Representation of emissions from European major population centres in MECO(n) - Lessons learned from EMeRGe-EU

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Take Home Messages

- We evaluated the MECO(n) model using the EMeRGe-EU measurements focusing on NO_y, CO, SO_2 and O_3.
  - Generally, the model performs well, but specific issues and biases exist.
- Several sensitivity simulations with changes of the model set-up were performed for instance with different emission inventories.
- While the performance of the model improves/deteriorates for individual flights with some changes, the overall performance does not change systematically.
- The ozone source attribution results react much more sensitive on specific model changes compared to the simulated trace gas mixing ratios.
- Accordingly, source attribution results can, especially when sampled only at specific locations, show larger differences of up to 20 %.
  - The largest sources of uncertainties are emissions and the model dynamics.
- Nevertheless, the source attribution results provide important insights into the tropospheric ozone budget and help to understand model biases.

Abstract/Motivation

- Comprehensive regional chemistry-climate or chemistry transport models are needed to study the impact of emissions from major population centres (MPC) and test mitigation options for the MPC emissions.
- Of special interest are model based diagnostics, such as source attribution.
- Before such tools can be employed their performance compared to observations needs to be investigated.
- This comparison helps not only in judging the performance of the models, but allows testing our understanding of chemical and physical processes in the atmosphere.
- A prerequisite for an extensive evaluation of models are the availability of temporally and spatially highly resolved observational data. Such a data set was obtained during the EMeRGe-EU mission.
- We used these data to evaluate the MECO(n) model including analyses of the uncertainties of the source attribution results.

MECO(n) model system

- The MECO(n) model system consists of the global chemistry-climate model EMAC and the regional scale chemistry-climate model COSMO-CLM/MESSy (Kerkweg & Jöckel 2012a/b, Hoffman et al., 2012, Mertens et al., 2016)
- The coupling allows a seamless ‘zooming’ from the global scale into specific areas down to resolutions of around 1 km.
- The coupling between the global and the regional model is performed during runtime.
- For the current study a MECO(3) set-up is applied with three nesting steps over Europe (see Fig.1) :
    - 50 km resolution, 12 km resolution, 7 km resolution
- In the *REF* simulation the EDGAR 4.3.1 emission inventory is applied

Fig 1: Computational domains of the model set-up

Sensitivity studies

- To study the influence of specific model setups systematically, different sensitivity studies were performed.
- Generally, the finest nesting step of these sensitivity studies were 12 km. Therefore, all analyses are performed for the model results at 12 km horizontal resolution.

- The performed simulations are:

- *EMIS*: Change of anthropogenic emissions (VEU2 emission inventory instead of EDGAR 4.3.1).
- *DYN*: EMAC is ‘nudged’ against the ECMWF operational analyses data instead of ERA-Interim.
- *RESO*: The vertical resolution of COSMO is increased from 40 to 50 vertical layers.
- CH4EMIS: The EDGAR 5.0 emissions are used for CH_4 in COSMO instead of prescribed surface CH_4 concentrations.

EMeRGe-EU measurement campaign

- To evaluate the MECO(n) model we used the measurement results of the EMeRGe-EU campaign of the HALO research aircraft.
- The campaign took place in July 2017, focussing on plumes of European cities.
    - Main areas of foci: Benelux, London, Po Valley, Barcelona

Fig 2: Flight tracks (blue) of the EMeRGe-EU campaign (figure taken from halo-db.pa.op.dlr.de/mission/95)

Evaluation of model results (CO)

- Model data are sampled online along the HALO flight track.
- From the results of the different simulations an 'ensemble' mean and min/maximum values are calculated to assess the spread of the model results among the different simulation results.
- For CO the model shows in general an underestimation of CO for mixing ratios above 80 nmol mol^{-1} (see Fig. 3).

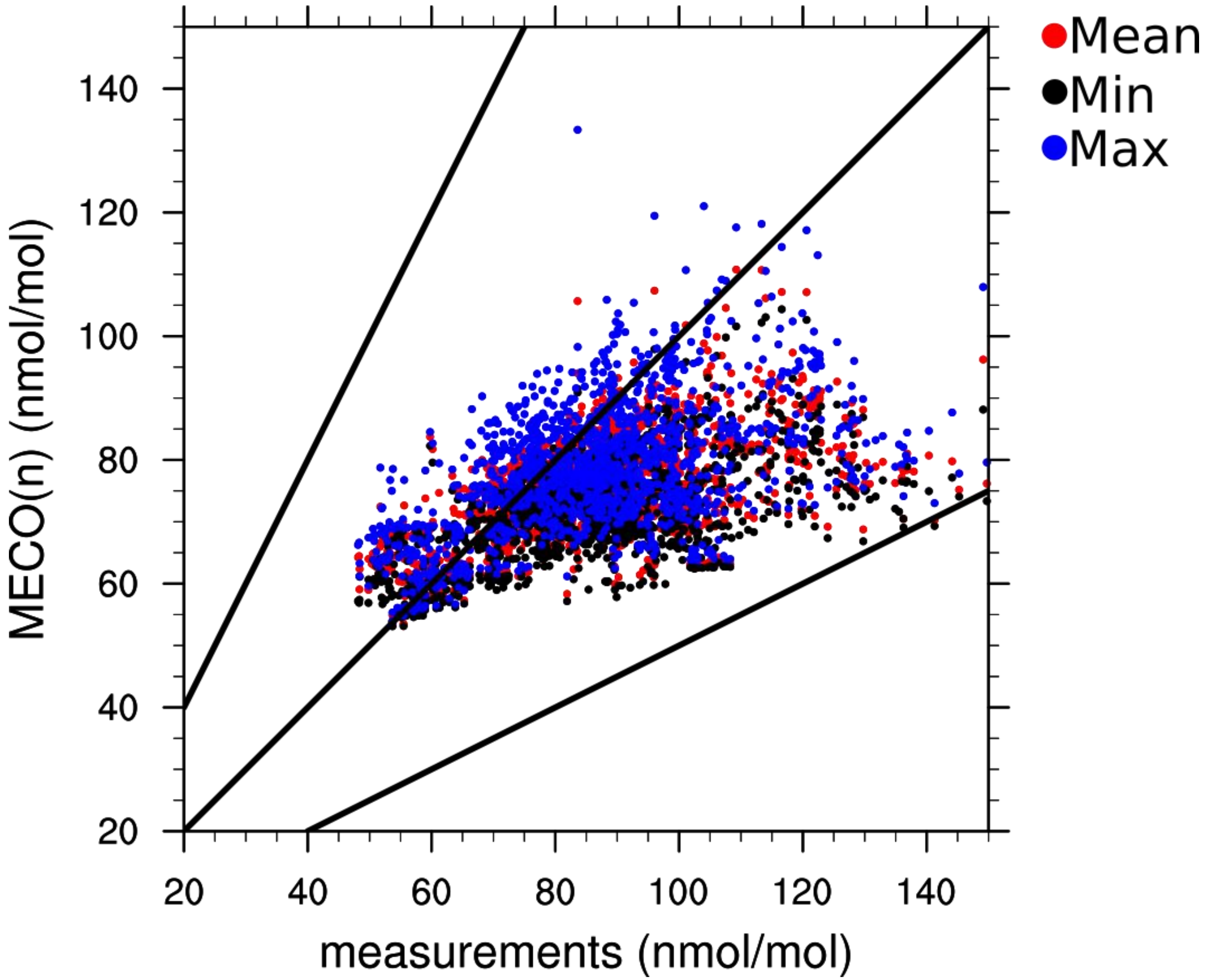

Fig. 3: Scatter plot for measured and simulated CO mixing ratios (nmol/mol).

Evaluation of model results (NO_y)

- Model data are sampled online along the HALO flight track.
- From the results of the different simulations an ‘ensemble’ mean and min/maximum values are calculated to assess the spread of the model results among the different simulation results.
- For NO_y mixing ratios below 2 nmol mol^{-1} measurements and model results agree well (see Fig. 4).
- For several situations a mismatch between model and measured plumes exist (large spread for larger mixing ratios).

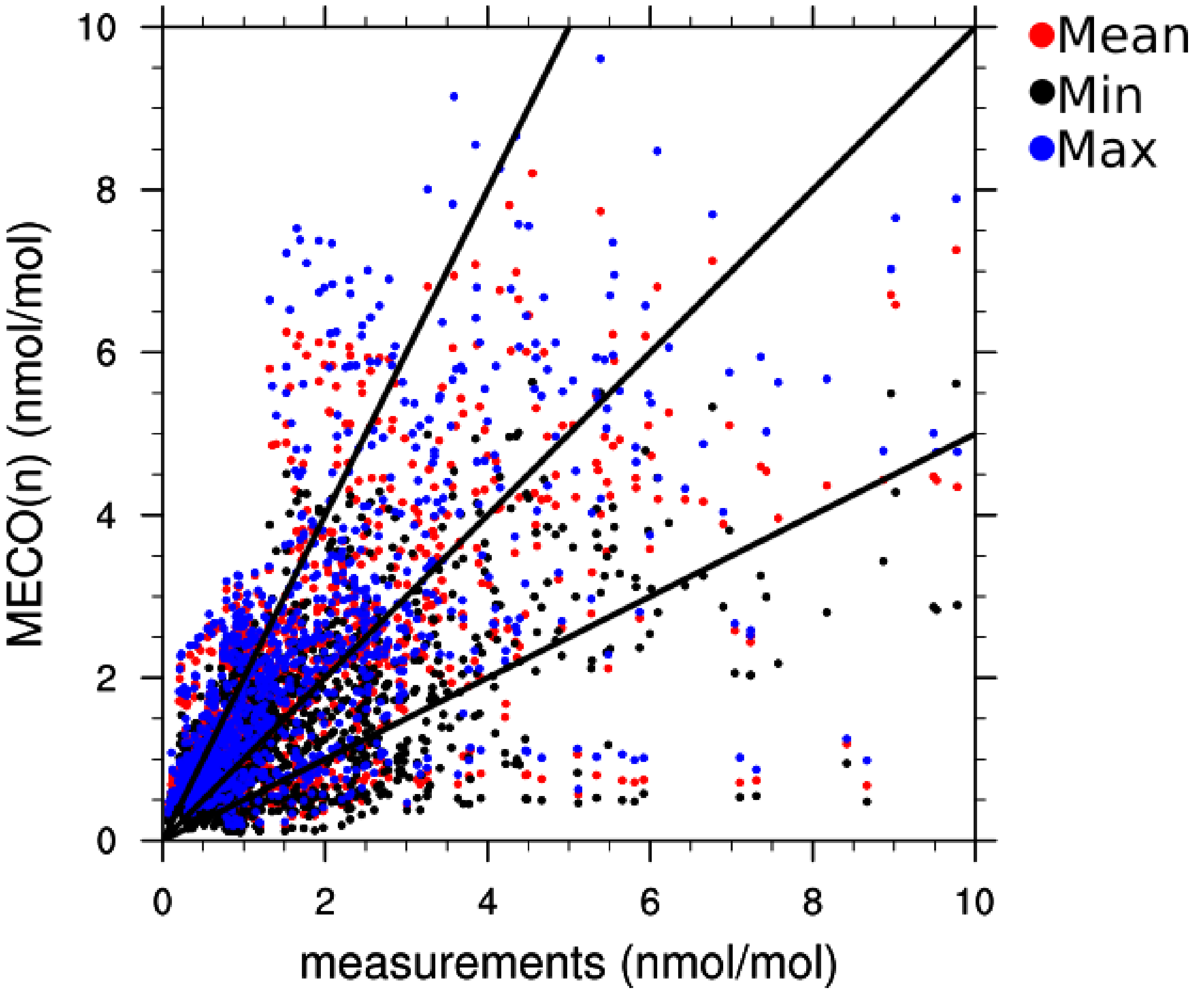

Fig. 4: Scatter plot for measured and simulated NO_y mixing ratios (nmol/mol)

Evaluation of model results (O_3)

- Model data are sampled online along the HALO flight track.
- From the results of the different simulations an ‘ensemble’ mean and min/maximum values are calculated to assess the spread of the model results among the different simulation results.
- The model shows in general a positive ozone bias among all measured mixing ratios (see Fig. 5).

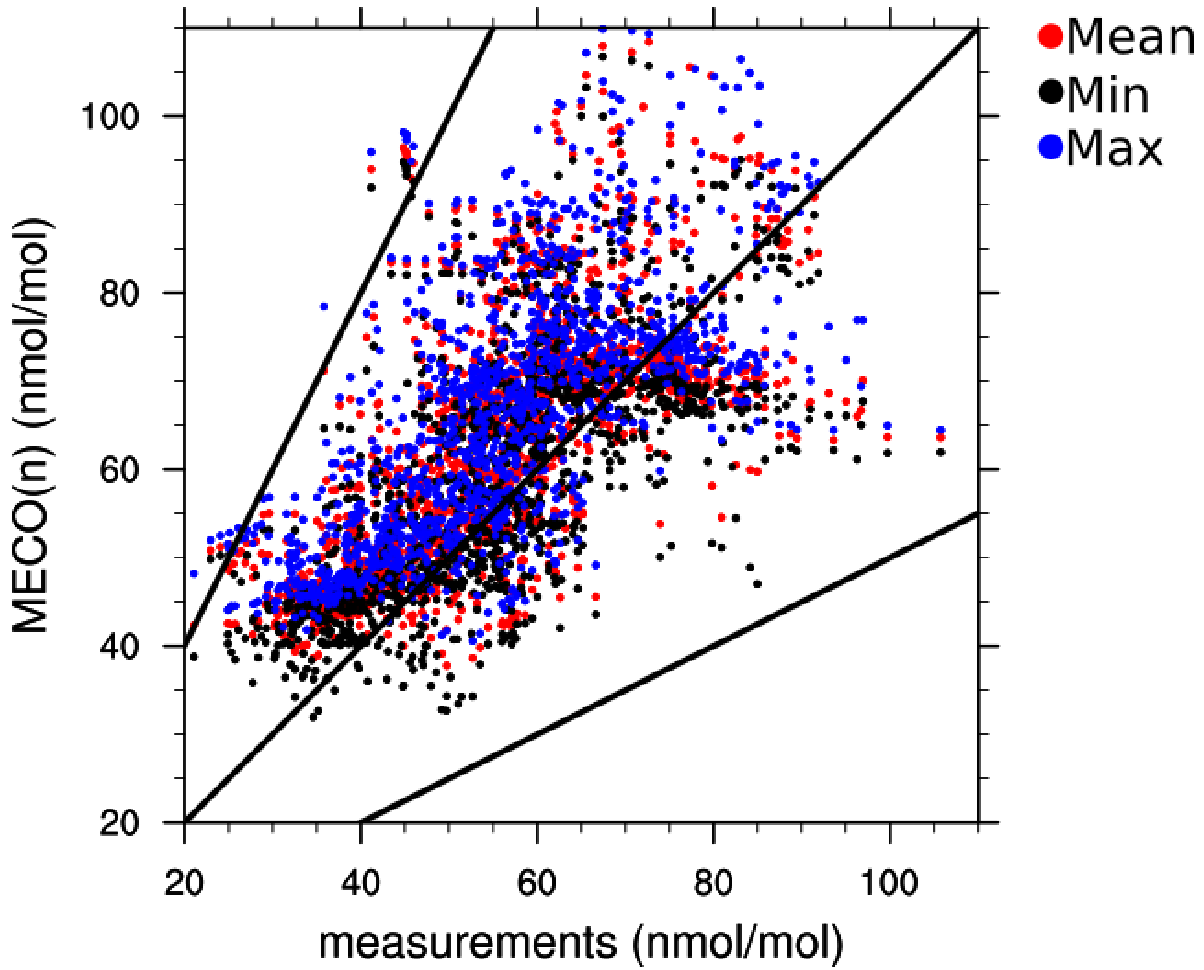

Fig. 5: Scatter plot for measured and simulated O_3 mixing ratios (nmol/mol)

Evaluation of model results (SO_2)

- Model data are sampled online along the HALO flight track.
- From the results of the different simulations an ‘ensemble’ mean and min/maximum values are calculated to assess the spread of the model results among the different simulation results.
- Similar as for NO_y the background values agree well, but a large spread between measured and simulated mixing ratios exist s (see Fig. 6).
    - Mismatch between measured/simulated city plumes

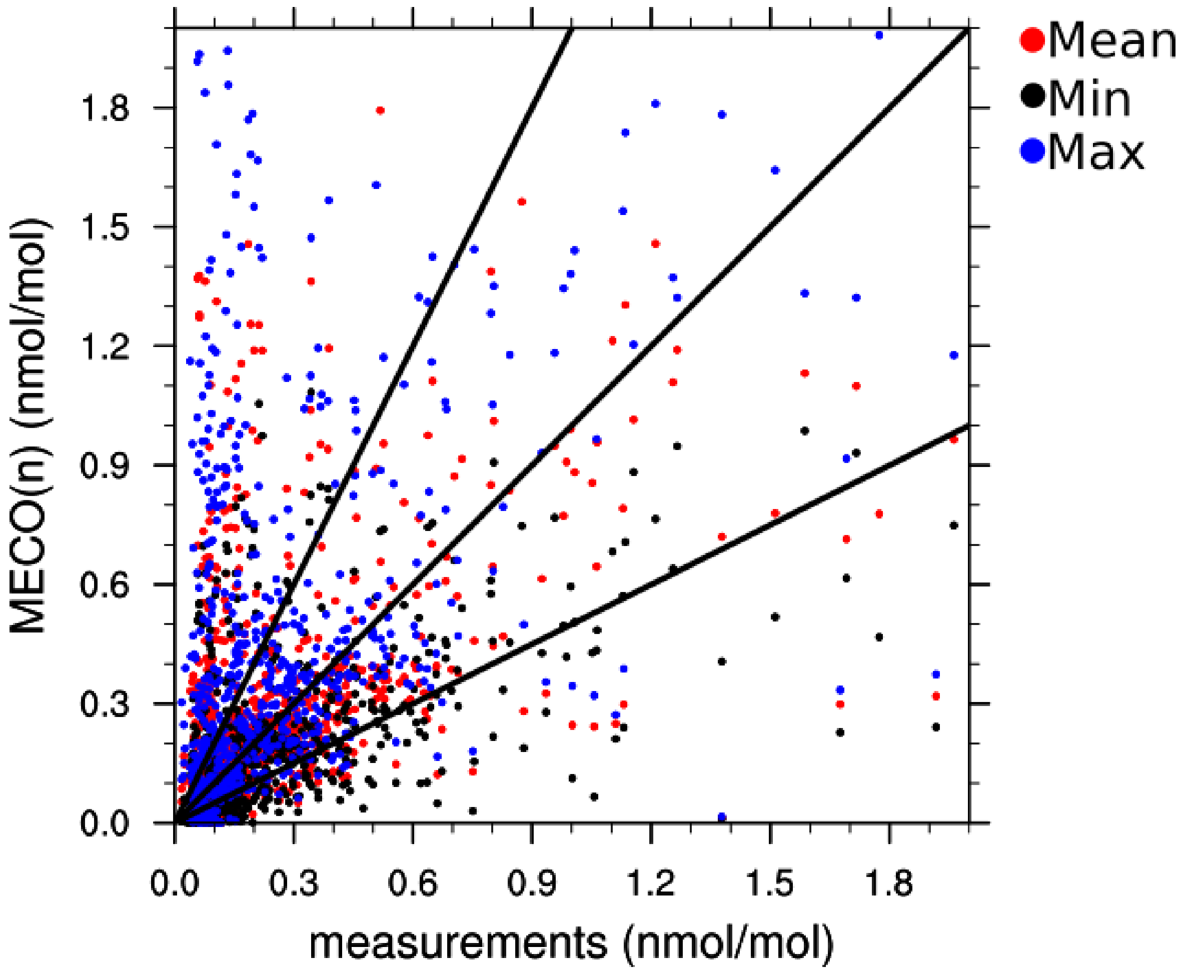

Fig. 6: Scatter plot for measured and simulated SO_2 mixing ratios (nmol/mol)

Evaluation of model results

- Generally, model results and measurements agree well, but specific problems exists.
- Table 1 lists the mean bias errors (MBE) compared to the measurements for all different simulation results.
- Specific model changes improve/deteriorate the representation of specific trace gases or specific events (such as plumes of specific cities).
- None of the model changes leads to an overall improvement of the model results.

	MBE NO_y (nmol mol^{-1})	MBE O_3 (nmol mol^{-1})	MBE CO (nmol mol^{-1})	MBE SO_2 (nmol mol^{-1})
REF	0.01	6.98	-12.8	-0.0015
EMIS	0.26	7.74	-10.1	0.010
DYN	-0.11	6.29	-13.0	0.0200
RESO	0.12	7.74	-12.9	0.0420
CH4EMIS	-0.01	7.25	-12.9	-0.0031

Table 1: Mean bias errors (MBE) in nmol/mol for different species averaged for all flights

Source attribution for ozone

- We apply the TAGGING method of Grewe et al. 2017 (see also Mertens et al, 2020) for source attribution of ozone and ozone precursors. In the applied set-up 12 different emission / source regions are distinguished.
- Fig. 7 depicts the relative contributions of different emission sources to ground-level ozone for July 2017 (*REF* simulation).

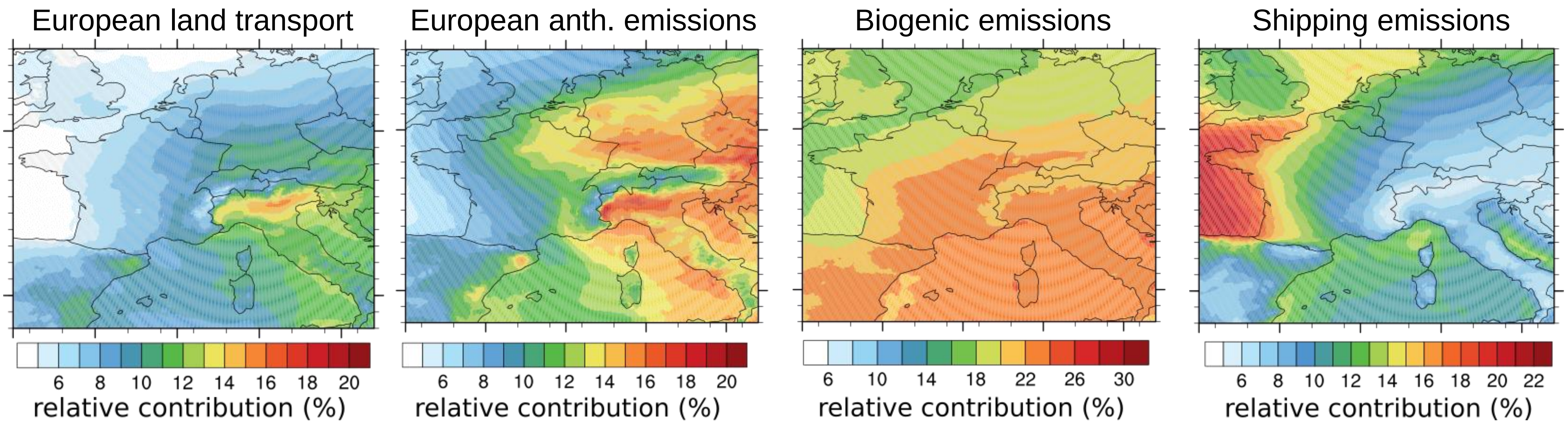

Figure 7: Relative contributions of different emissions sources (in %) to ground-level O_3 averaged for July 2017 (*REF* simulation).

Source attribution for ozone

- These source attribution results are analysed also for the model results sampled along the flight track of HALO.
- These results help to attribute the measured ozone mixing ratios to specific emission sources.
- Further, these results help to understand the simulated ozone budget in more detail and reveal potential reasons for model biases.
- Table 2 gives the average contribution along all model data sampled along the flight track.

	EU land anthropogenic (%)	EU land transport (%)	Stratosphere (%)	Shipping (%)	Biogenic (%)
REF	8.1 %	6.5 %	6.7 %	6.7 %	19.8 %

Table 2: Relative contribution (%) of different emission sources to O_3 averaged for all model data sampled along the HALO flight tracks of the EMeRGe-EU campaign. Results of the *REF* simulation.

Source attribution for ozone

- To investigate the sensitivity of the attribution results on the different changes of the model set-up, Table 3 lists the relative changes of the source attribution results compared to the *REF* simulation results.
- Generally, the contributions are much more variable compared to the mixing ratios of trace gases, and differences in the model set-ups lead to larger differences compared to the trace gases.
- The strongest source of uncertainties for the source attribution are emissions and the model dynamics. The latter is due to geographical/temporal shifts of certain features (such as emission plumes) caused by differences of the model dynamics. In these cases features are not ‘measured’ by the virtual HALO flights.

	Change of contribution from EU anthropogenic (%)	Change of contribution from EU land transport (%)	Change of contribution from Stratosphere (%)	Change of contribution from Shipping (%)	Change of contribution from Biogenic (%)
EMIS	0.1	**+16**	-1.4	-6.2	1.2
DYN	-0.3	**-5.4**	-0.4	**+11**	-0.8
RESO	+ 3.0	+ 1.0	2.2	**-5,8**	+0.2
CH4EMIS	-0.1	-0.5	-1.9	1.2	-0.6

Table 3: Relative change of the relative contributions (%) of different emission sources to O_3 compared to the *REF* simulation. Data are averaged for all model data sampled along the HALO flight tracks of the EMeRGe-EU campaign.

Source attribution for ozone

- The large sensitivity of the source attribution results can also be observed in the monthly average data. As an example, the O_3 mixing ratios of the *REF* and *EMIS* simulations show only small differences. The differences between the absolute contributions of land transport emissions, however, is larger than for O_3.
- This indicates that source attribution results are very sensitive on different model uncertainties, which must be kept in mind when analysing results.

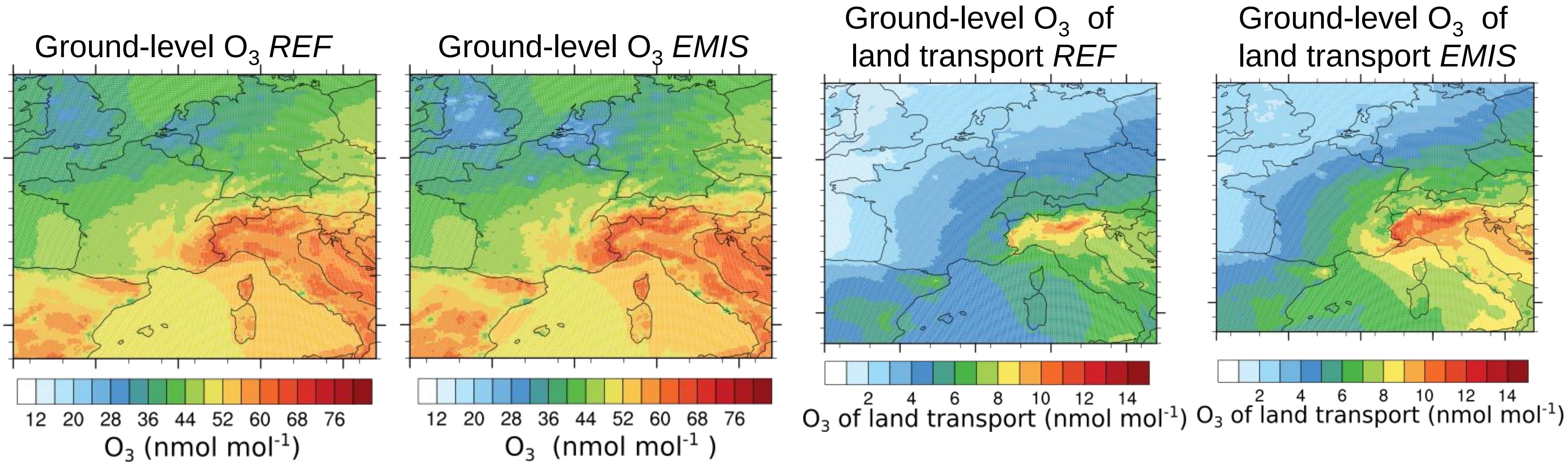

Figure 8: Ground-level O_3 and absolute contribution of land transport emissions to O_3 (both in nmol/mol) averaged for July 2017 for the *REF* and *EMIS* simulation.

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Outlook

- For individual flights more detailed investigations of the different sensitivity studies will be performed to investigate, if specific physical/chemical processes are captured well by the model.
- Ground-level observations will be included in the study to judge the performance of the different emission inventories in more detail.
- Similar analyses are ongoing for EMeRGe-ASIA (March/April 2018).
- All model results are available for the EMeRGe community.

References

- Grewe, V., Tsati, E., Mertens, M., Frömming, C., & Jöckel, P.: Contribution of emissions to concentrations: the TAGGING 1.0 submodel based on the Modular Earth Submodel System (MESSy 2.52), Geoscientific Model Development, 10, 2615–2633, doi: 10.5194/gmd-10-2615-2017, URL https://www.geosci-model-dev.net/10/2615/2017/ (2017)
- Kerkweg, A. & Jöckel, P.: The 1-way on-line coupled atmospheric chemistry model system MECO(n) – Part 2: On-line coupling with the Multi-Model-Driver (MMD), Geoscientific Model Development, 5, 111–128, doi: 10.5194/gmd-5-111-2012, URL http://www.geosci-model-dev.net/5/111/2012/ (2012a)
- Kerkweg, A. & Jöckel, P.: The 1-way on-line coupled atmospheric chemistry model system MECO(n) – Part 1: Description of the limited-area atmospheric chemistry model COSMO/MESSy, Geoscientific Model Development, 5, 87–110, doi: 10.5194/gmd-5-87-2012, URL http://www.geosci-model-dev.net/5/87/2012/ (2012b)
- Hofmann, C., Kerkweg, A., Wernli, H., & Jöckel, P.: The 1-way on-line coupled atmospheric chemistry model system MECO(n) – Part 3: Meteorological evaluation of the on-line coupled system, Geoscientific Model Development, 5, 129–147, doi: 10.5194/gmd-5-129-2012, URL http://www.geosci-model-dev.net/5/129/2012/ (2012)
- Mertens, M., Kerkweg, A., Jöckel, P., Tost, H., & Hofmann, C.: The 1-way on-line coupled model system MECO(n) – Part 4: Chemical evaluation (based on MESSy v2.52), Geoscientific Model Development, 9, 3545–3567, doi: 10.5194/gmd-9-3545-2016, URL http://www.geosci-model-dev.net/9/3545/2016/ (2016)
- Mertens, M., Kerkweg, A., Grewe, V., Jöckel, P., & Sausen, R.: Are contributions of emissions to ozone a matter of scale? – a study using MECO(n) (MESSy v2.50), Geoscientific Model Development, 13, 363–383, doi: 10.5194/gmd-13-363-2020, URL https://www.geosci-model-dev.net/13/363/2020/ (2020)