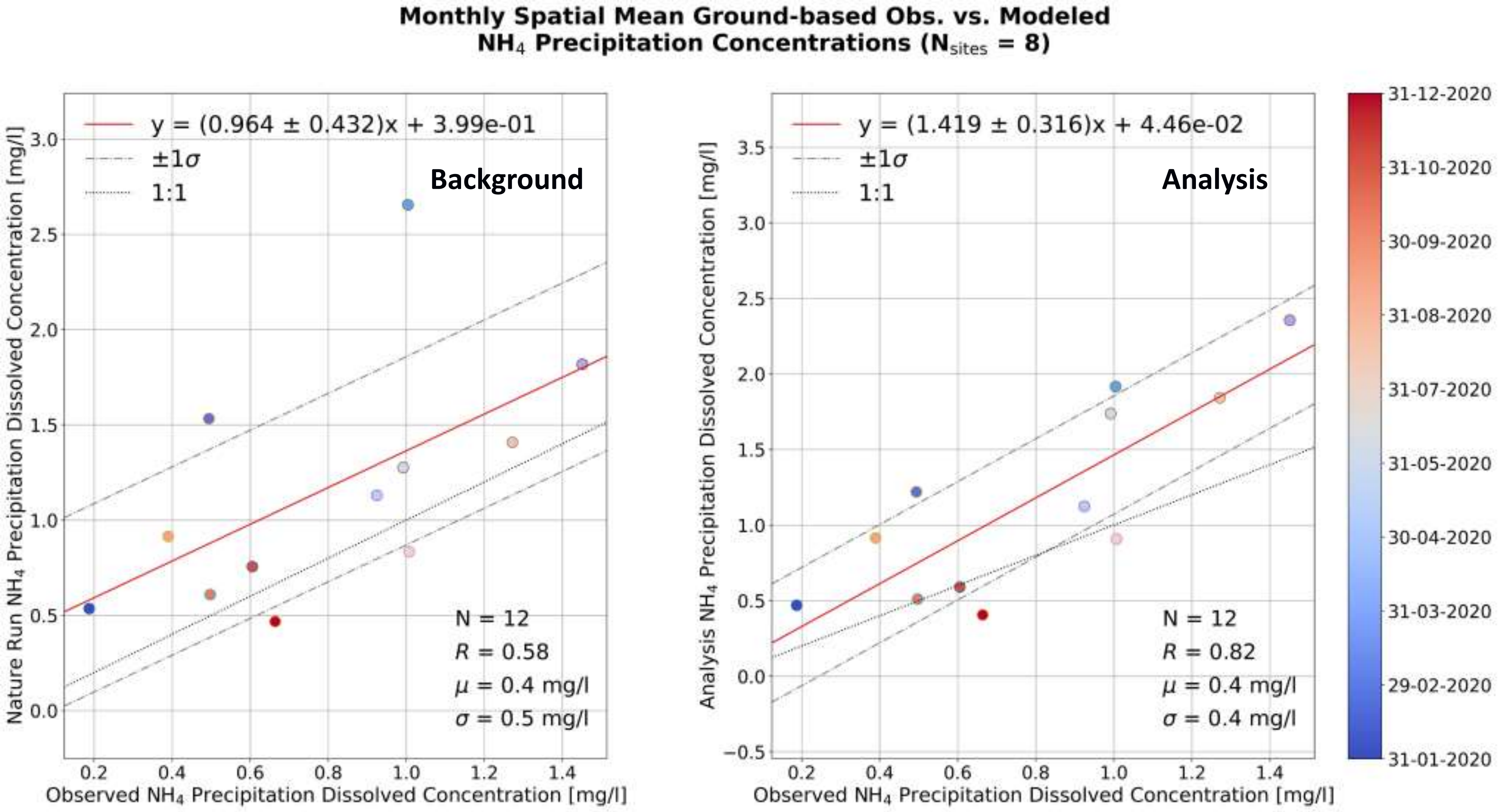
Improvement on diurnal cycle of NH_3, even though only morning/early afternoon overpasses were used
Mean of the observations still shows a difference

Results – NH_3 Surface Concentrations - Temporal



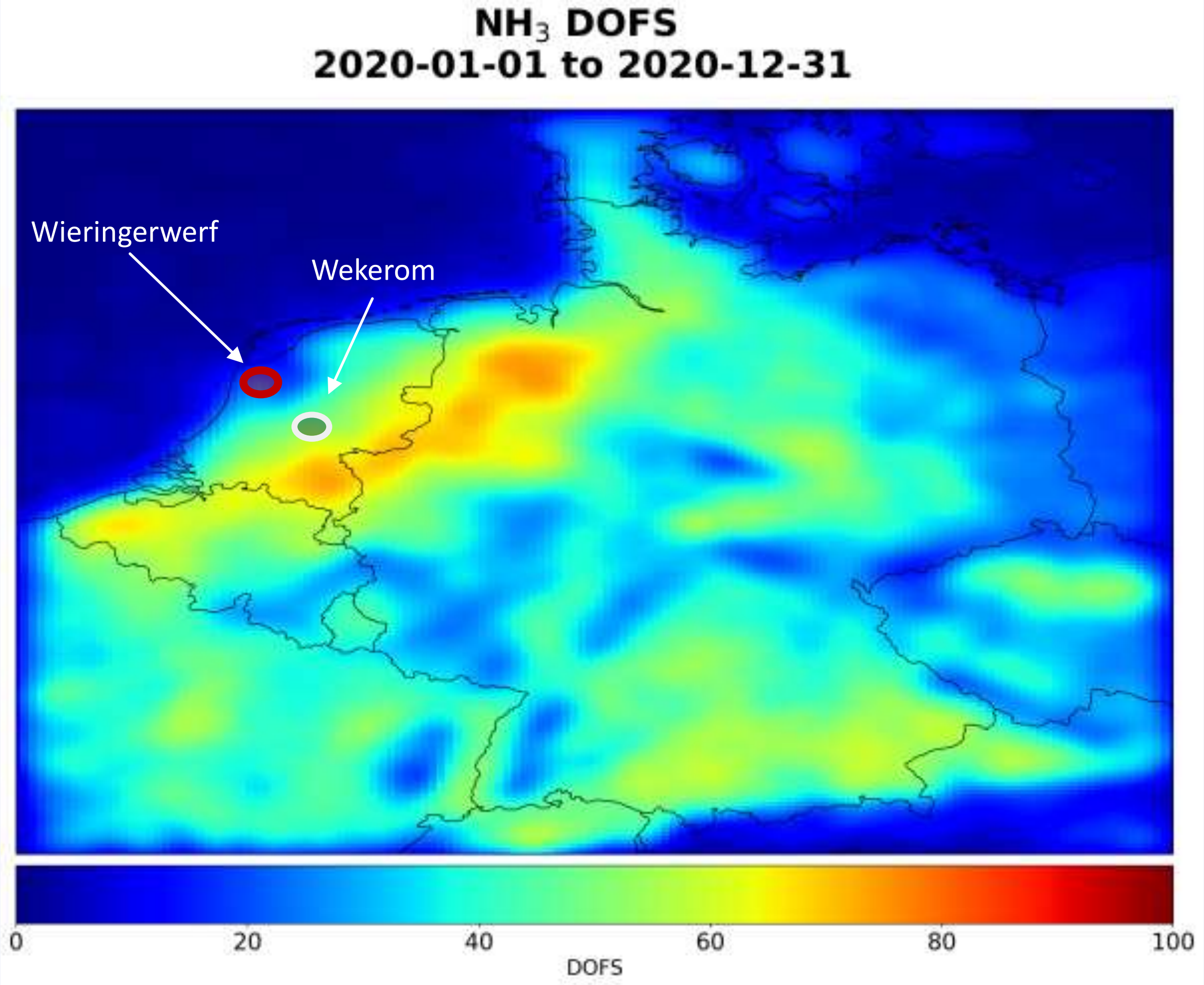
Monthly averages for all sites show broad improvement in surface NH_3 concentrations.

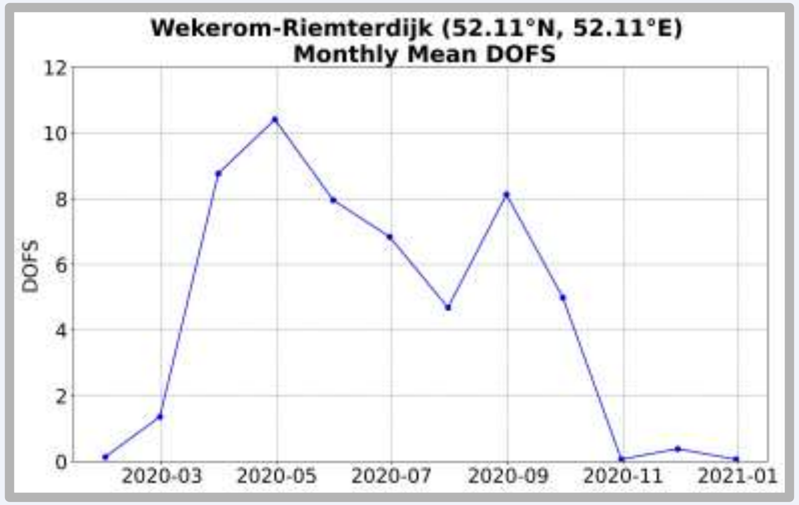
Results – NH_4+ Wet Deposition - Spatial

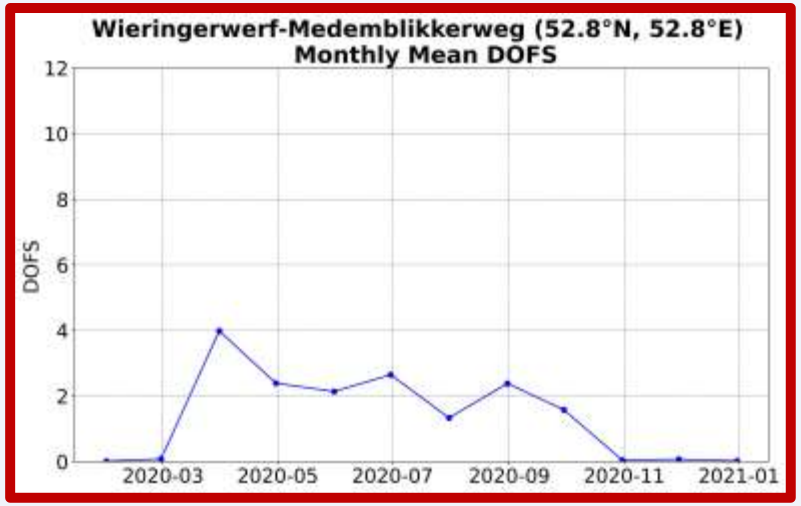


Temporal means of NH4+ wet deposition did not show large differences, but the spatial means show a notable improvement in the correlations.

Results – Degrees of Freedom







Limitation to available information at locations right on the coast & islands due to lack of observations.

Positive: Even in worst case, satellite still provides a solid 2 bits of information (summer/spring), (e.g. comparable to >2 passive samplers)

Conclusions

- Co-assimilated IASI & CrIS NH_3 + TROPOMI-NO_2.
- LETKF able to pick up on “limited” shifts in emissions timing and level.
- Strong improvements compared to hourly observations (LML).
- Limited value in coastal / island regions / wintertime (low NH_3 anyway).
- Limited impact of co-assimilating with NO_2 (region is not NH_3 limited) – few co-emitting species.

Outlook

- Full OSSE underway to understand the actual performance of the system in detail.
- Further validation with in-situ deposition and monthly samplers data to be added.
- Future comparison to other inversion methods for trade off study between the various satellite estimates methods.
- Work on LETKF analysis of Iberian peninsula by Daniel Helm from University of Aveiro.

Questions?

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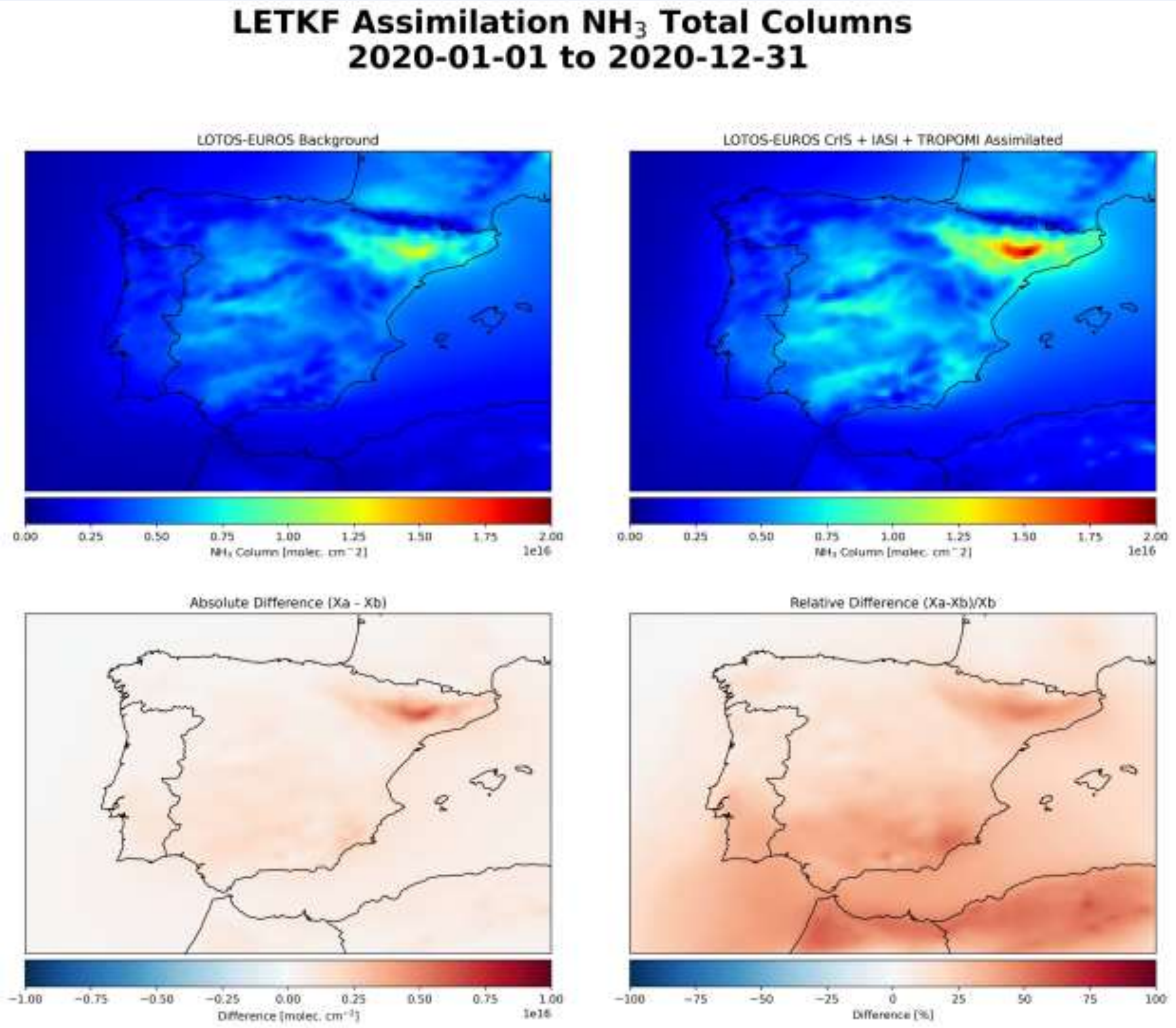
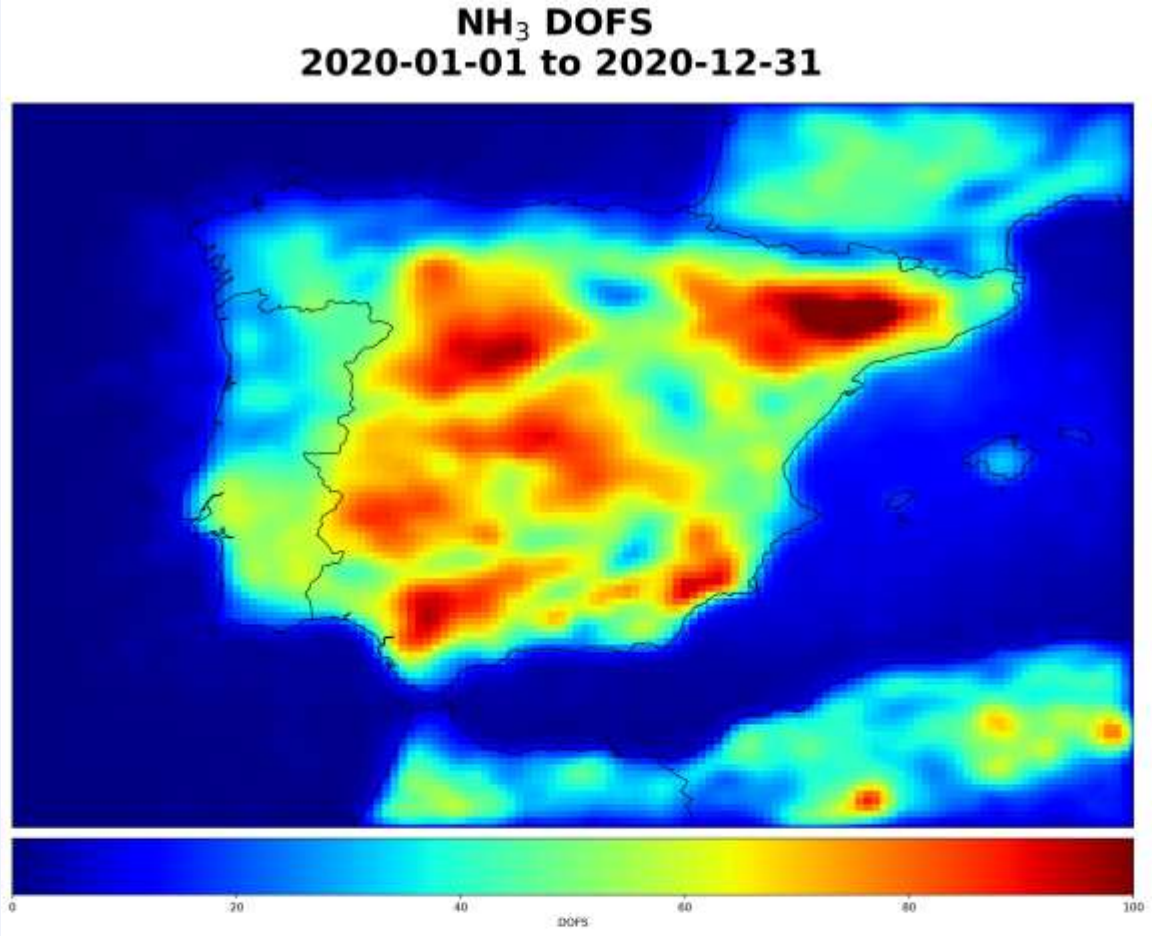
Tyler.Wizenberg@tno.nl

Results – Iberian Peninsula





LETKF not good at completely missing emissions, needs a base to adjust, limited impact on Portugal

Future work by Daniel Helm within FONDA

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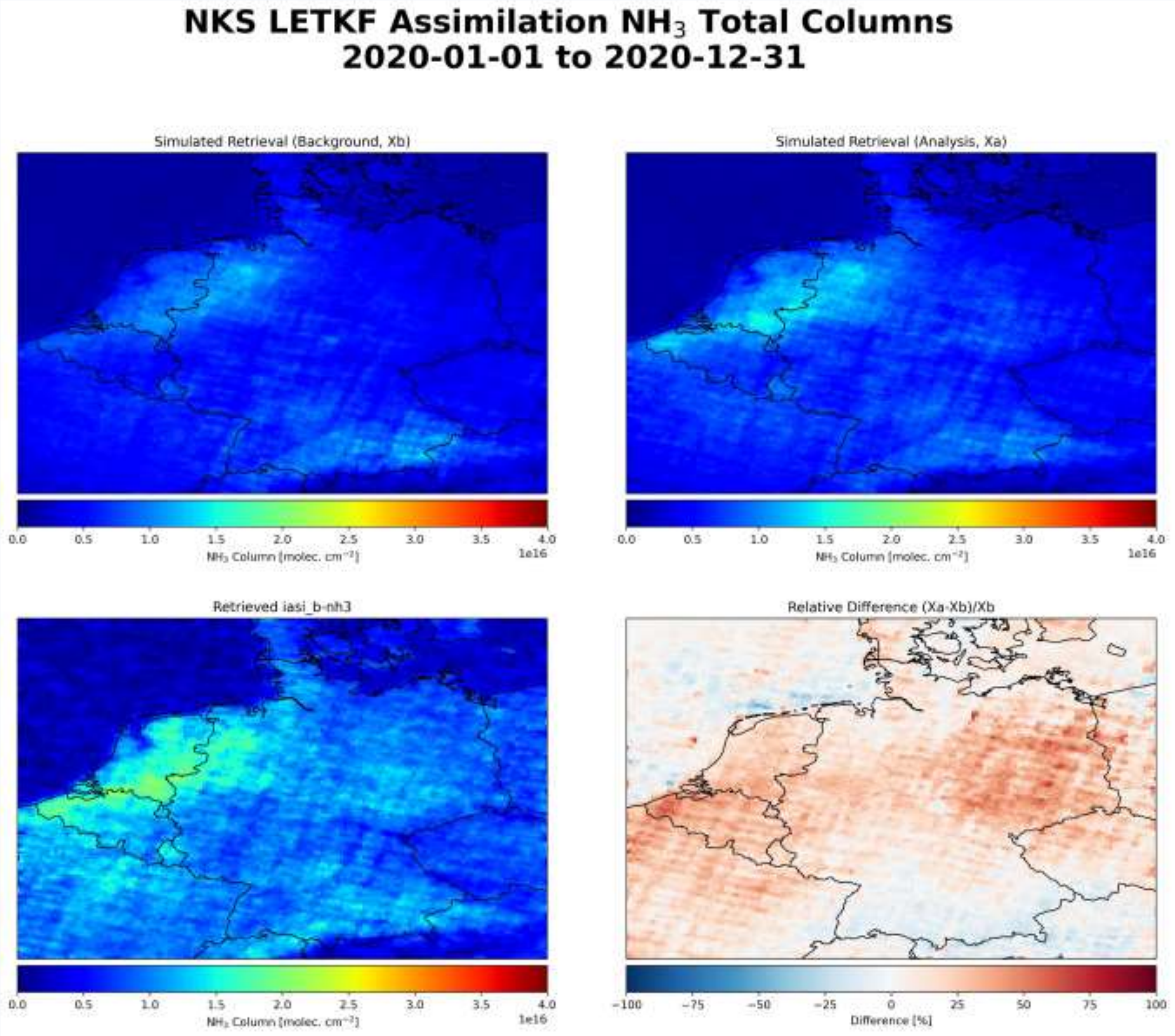
Results – Column level changes + emission totals



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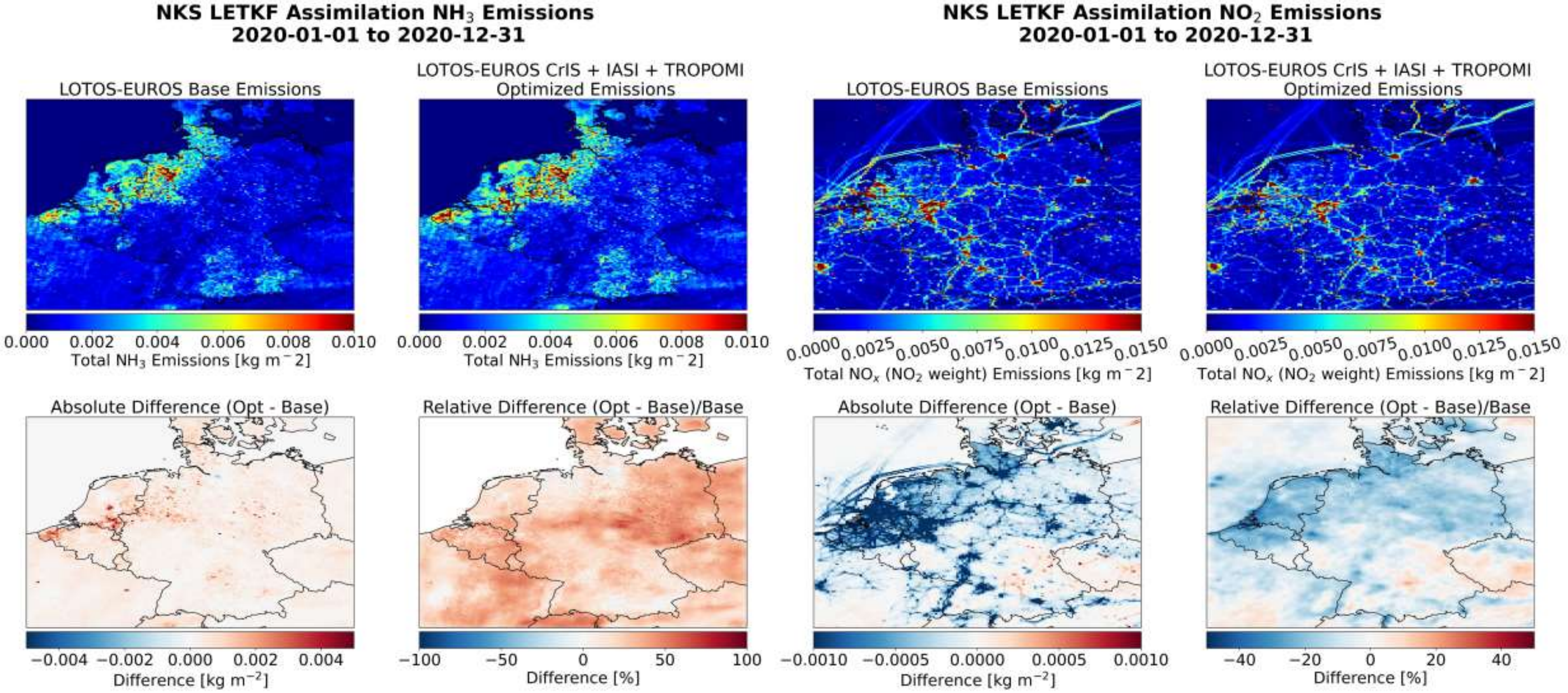
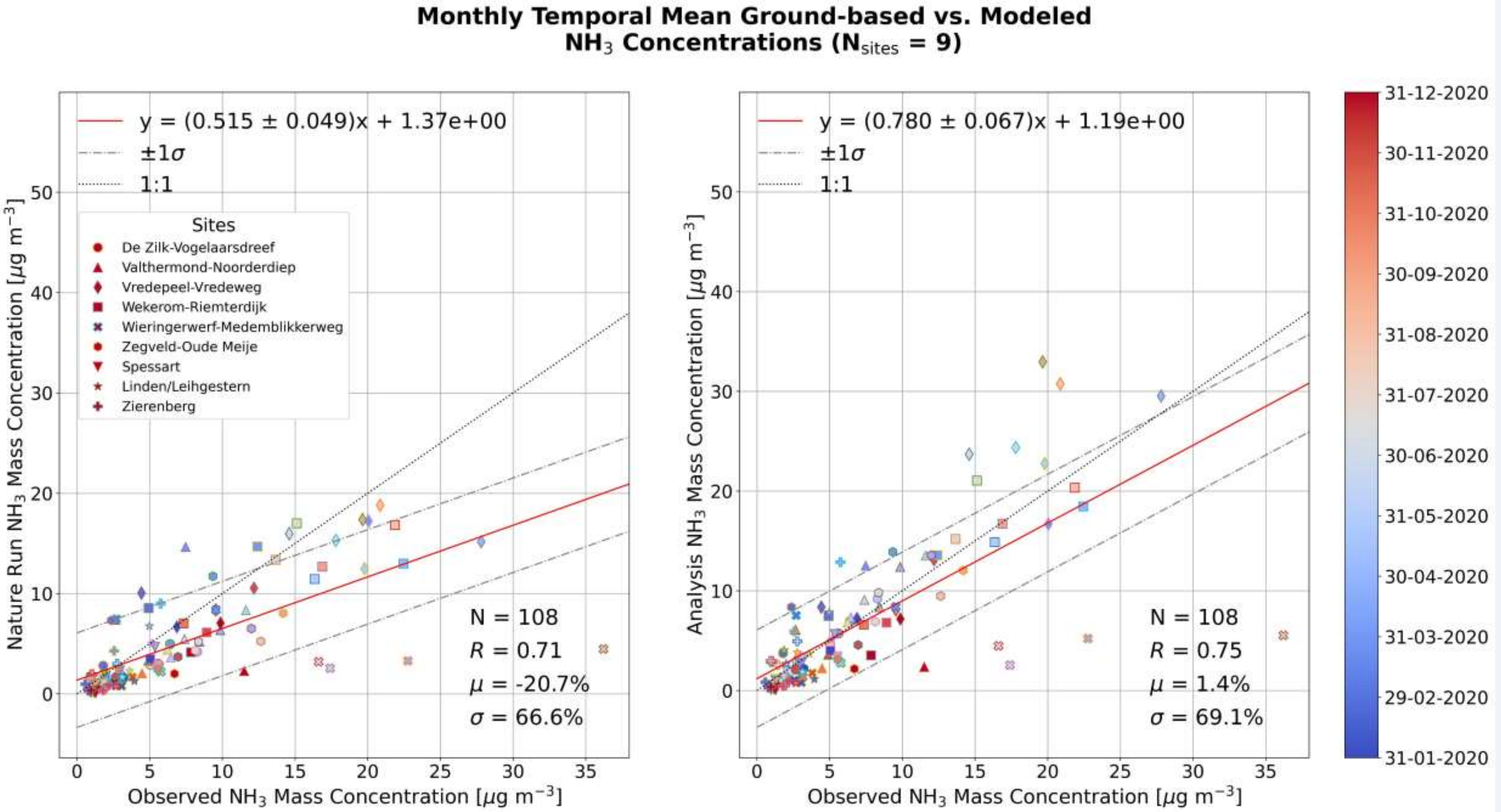
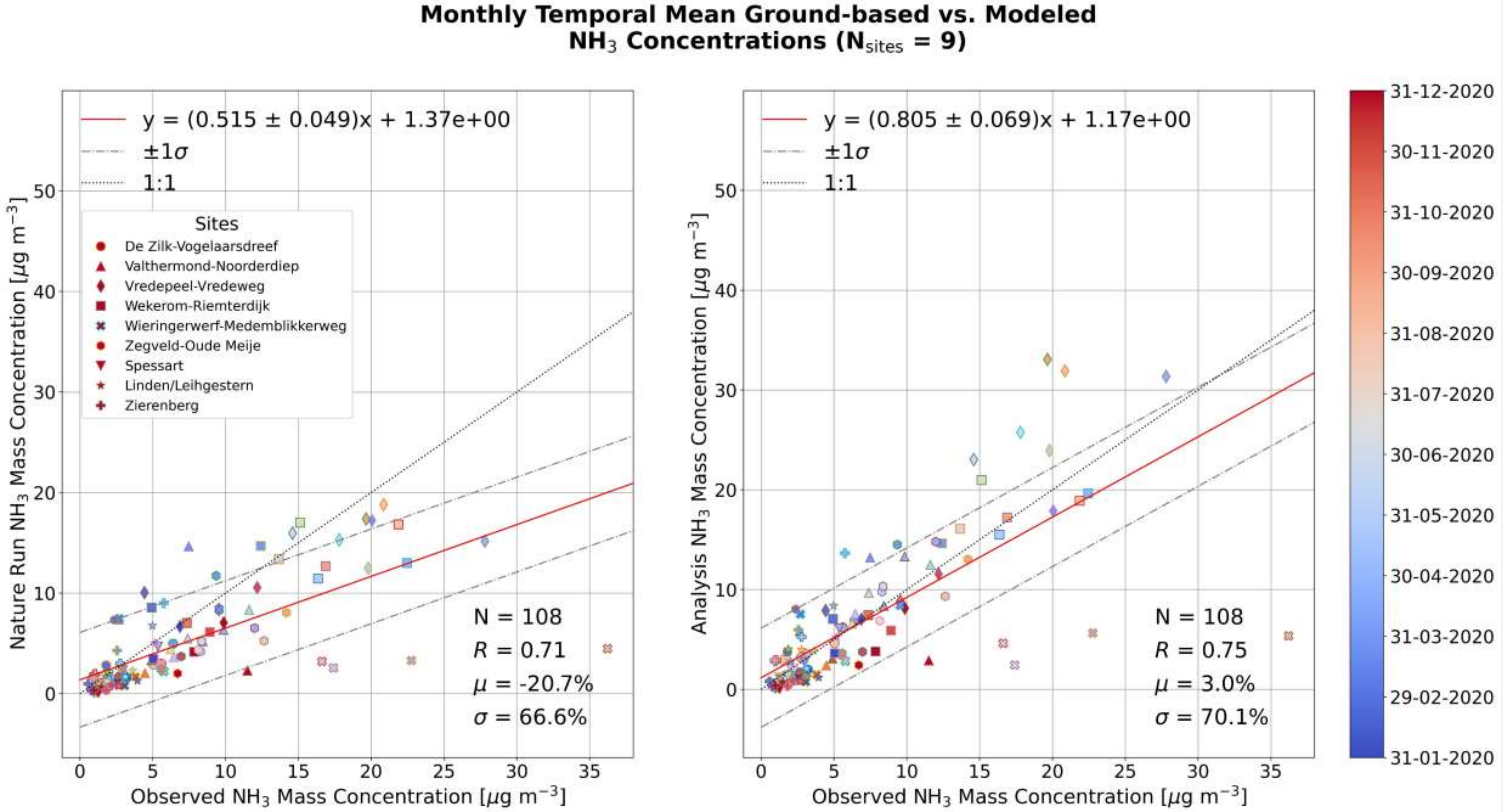


Results – Concentration after co-assimilation



Results – Concentration CrIS/IASI only



Calculation of DOFS for the LETKF

Approach of Chen et al. (2023; https://doi.org/10.5194/acp-23-5945-2023) was applied.

The averaging kernel **A** that describes the sensitivity of the solution to the true value is given by (Chen et al. 2023):

$$\mathbf{A} = \frac{\partial \hat{x}'}{\partial \boldsymbol{x}'} = \mathbf{I}_N - \hat{S}'\mathbf{S}_{\mathrm{a}}'^{-1},$$

Where I_{N} is the identity matrix, $\hat{S}'$ is the aposteriori covariance matrix, and S_a' is the a priori covariance matrix.

The trace of **A** quantifies the number of independent pieces of information gained from the observations (the DOFS).