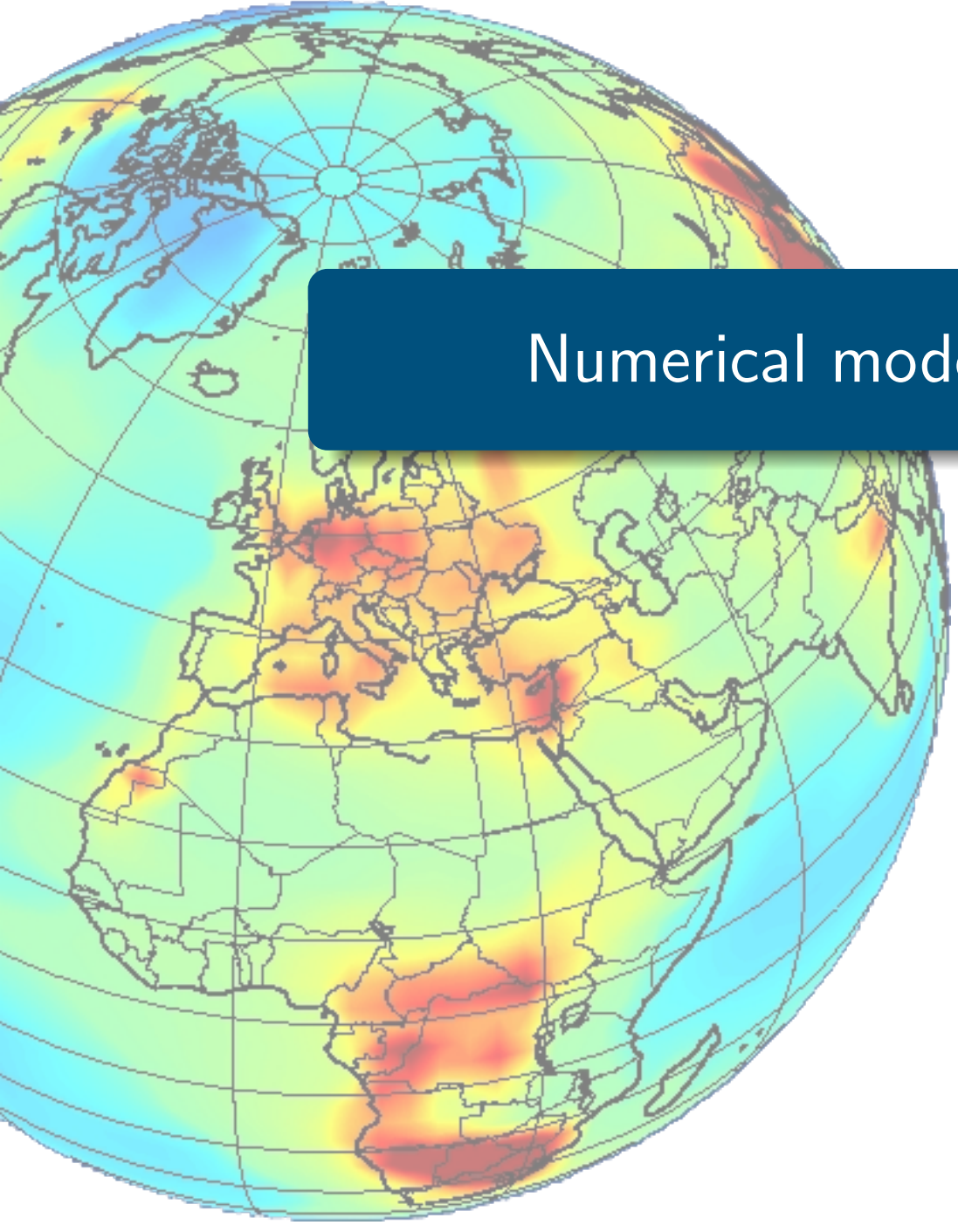


Numerical modelling of air quality

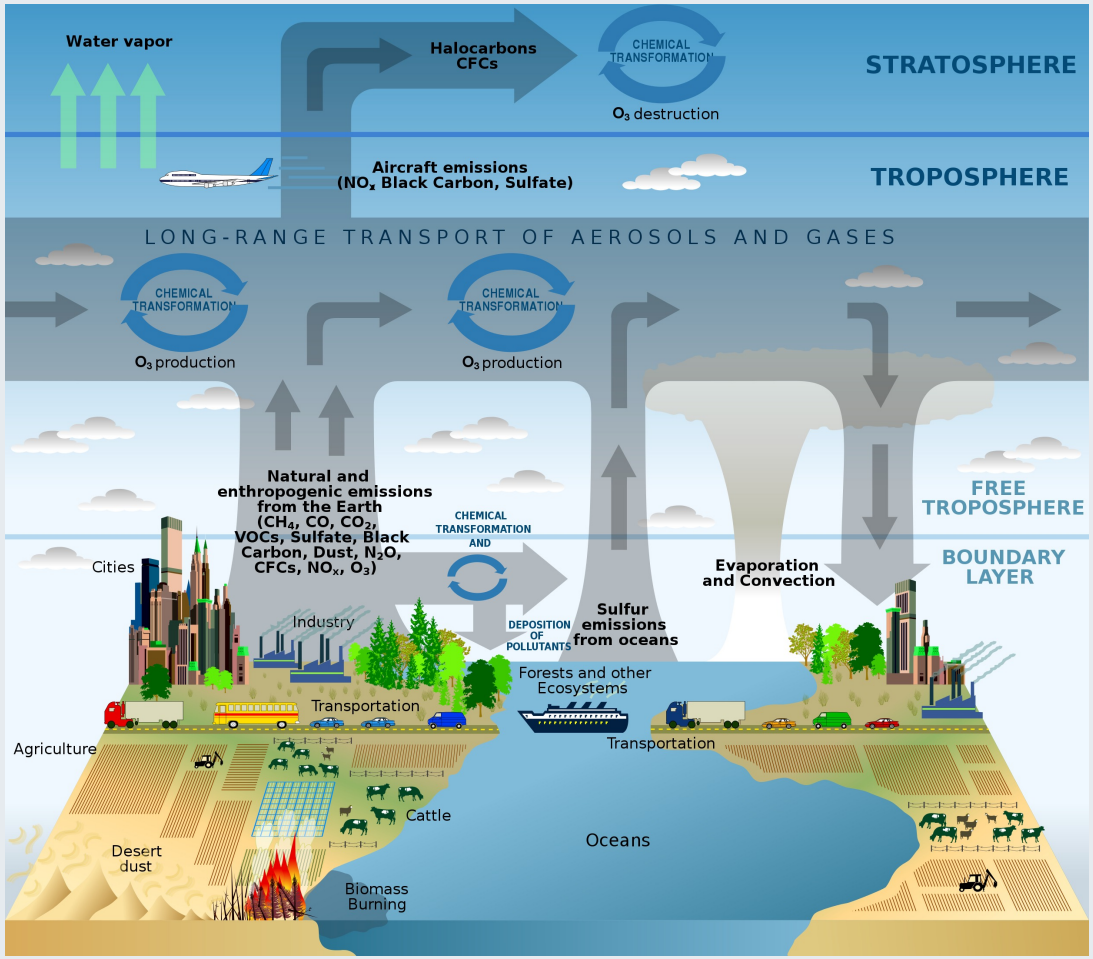
A. Pozzer

MPI for Chemistry & CARE-C CyI

19th October 2023

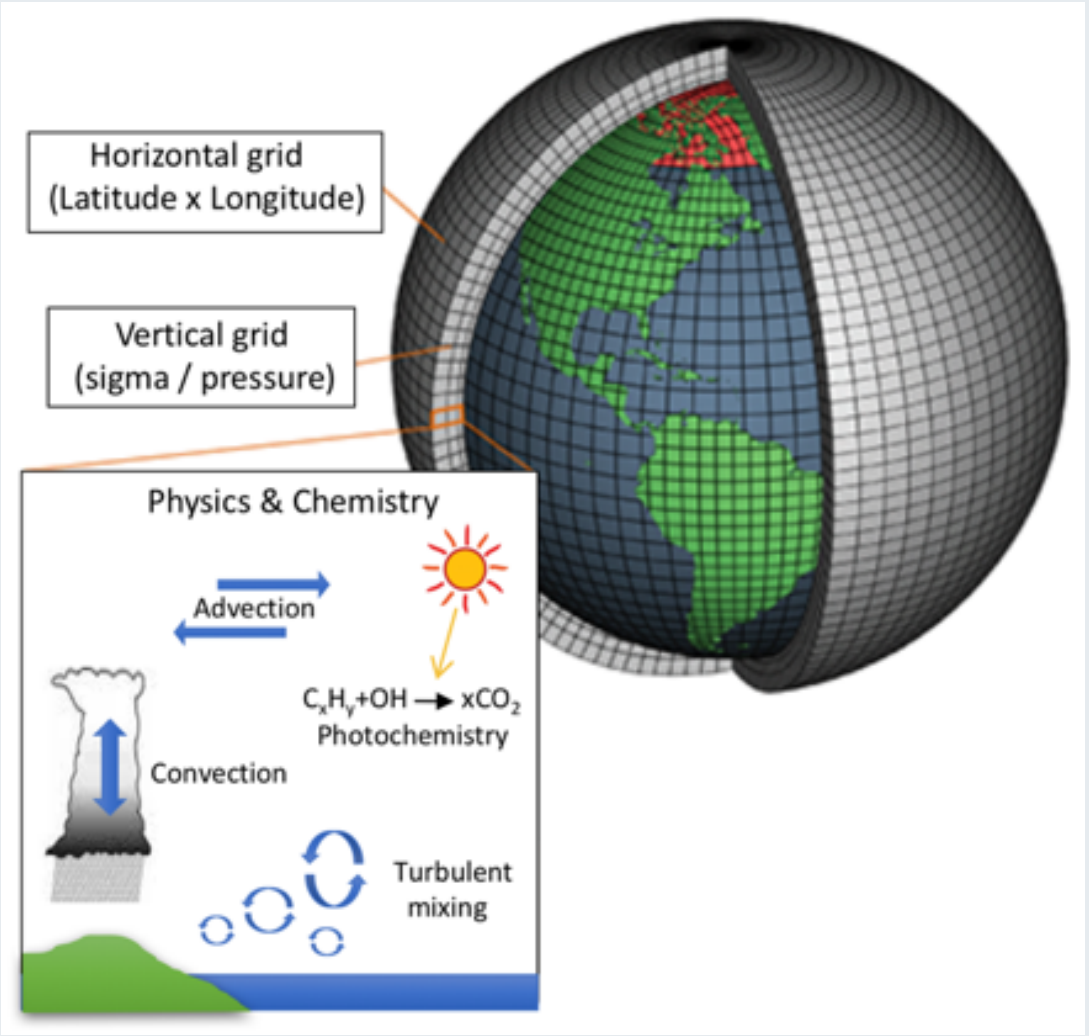
MAX-PLANCK-GESELLSCHAFT

The chemistry of the Atmosphere

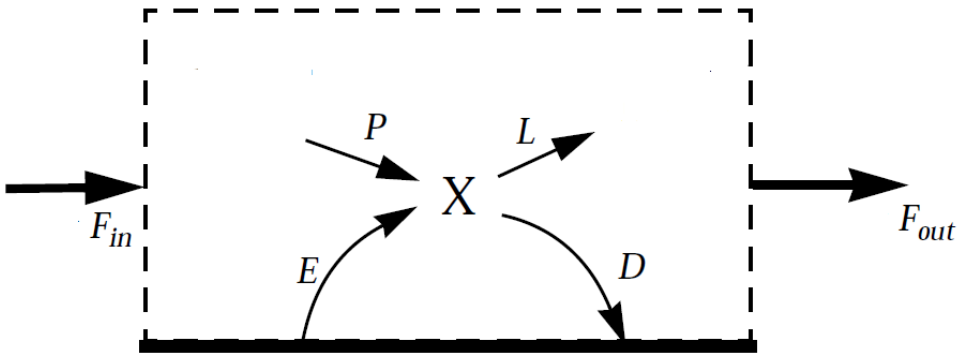


A. Pozzer

Numerical modelling



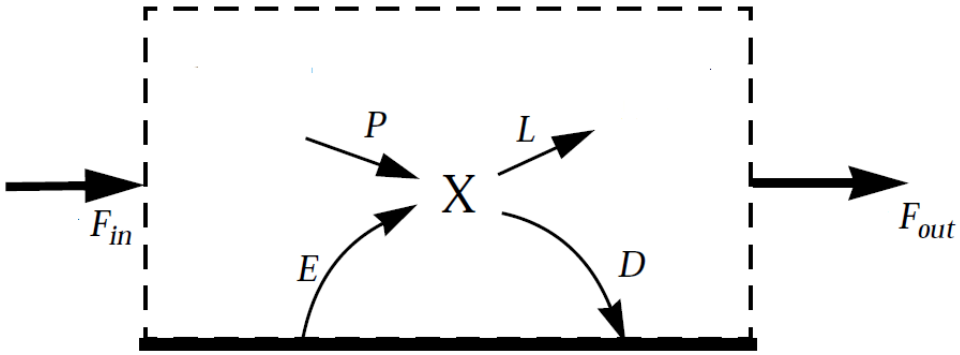
Simple Box Model



Concentration of X

- emission (E)
- transport (F_{in} and F_{out})
- reaction (Production an Loss)
- deposition (D)

Simple Box Model



Case studies

- Emission
- Deposition
- Transport

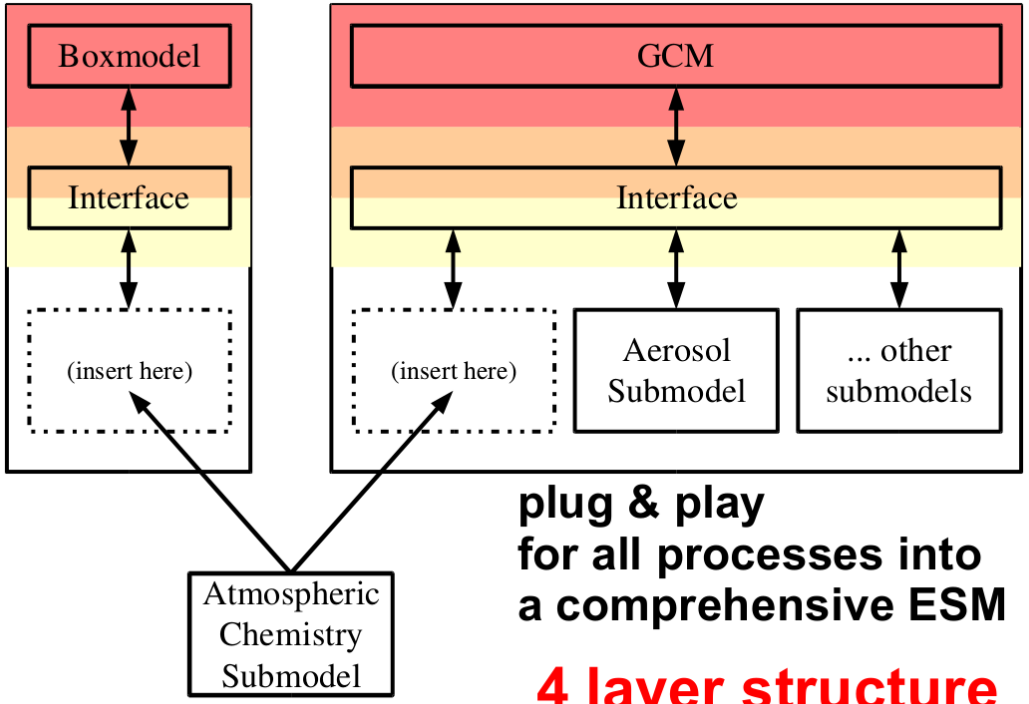
All work performed with the EMAC model

ECHAM5/MESSy for Atmospheric Chemistry

`www.messy-interface.org`

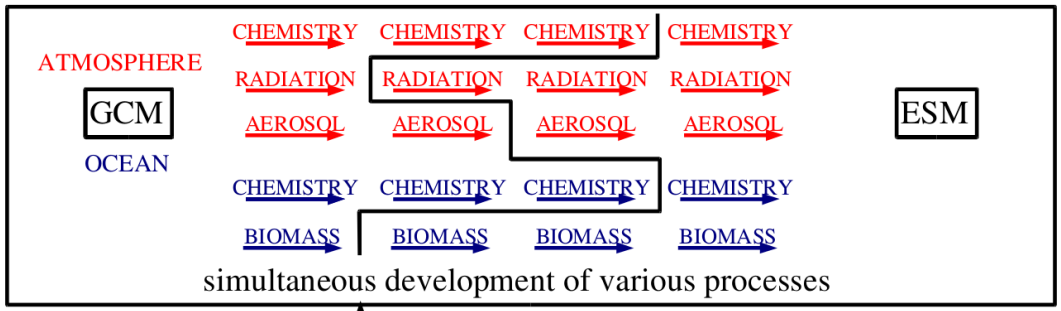
Main characteristics:

- Basemodel: General circulation model ECHAM5 (developed at the MPI for Meteorology in Hamburg).
- Chemistry submodels : MESSy, Modular Earth Submodel System

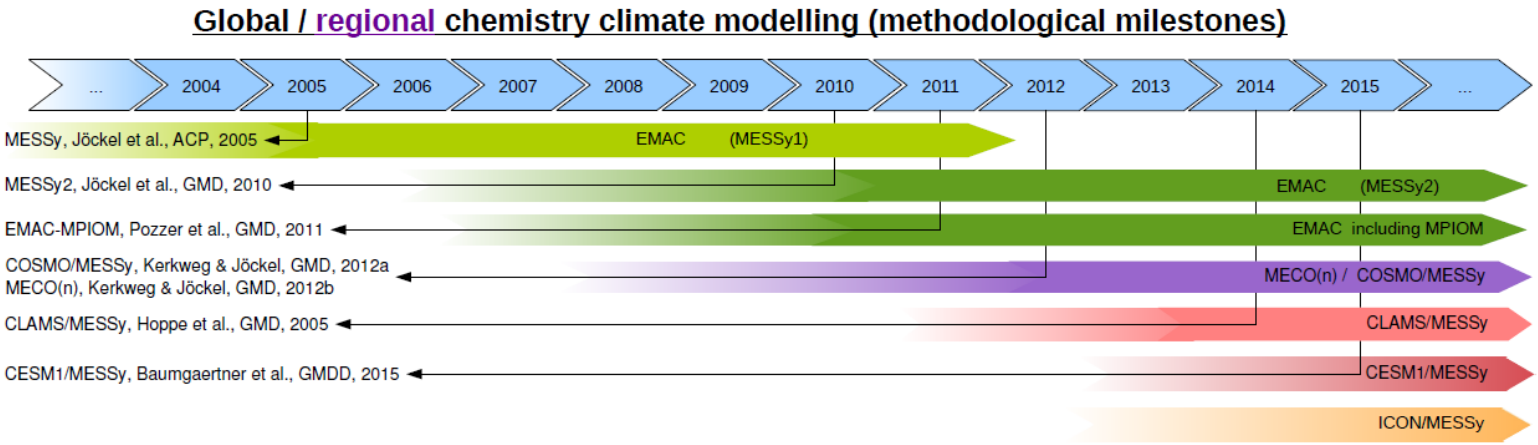


plug & play for all processes into a comprehensive ESM

4 layer structure



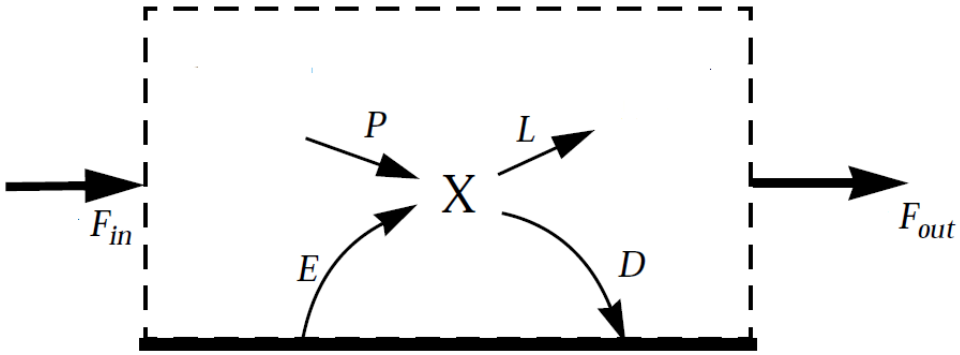
At any time during the development phase a "state-of-the-art" model for scientific applications is available.



Hence:

Flexible for different studies on atmospheric chemistry

Simple Box Model

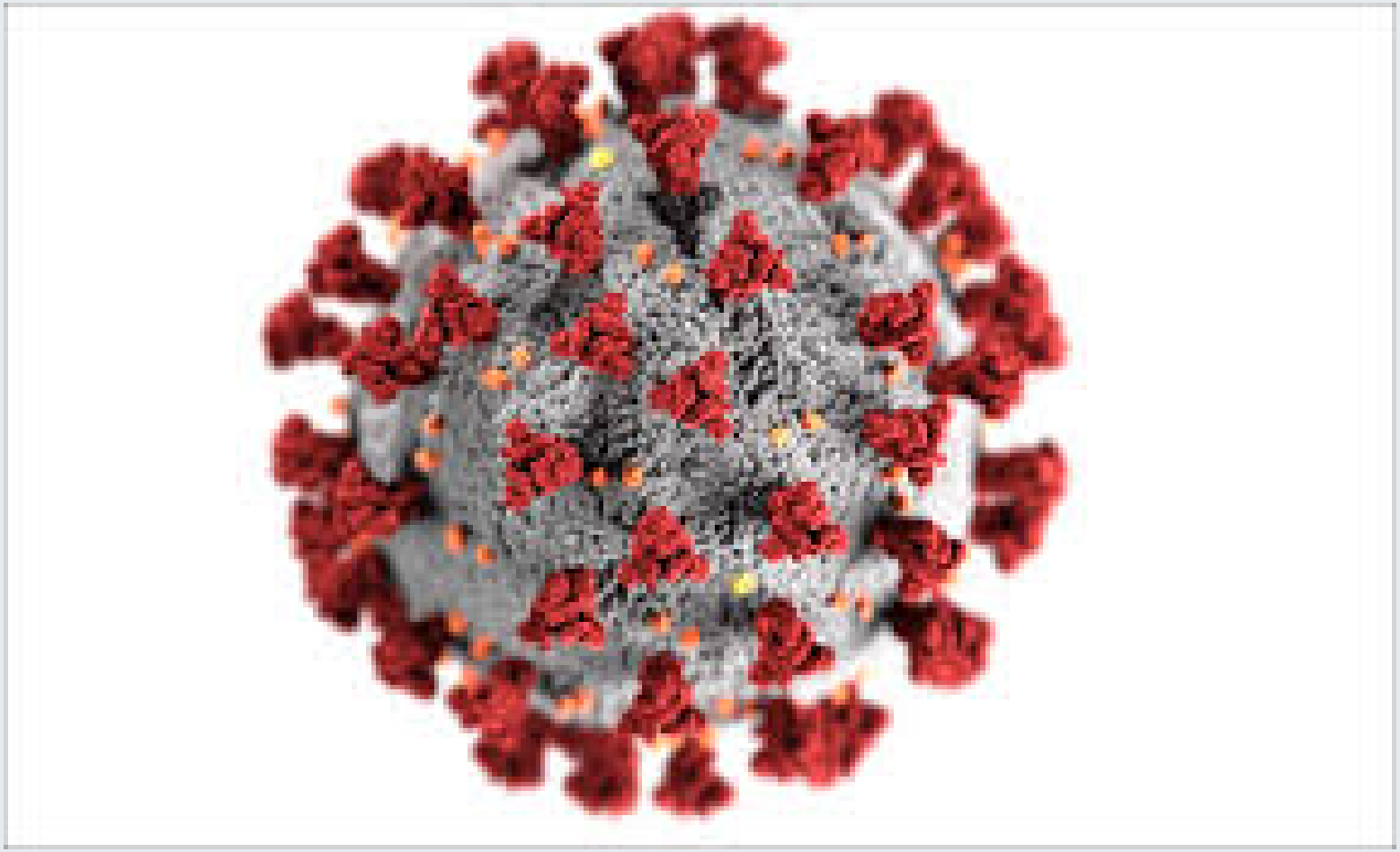


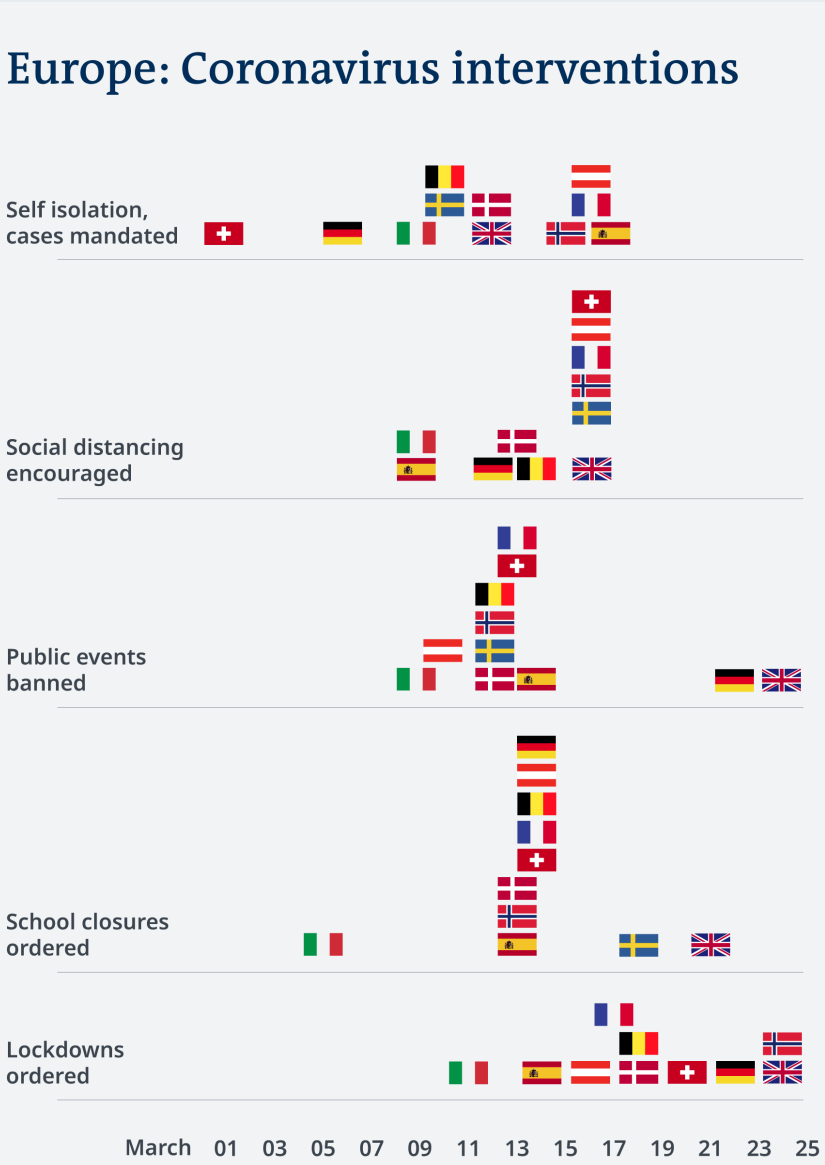
Case studies

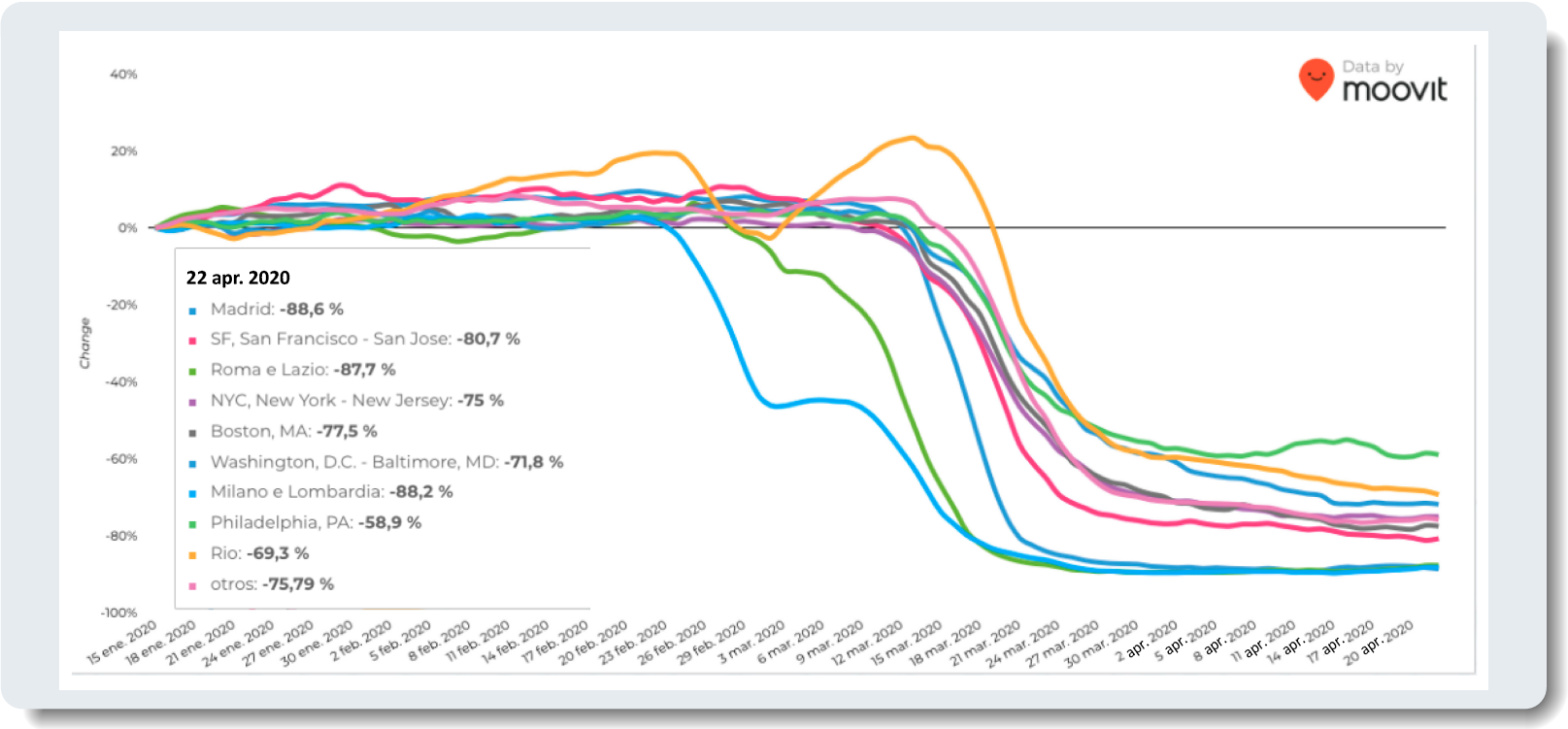
- Emission
- Deposition
- Transport

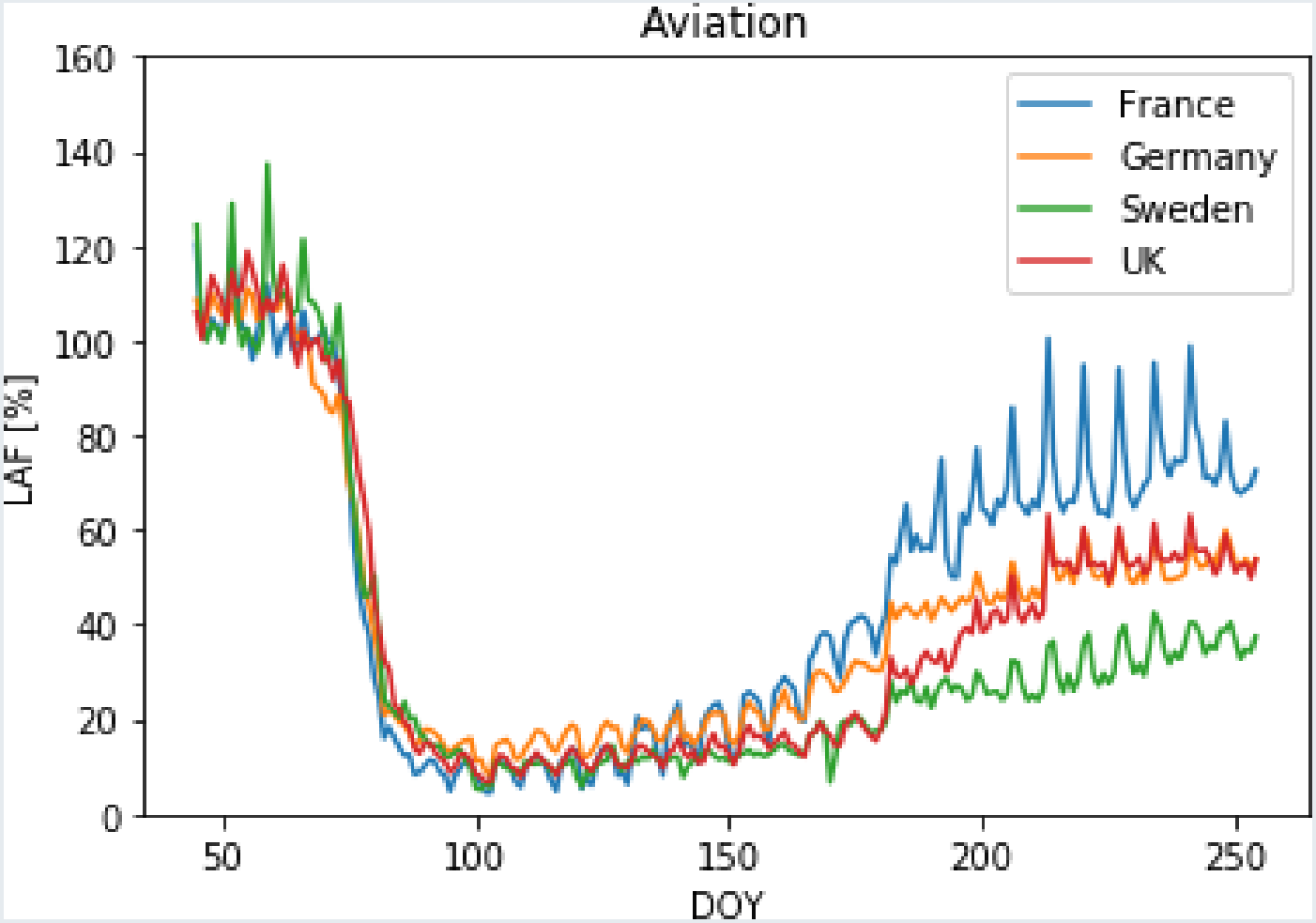
Can we prove the importance of emissions on air quality?
With real life experiment?

Strong influence on European emissions in 2020





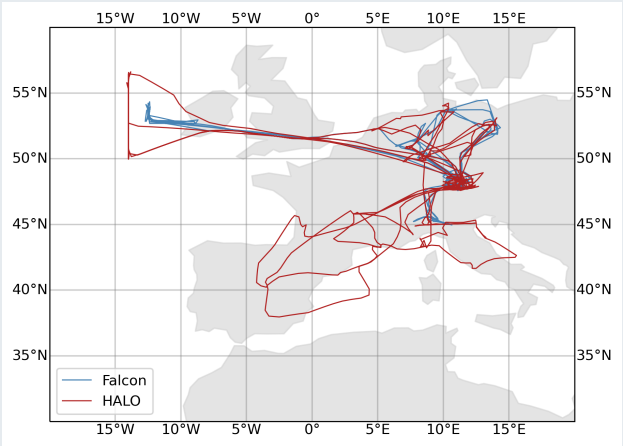




$\sim$ 90% decrease

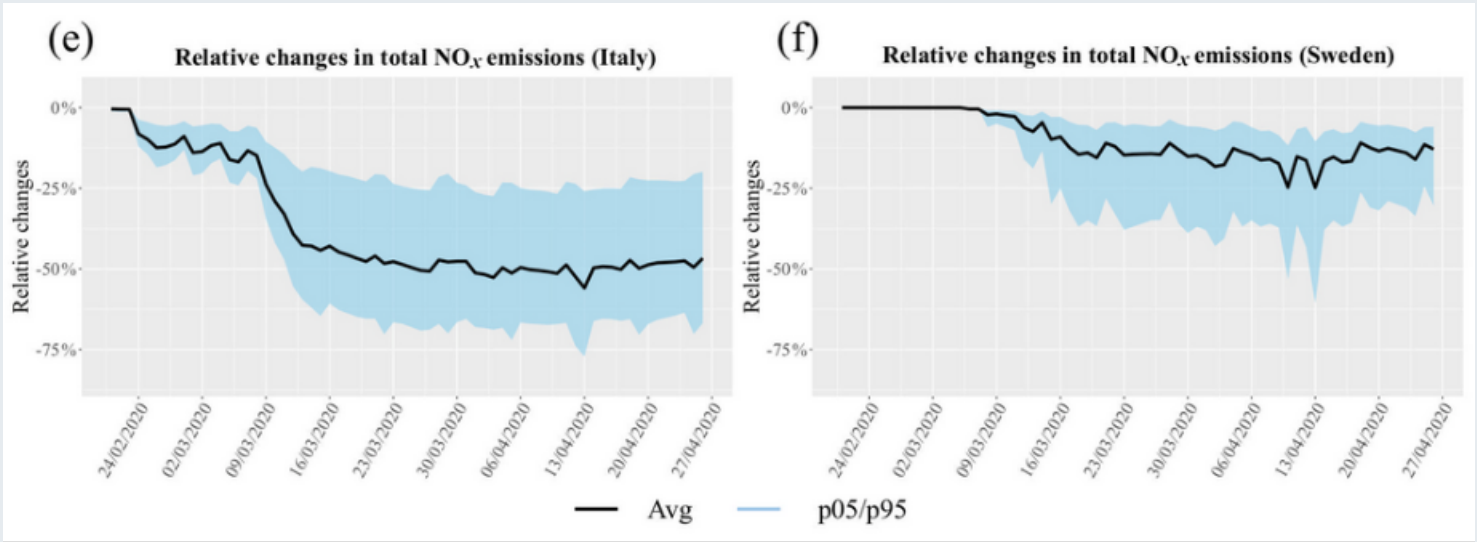
BLUESKY campaign

- 16th May - 9th June 2020
- Europe and the North Atlantic flight corridor
- High Altitude and Long Range (HALO) research aircraft
- Falcon research aircraft
- 8 and 12 flights were conducted with the HALO and the Falcon



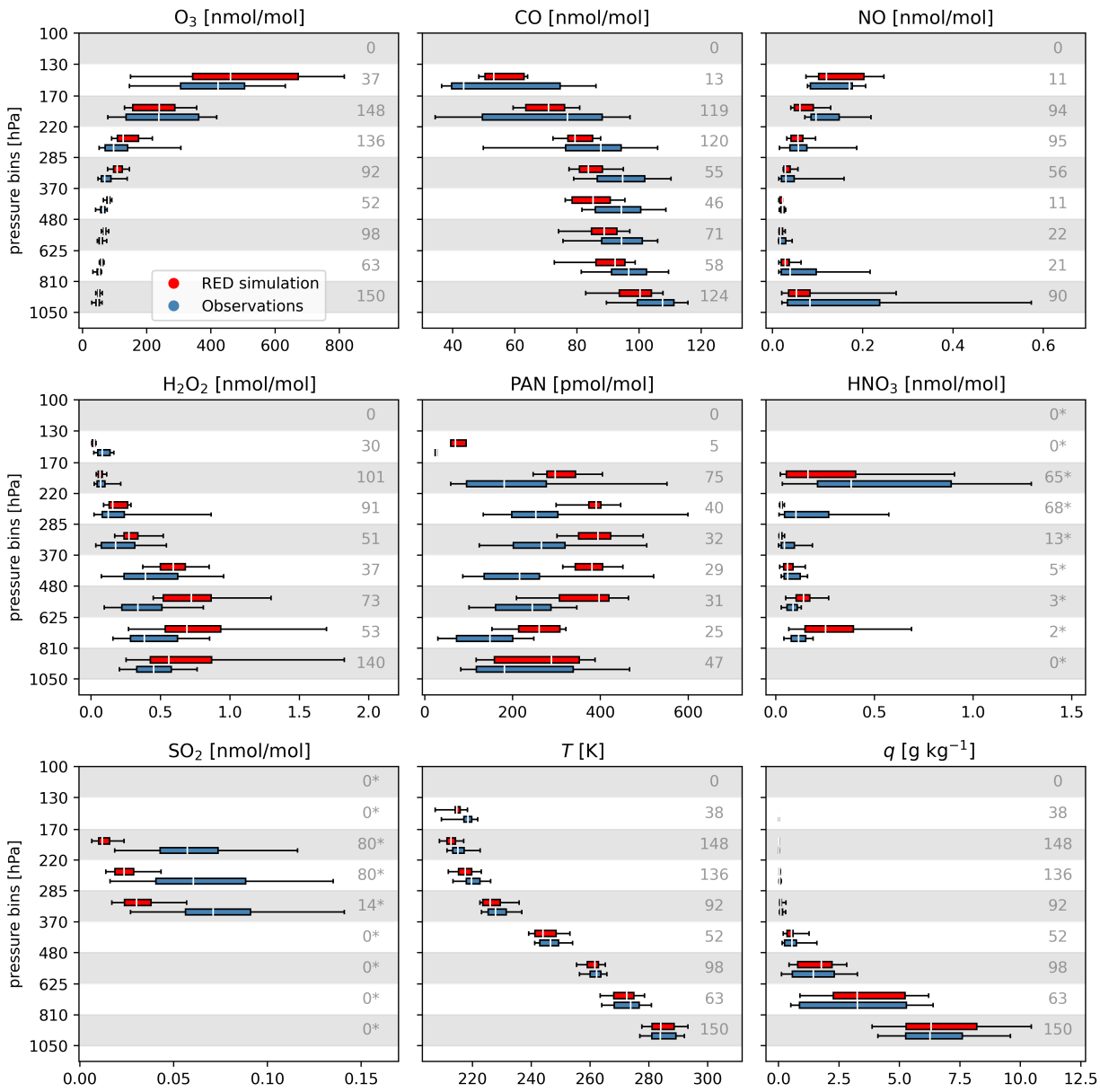
Model simulation

- Covering January-July 2020
- 1.8 degree resolution, 47 levels
- inclusion of stratosphere
- reduction emission coefficient for Europe
  - Industry
  - Energy
  - Transport
  - Aviation (special)

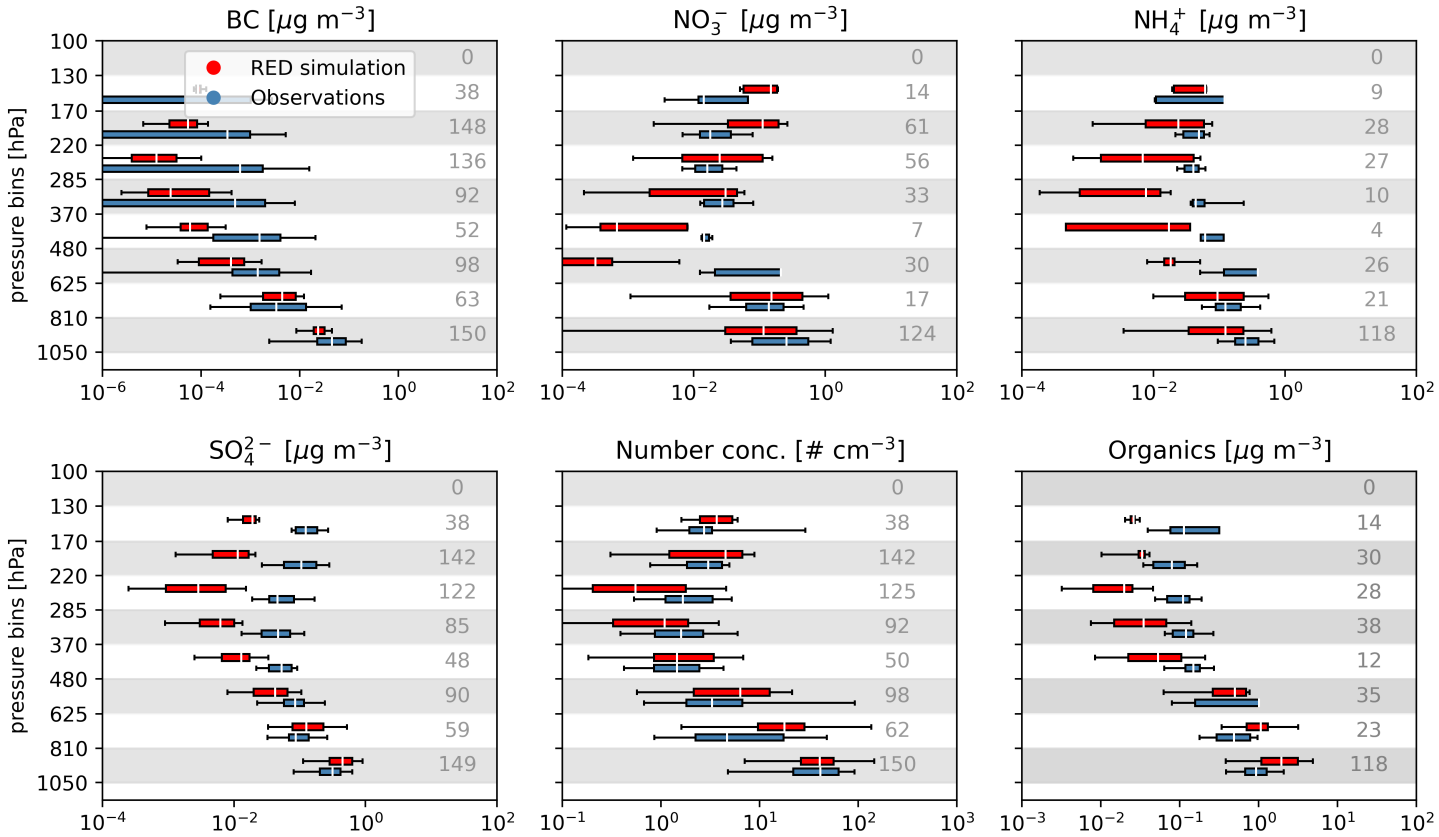


Guevara et al. (2021)

results - trace gases



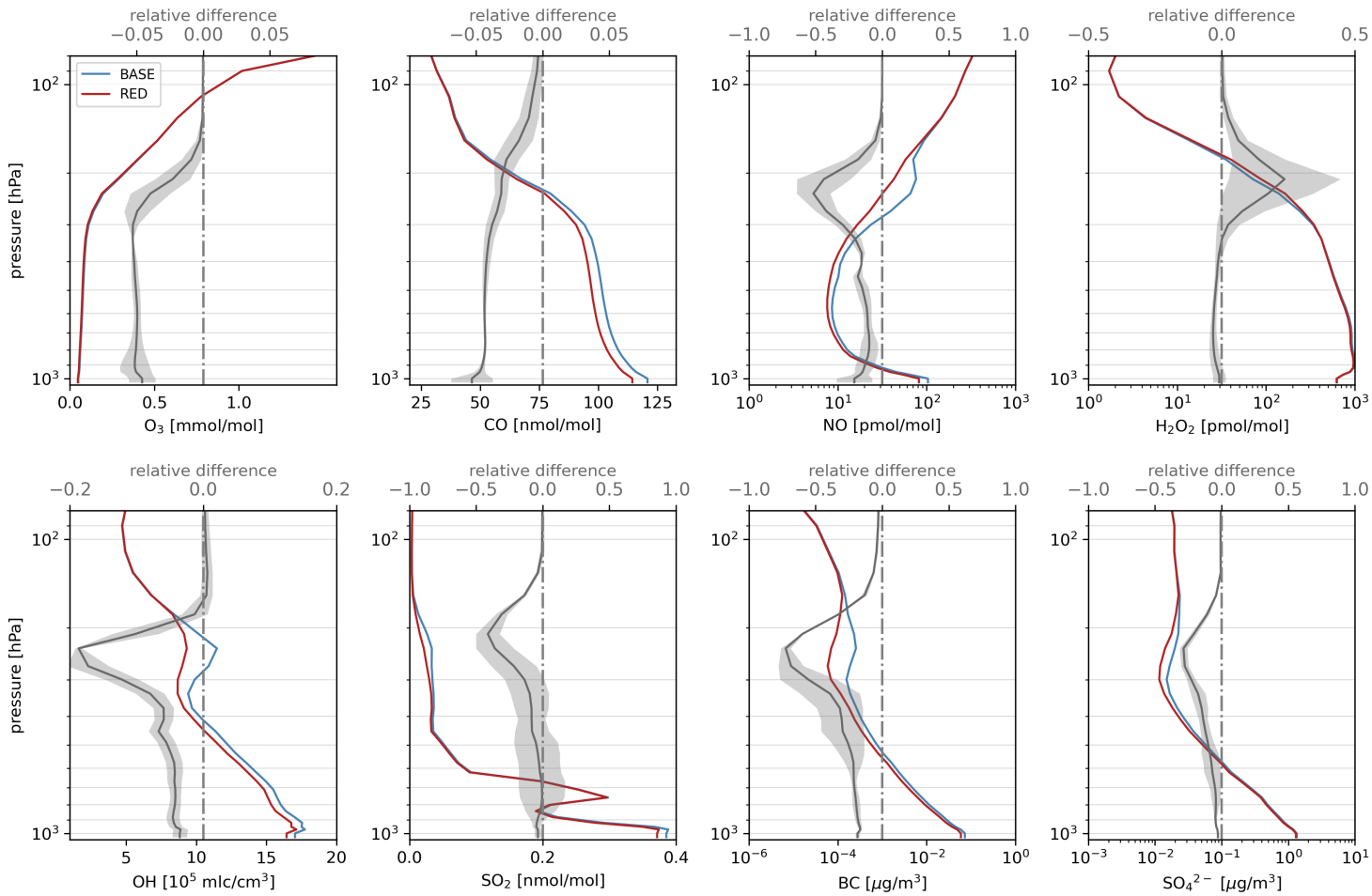
results - aerosols



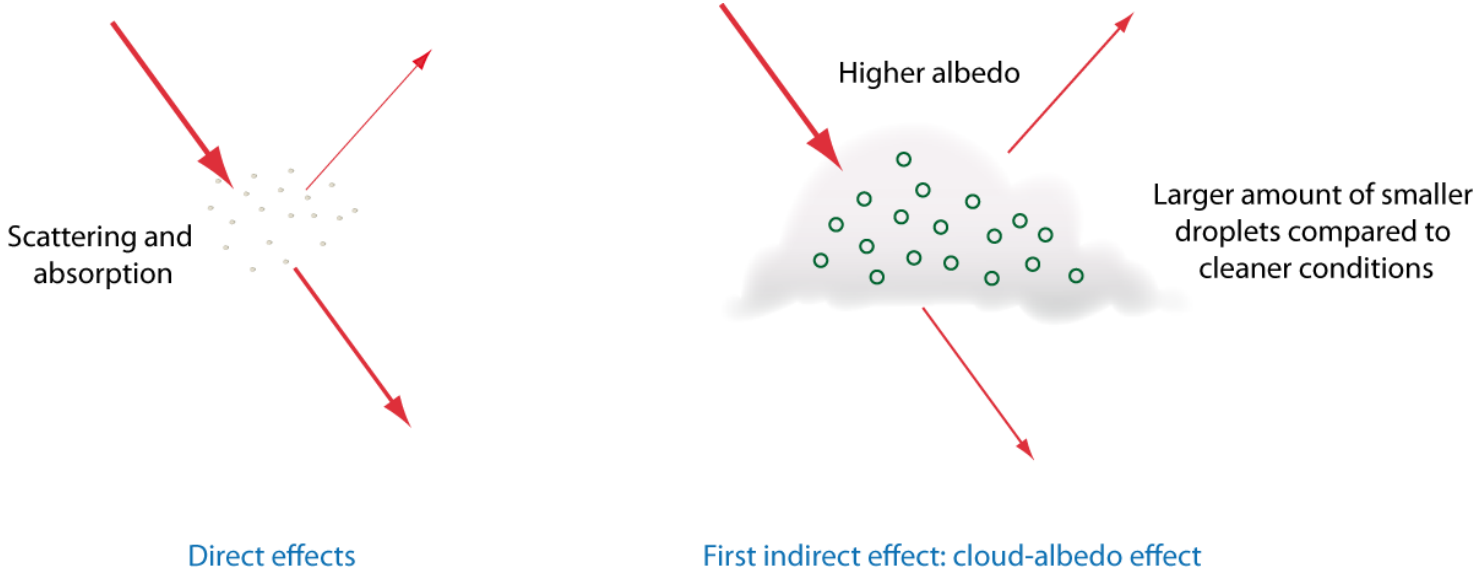
Reasonable comparison between model results and observations

Effect of reduced emissions

comparison with Business As Usual scenario



Effect of reduced emissions



Direct effects

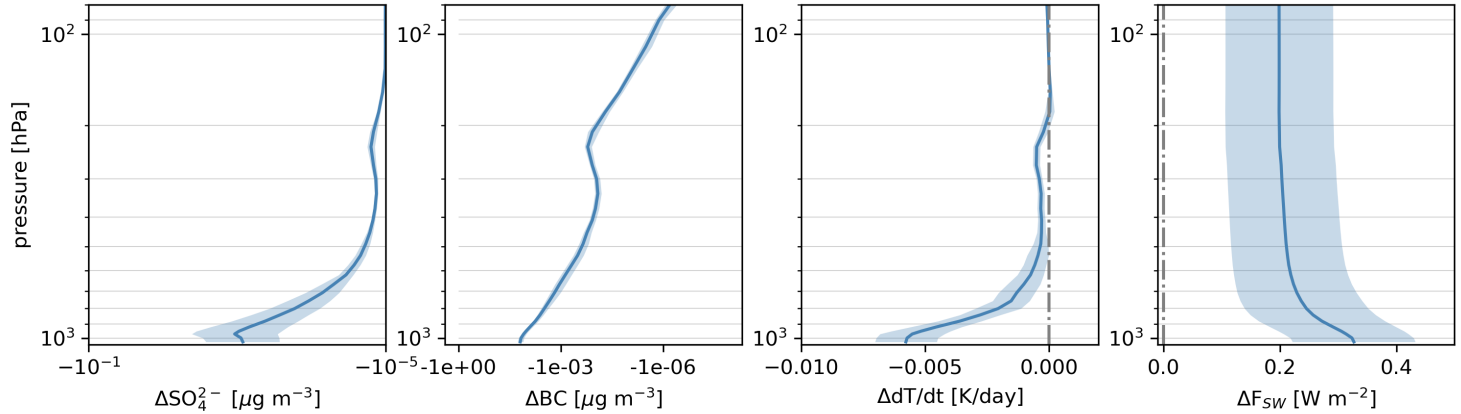
First indirect effect: cloud-albedo effect

Multiple simulation

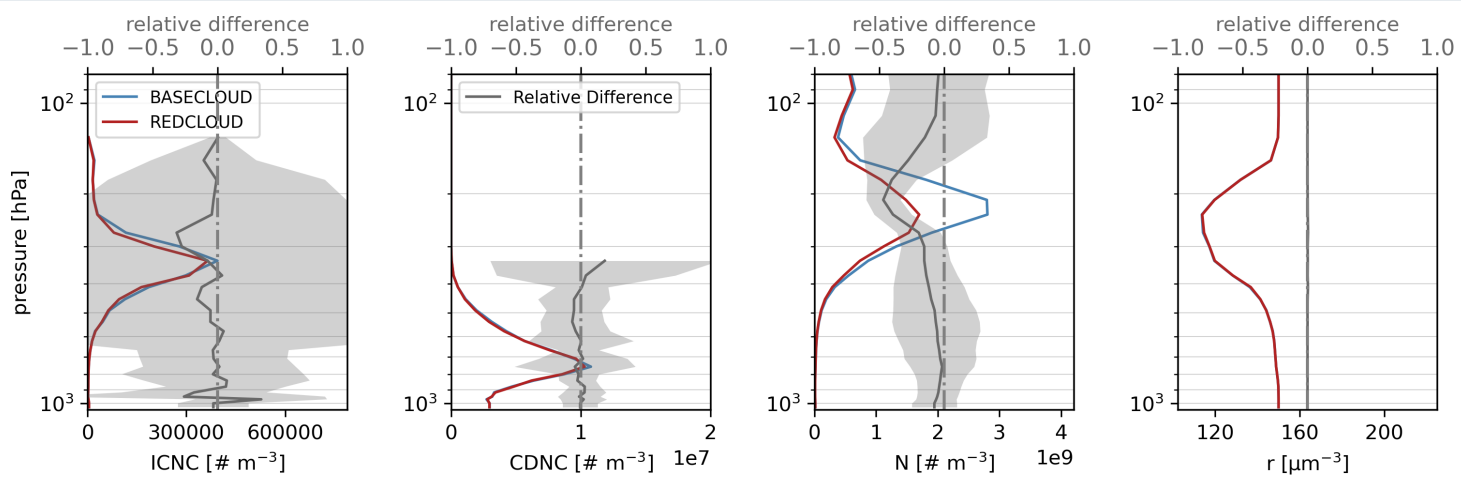
- without cloud interaction, BASE and RED
- with could interaction BASECLOUD and RECLOUD

Effect of reduced emissions

Without aerosol-cloud interaction



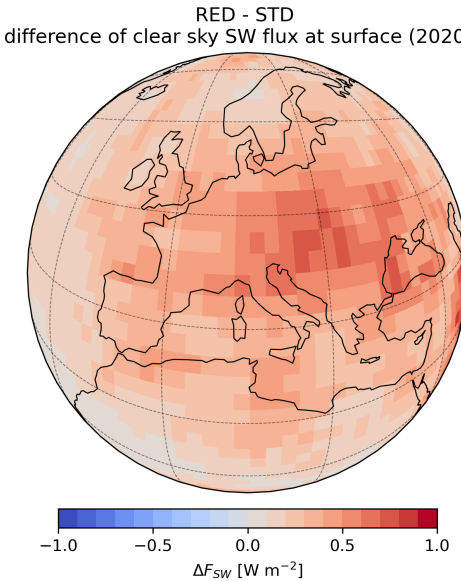
with aerosol cloud interaction



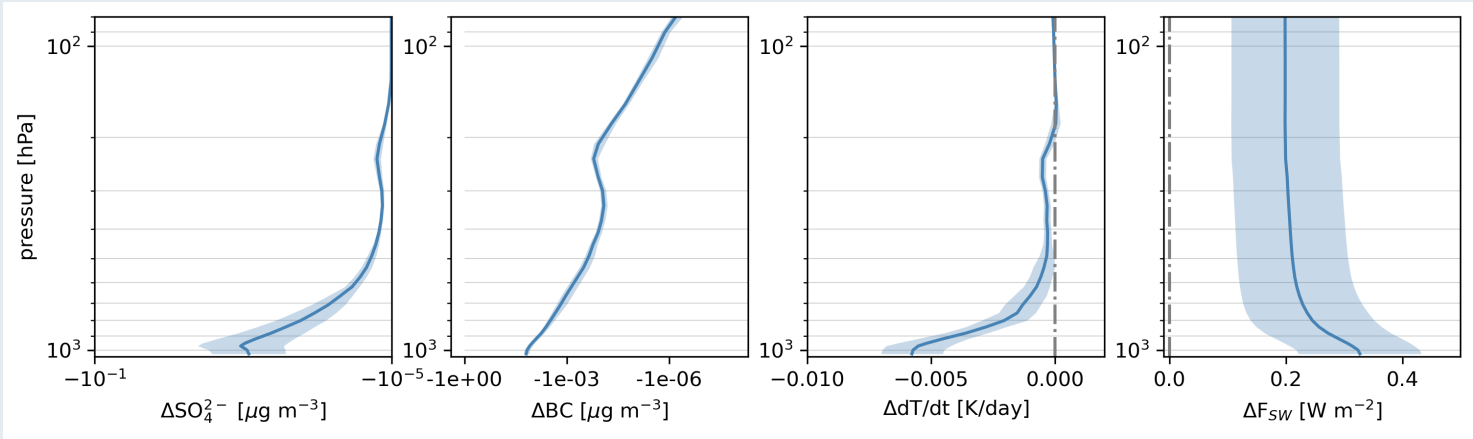
effect of reduced emissions

Aerosol direct and indirect effects on the shortwave radiation flux at the top of atmosphere (TOA) and surface (SRF) over Europe for May.

	RED−STD	REDCLOUD−STDCLOUD	
$\Delta F_{\mathrm{SW}}[Wm^{-2}]$	direct	indirect	total
TOA	0.090 ± 0.035	0.188 ± 0.759	0.281 ± 0.928
TOA clear sky	0.198 ± 0.092	0.000 ± 0.006	0.186 ± 0.106
SRF	0.209 ± 0.053	0.233 ± 1.089	0.443 ± 1.063
SRF clear sky	0.327 ± 0.105	0.001 ± 0.023	0.307 ± 0.115



Effect of reduced emissions

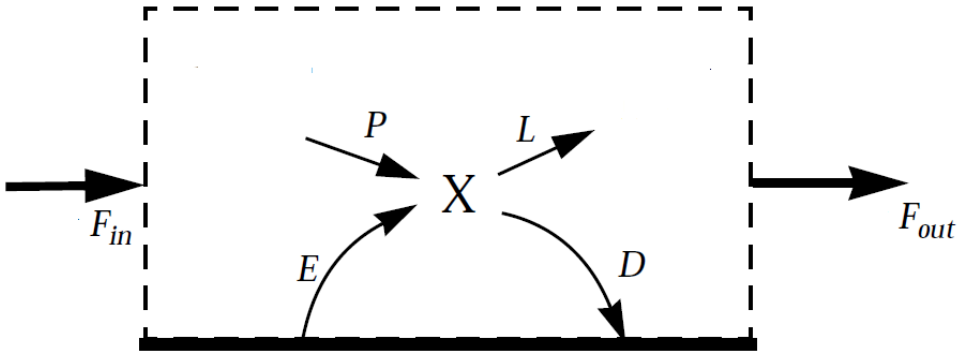


Conclusions:

- Large relative changes in the UT
- Large absolute changes at the surface

All results published here:
https://doi.org/10.5194/acp-22-10901-2022

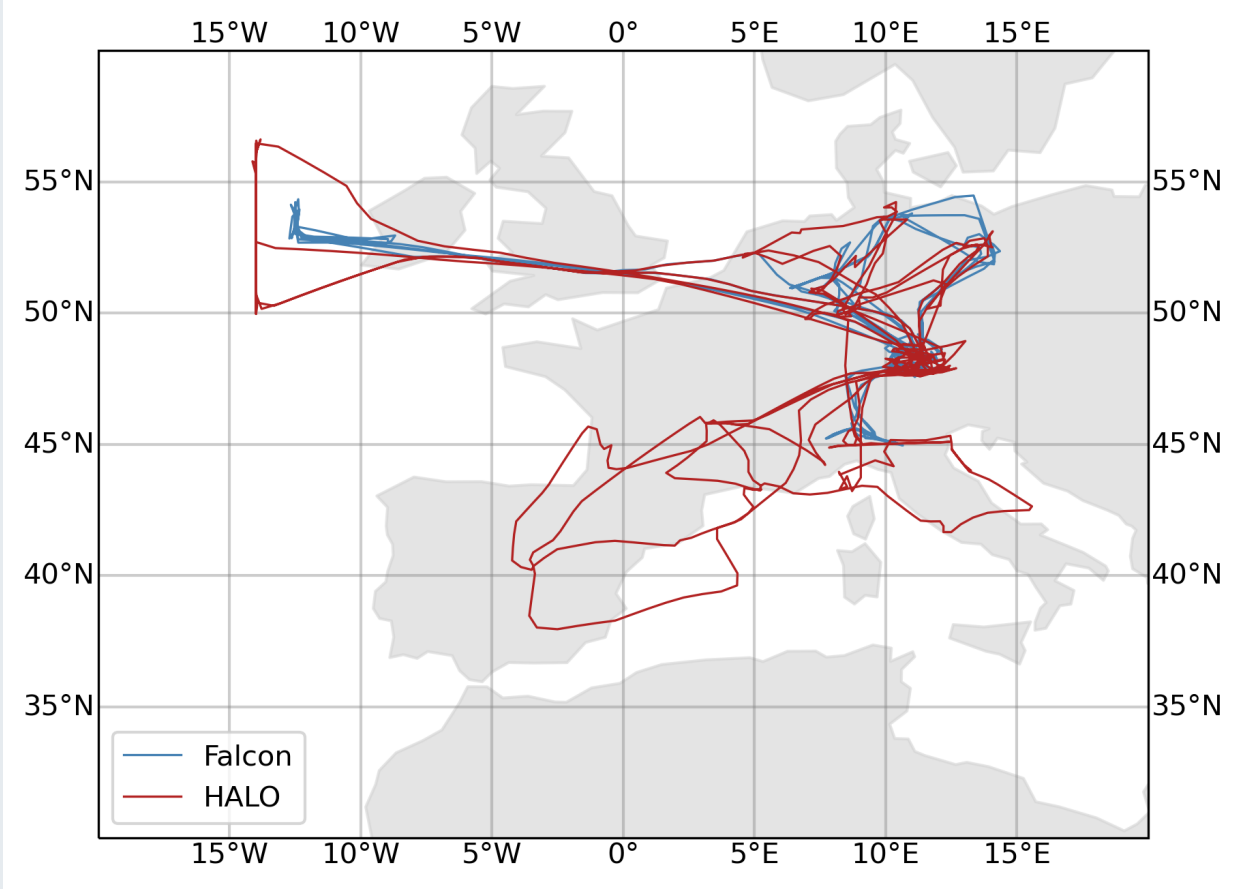
Simple Box Model



Case studies

- Emission
- Deposition
- Transport

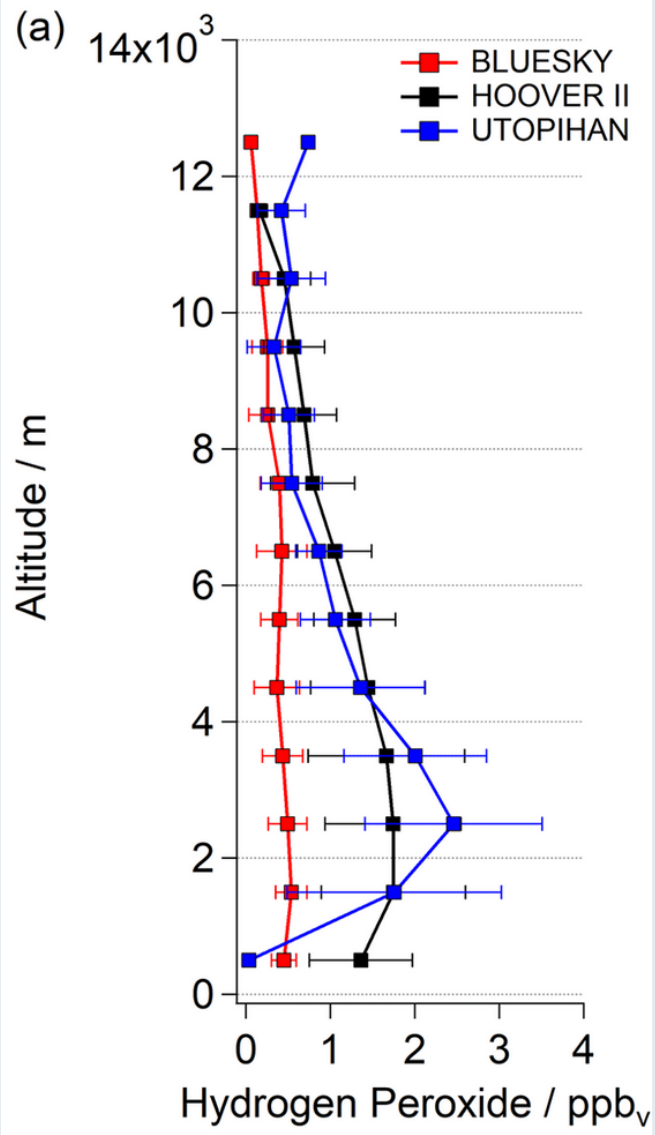
Observations



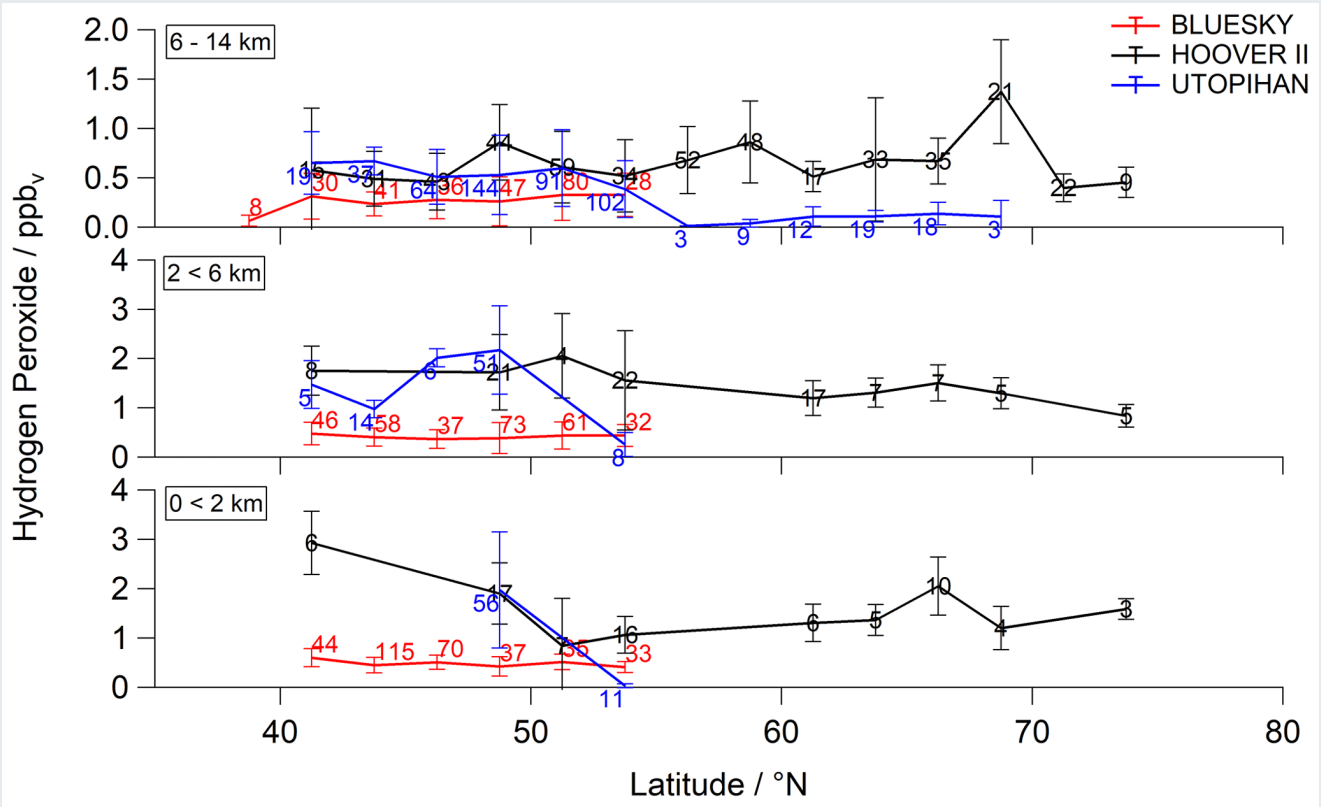
Observations

TRIHOP (TRacer In-situ quantum cascade laser absorption spectrometer/ Hydrogen and Organic Peroxide monitor)
Measurements of H_2O_2


Observations

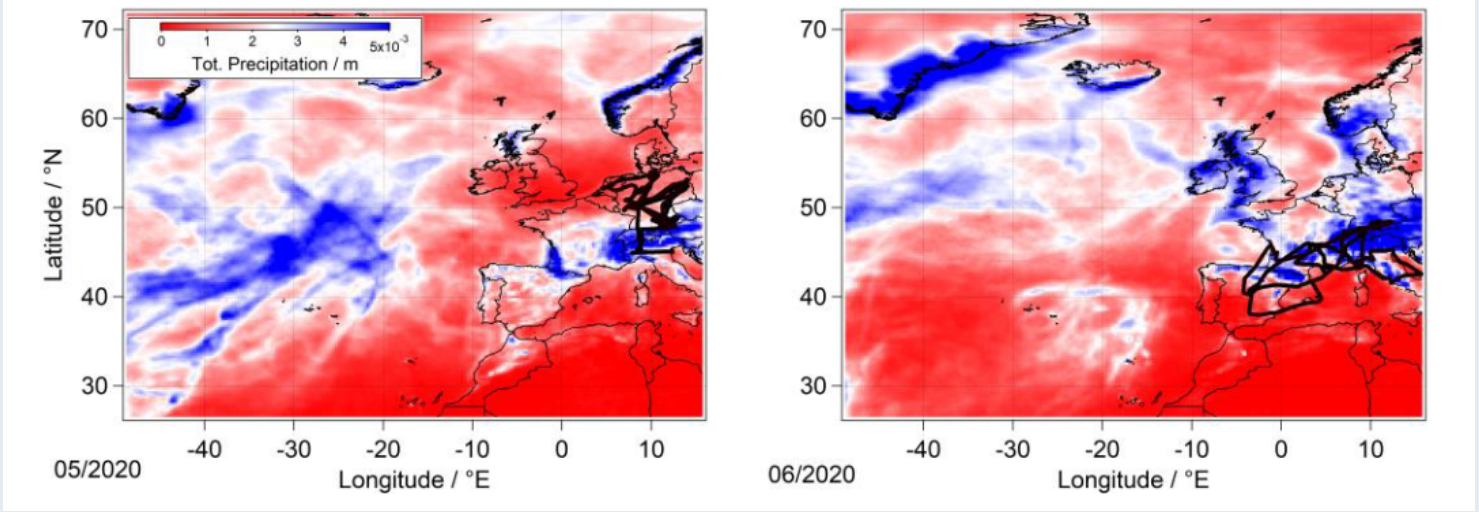


Observations

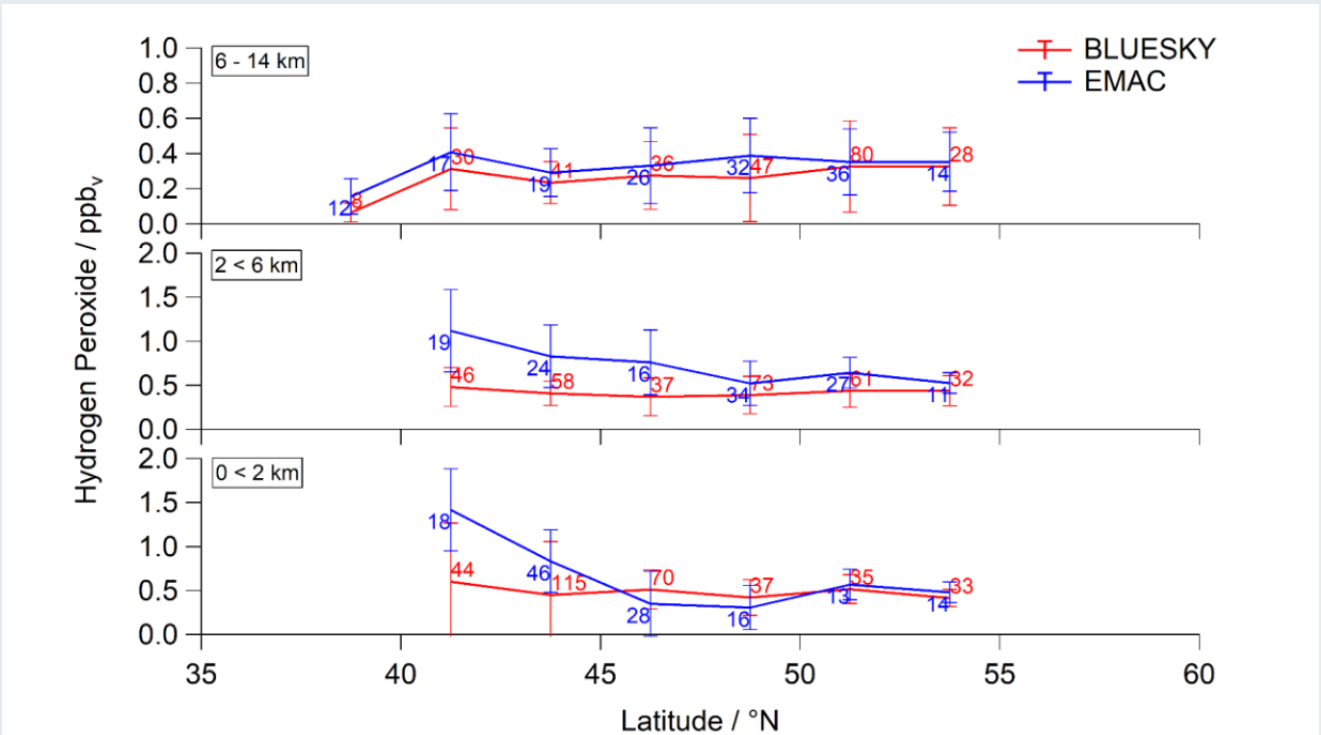


A. Pozzer

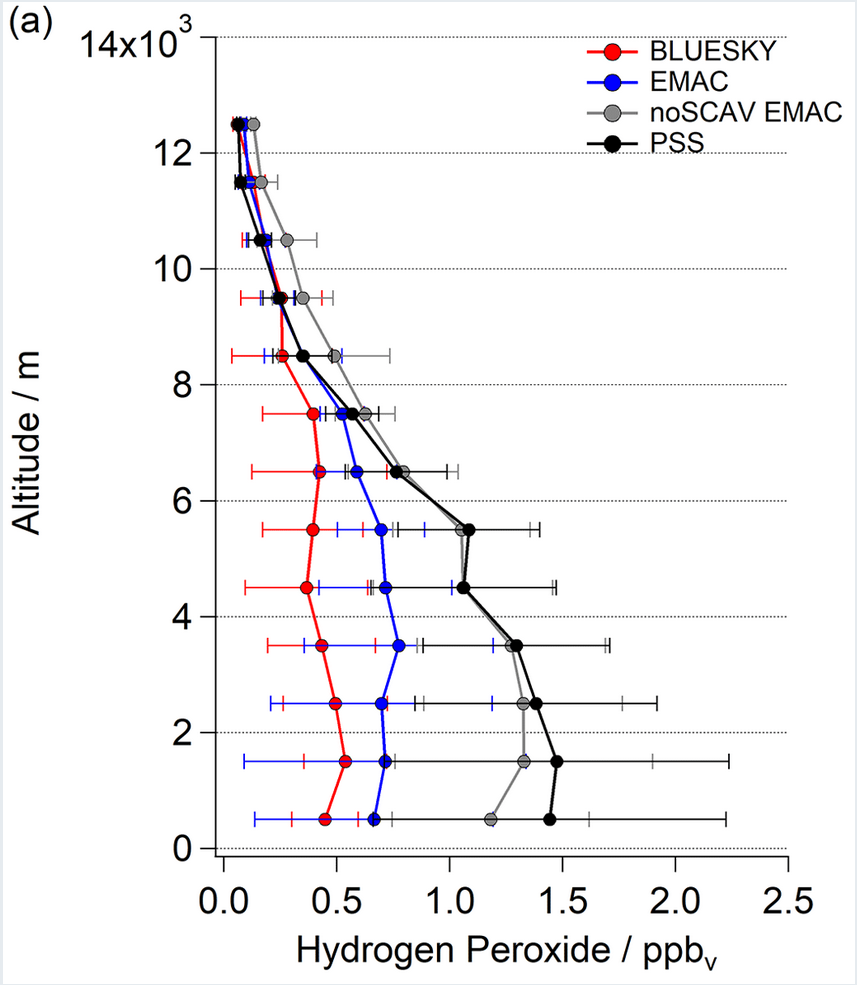
Observations



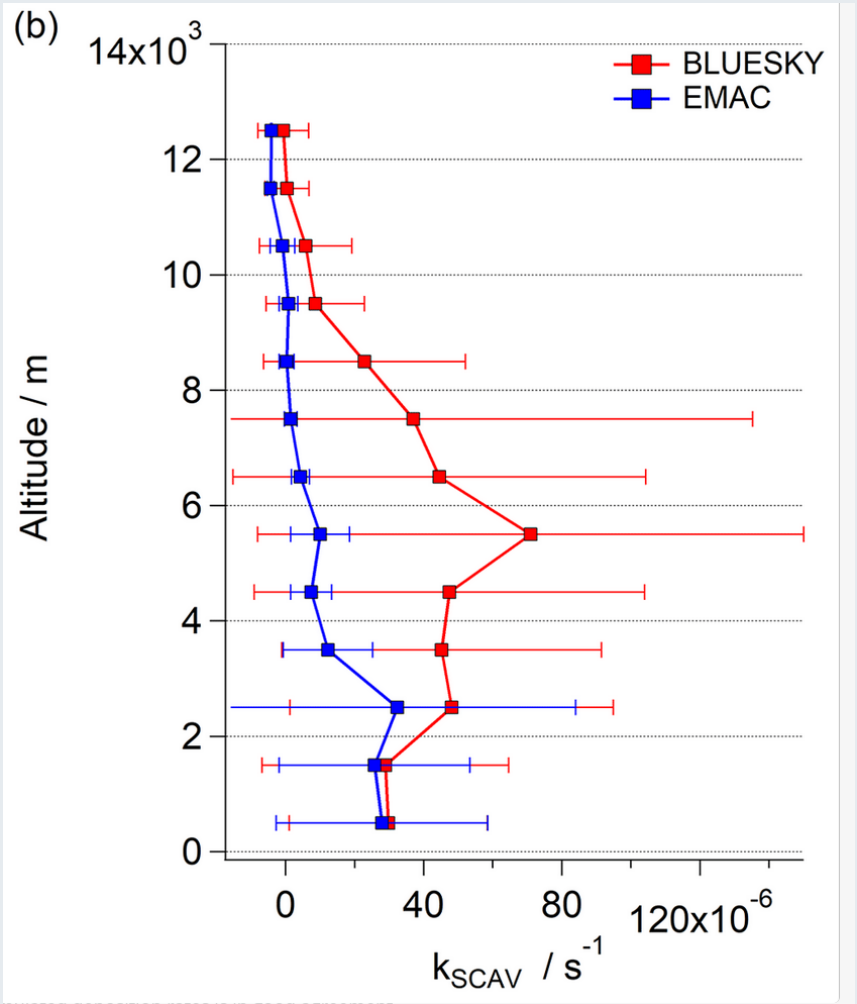
Model-Observations comparison



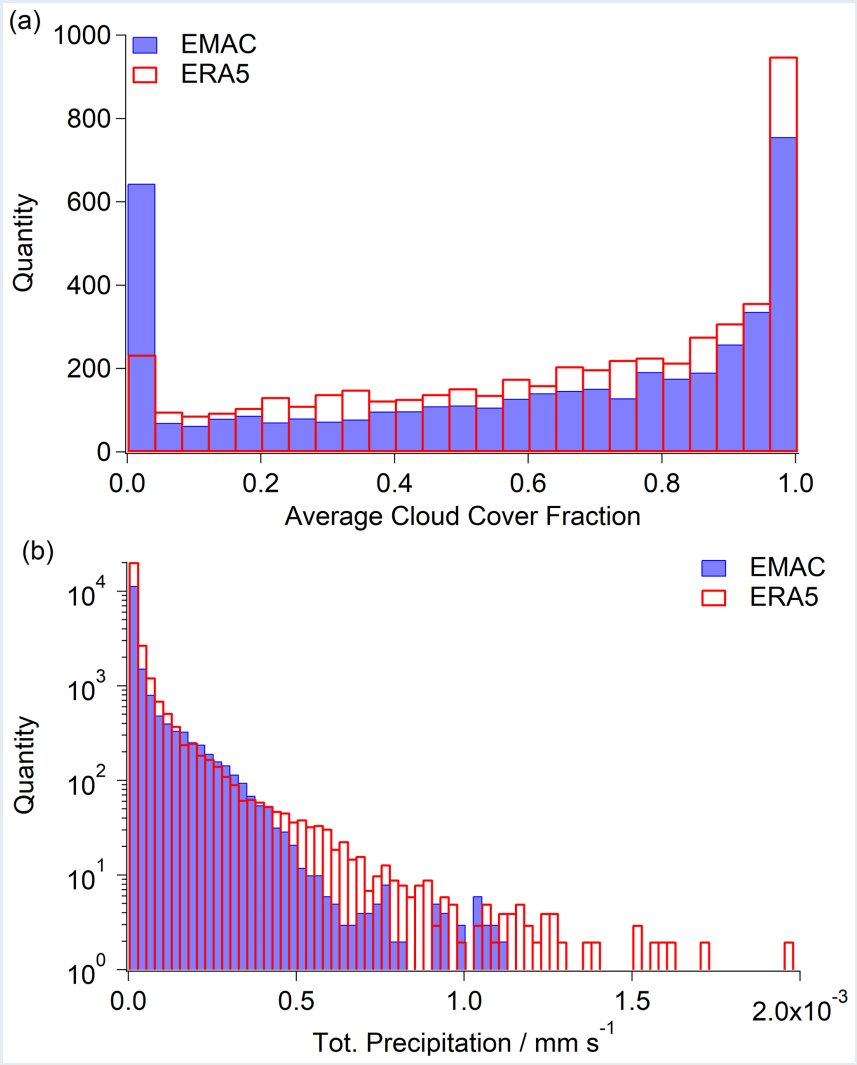
Model-Observations comparison



Effect of deposition



Effect of deposition



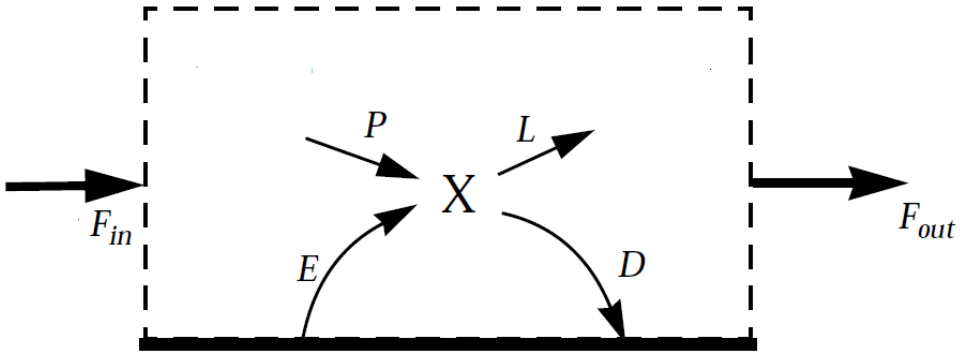
Effect of deposition

Conclusions:

- Precipitation (wet deposition) is important
- Dynamics must be correctly reproduced

See the publication:
https://doi.org/10.5194/acp-22-9483-2022

Simple Box Model



Case studies

- Emission
- Deposition
- Transport

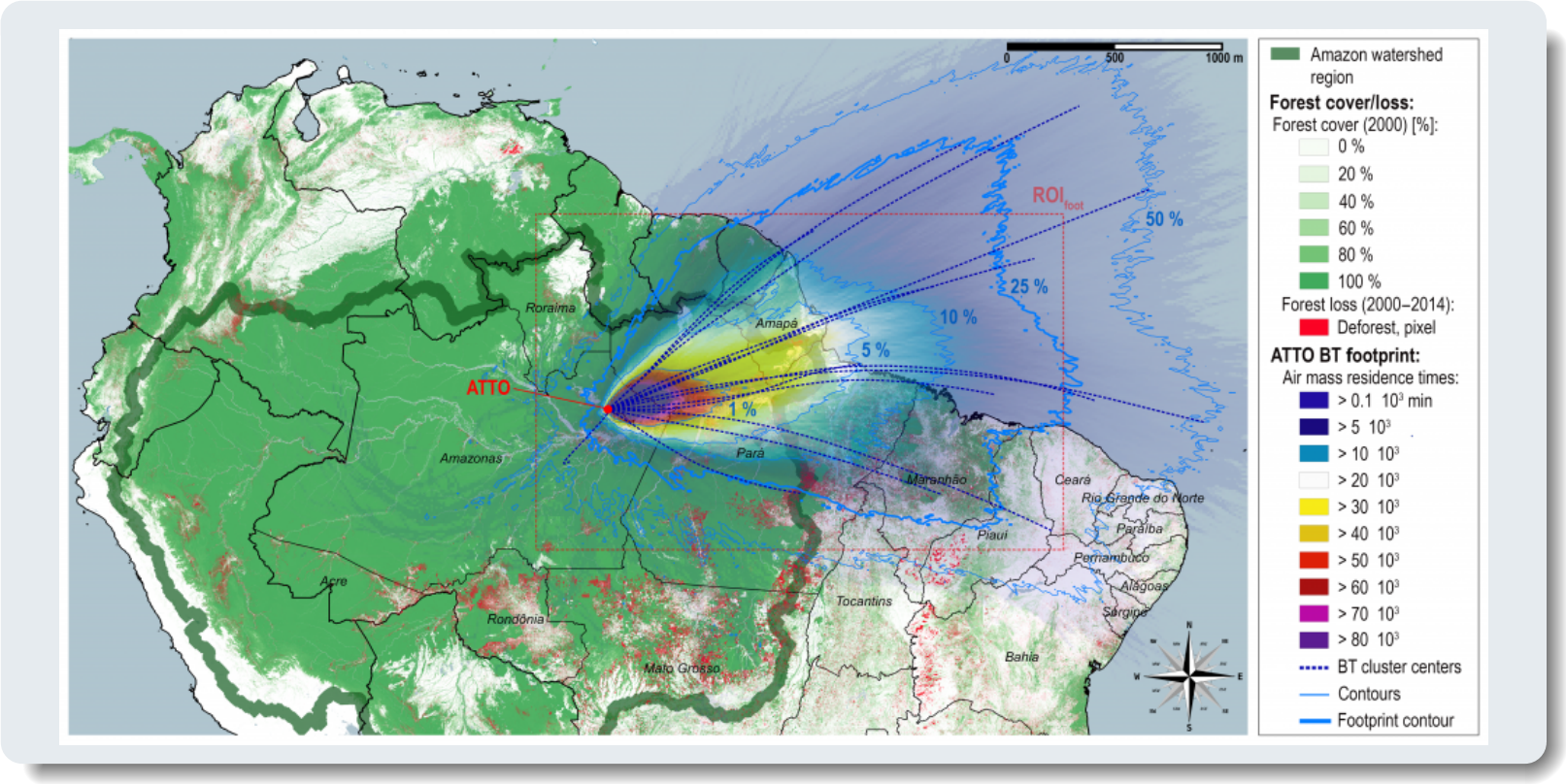
Atmospheric Transport

Is pollutant's transport important for air quality?

ATTO tower

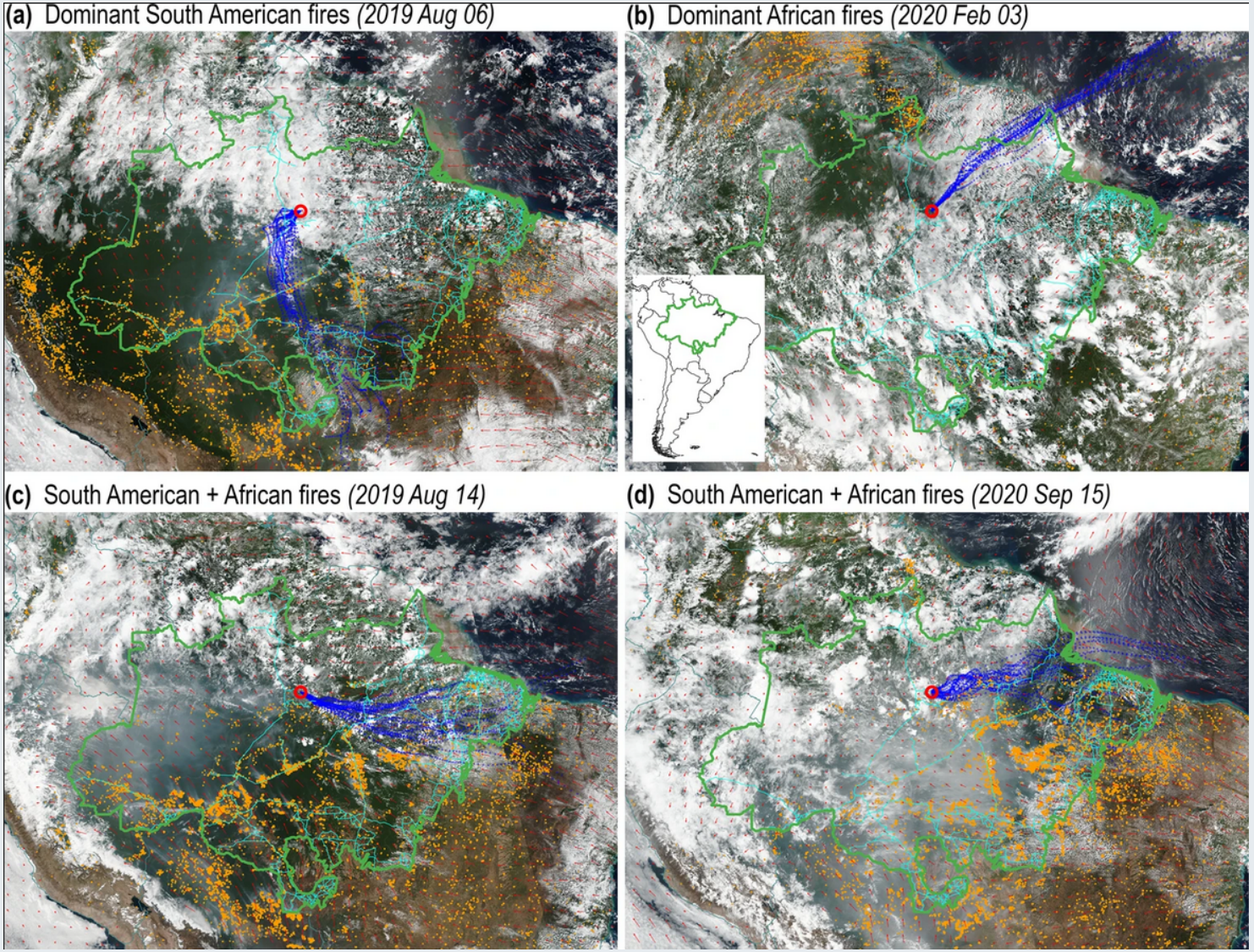
- 325-metre-tall tower in the rainforest
- samples from the soil surface to above the forest canopy
- equipped with a broad range of instruments

ATTO tower



A. Pozzer
30.08.2023

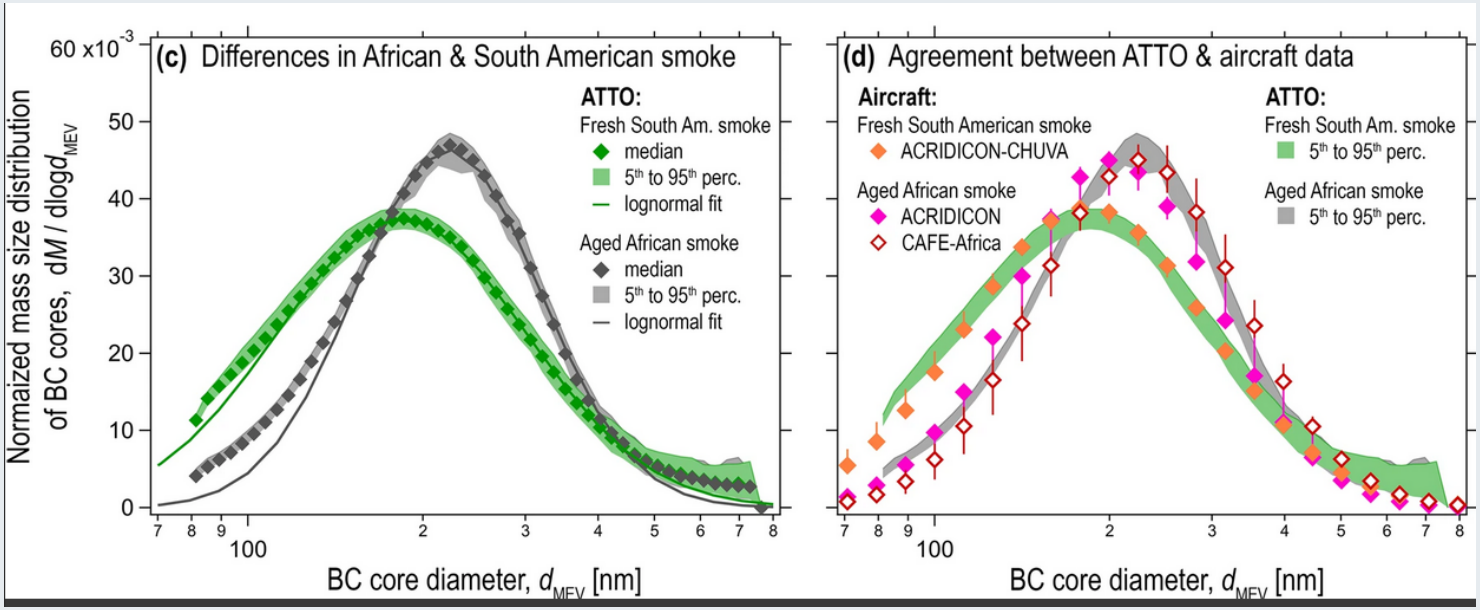
BC measurements



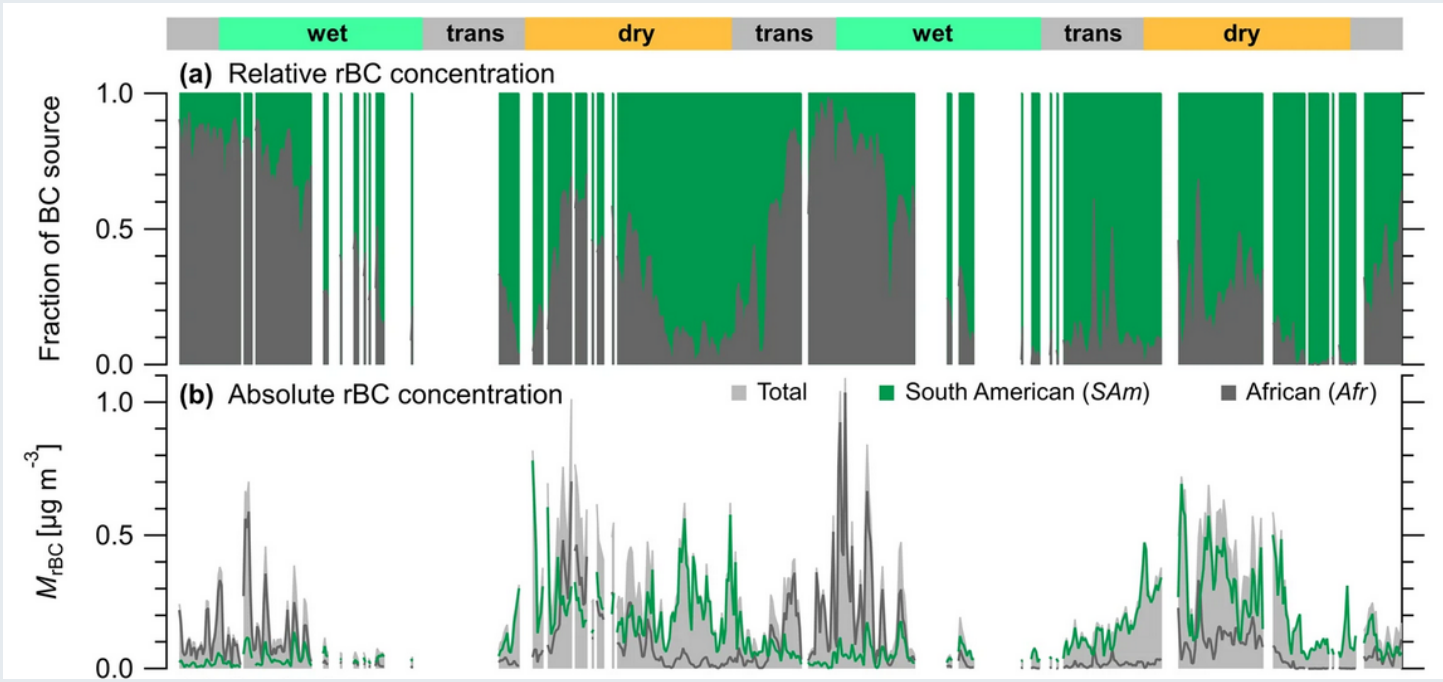
A. Pozzer

30.08.2023

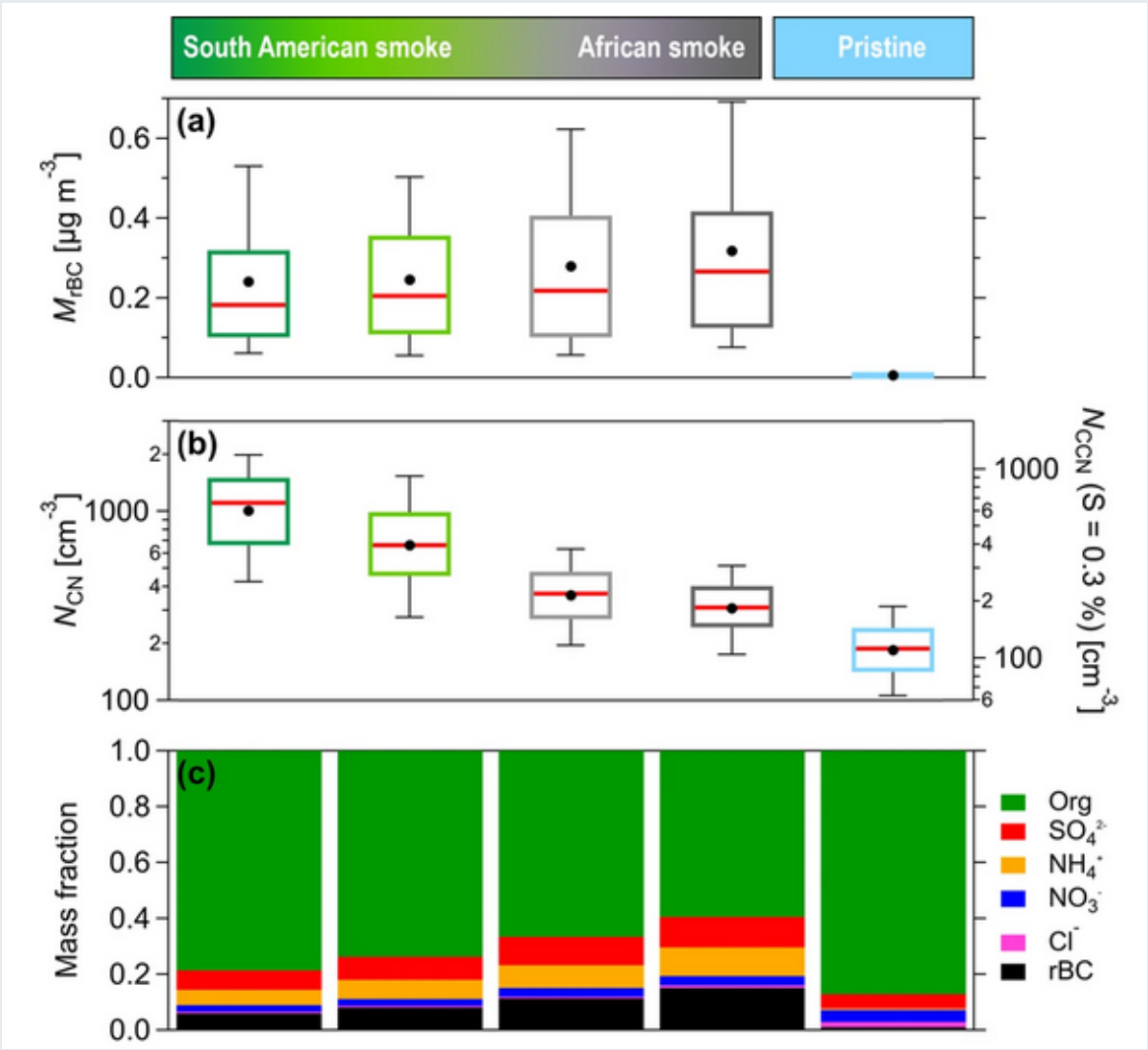
BC measurements



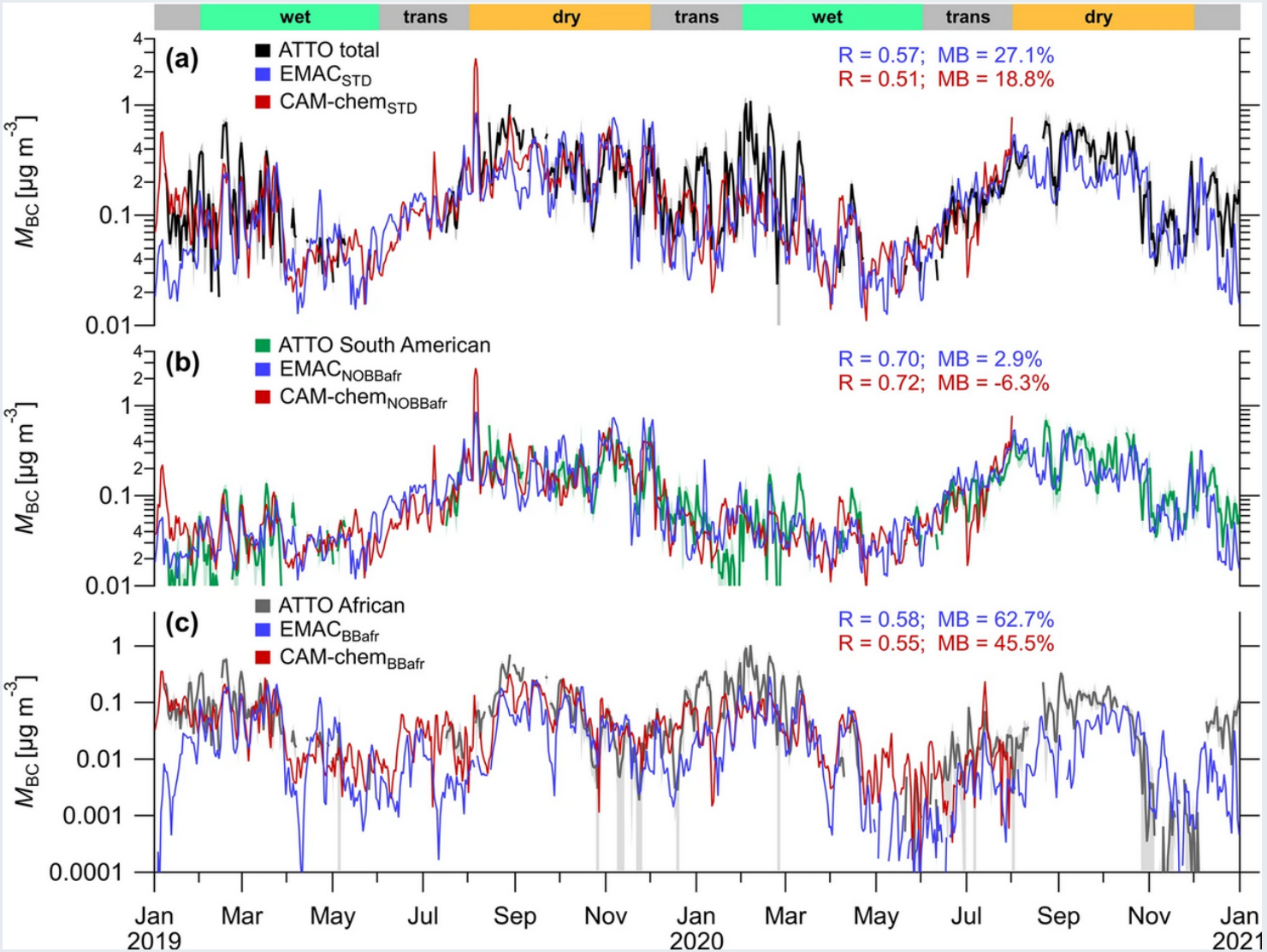
BC measurements



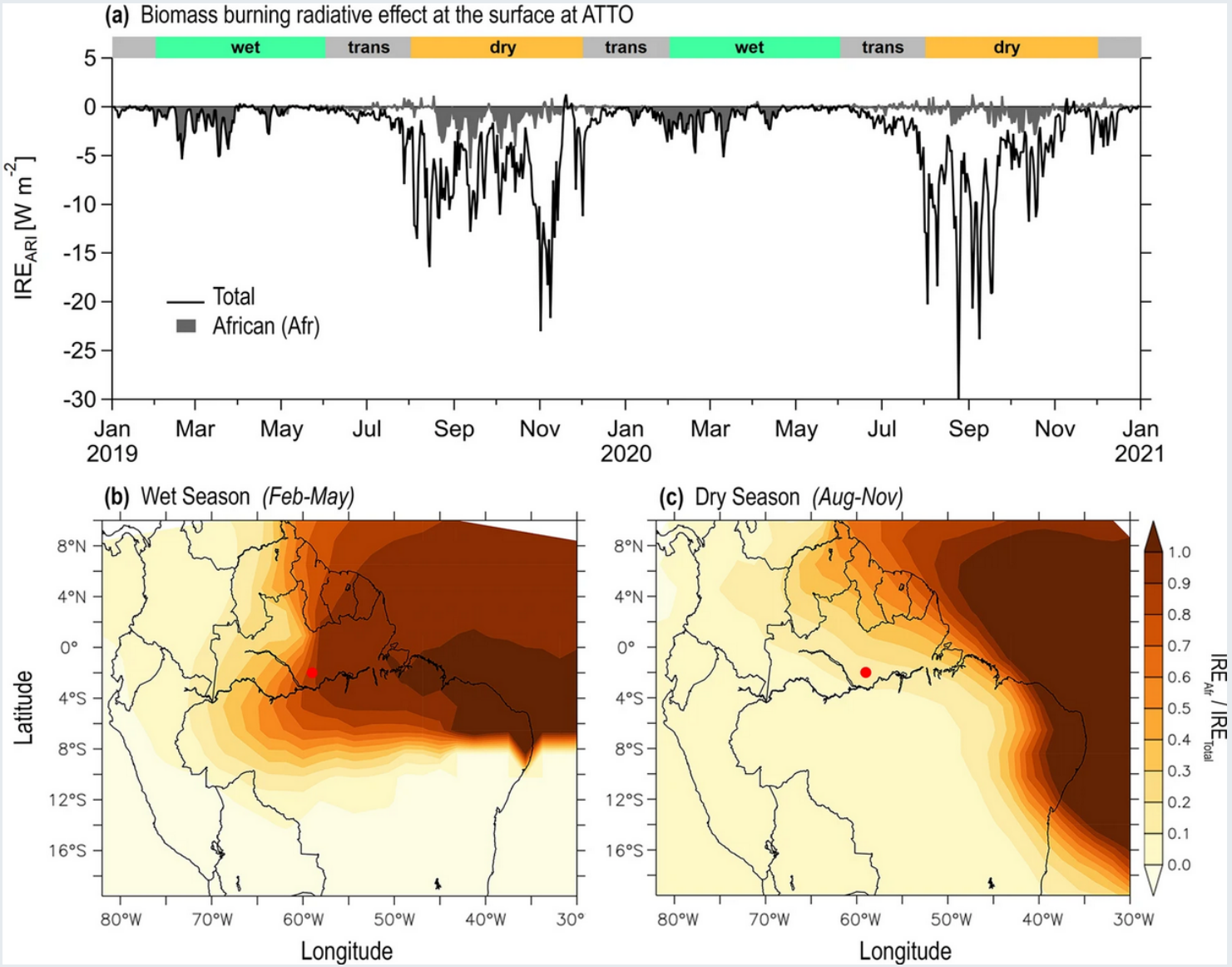
BC measurements



Comparison with the model



Model Results



A. Pozzer
30.08.2023

Transport

Conclusions:

- transport can move pollutants far away from the source region
- such pollutants can impact significantly the local concentration

See the publication:
https://doi.org/10.5194/acp-22-9483-2022

Conclusions

- Emissions, deposition and transport have direct impact on pollutants' concentration
- Multiple processes must be considered when simulating chemistry in the atmosphere
- Numerical model are essential to simulate all process simultaneously

Observations are necessary

- to evaluate the model
- to test the numerical results

Thank you for your attention!

Special thanks to the group at MPIC