

HARMO21

27 – 30 September 2022, Aveiro, Portugal

SO₂ and NO_x peak concentrations, vertical profiles and model-identified origins from distant sources

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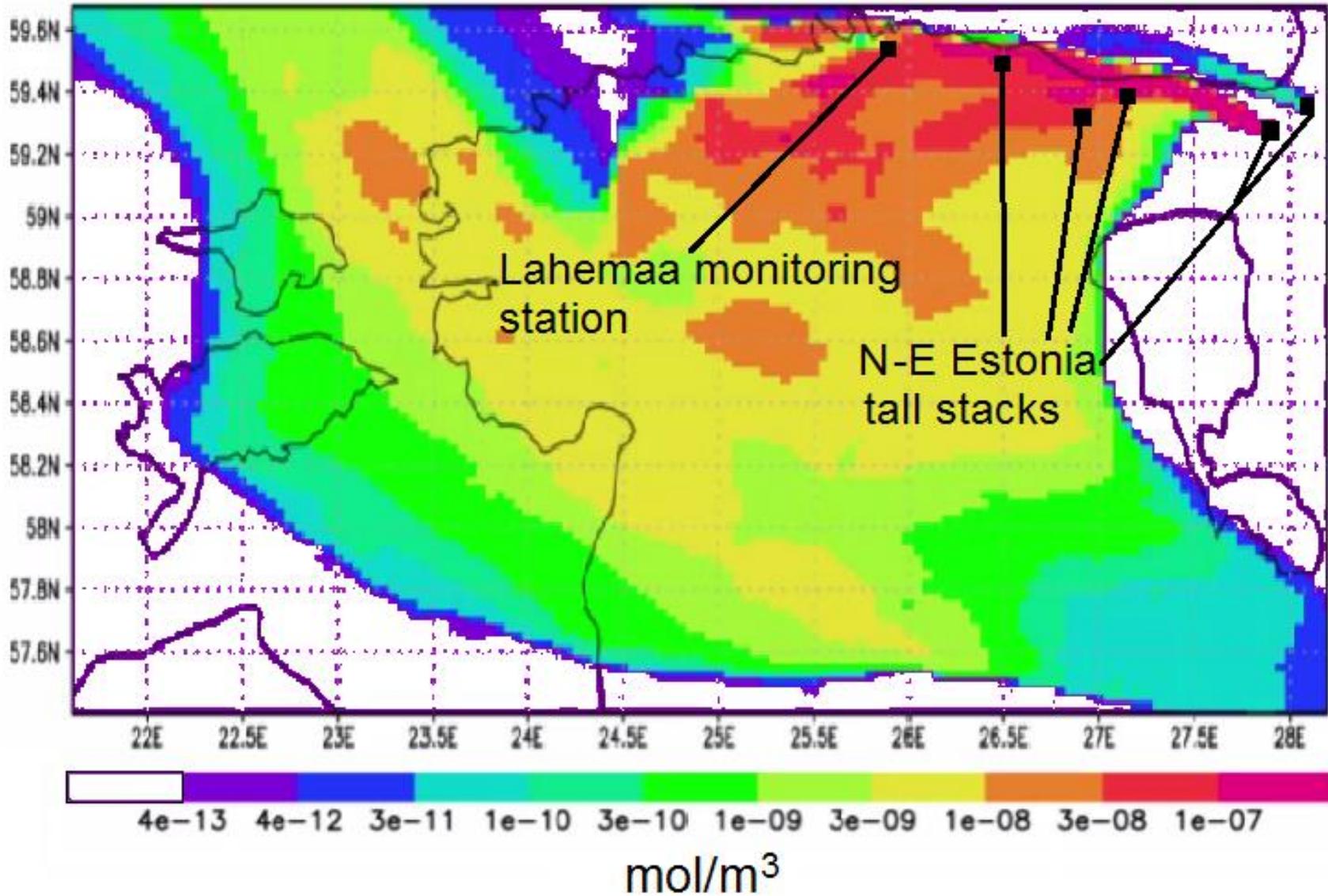
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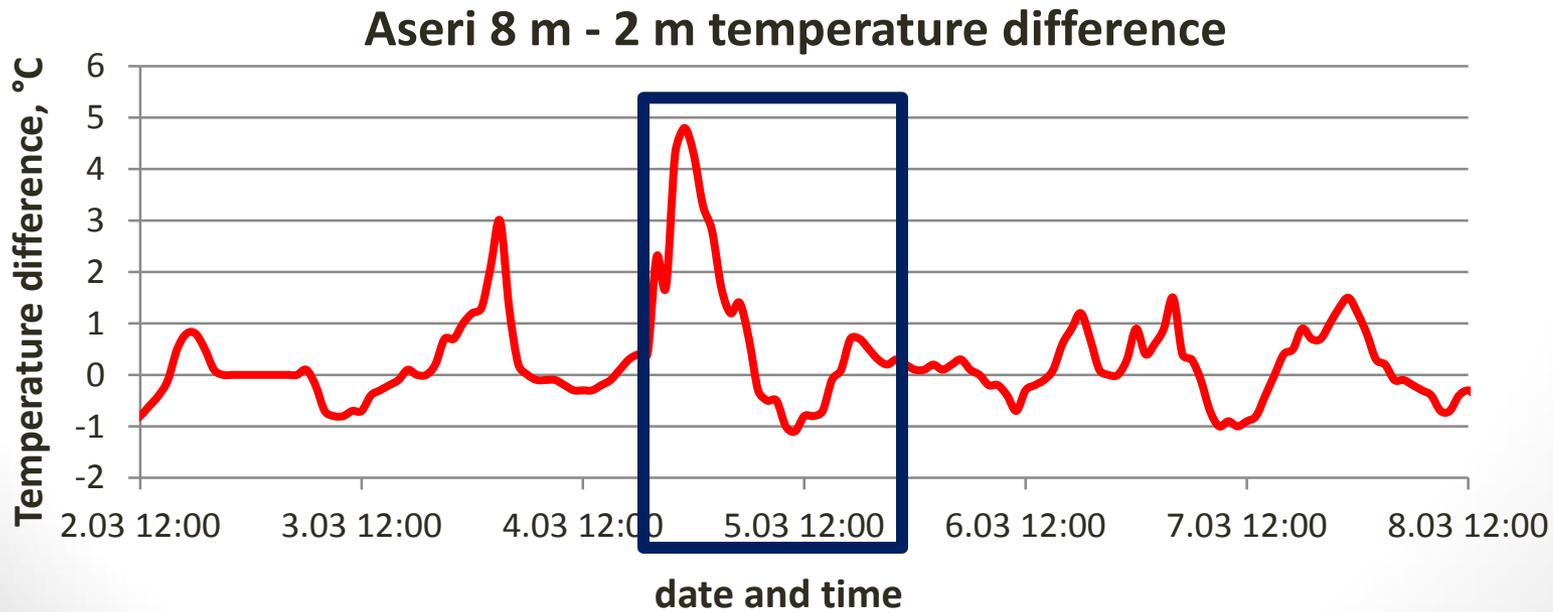
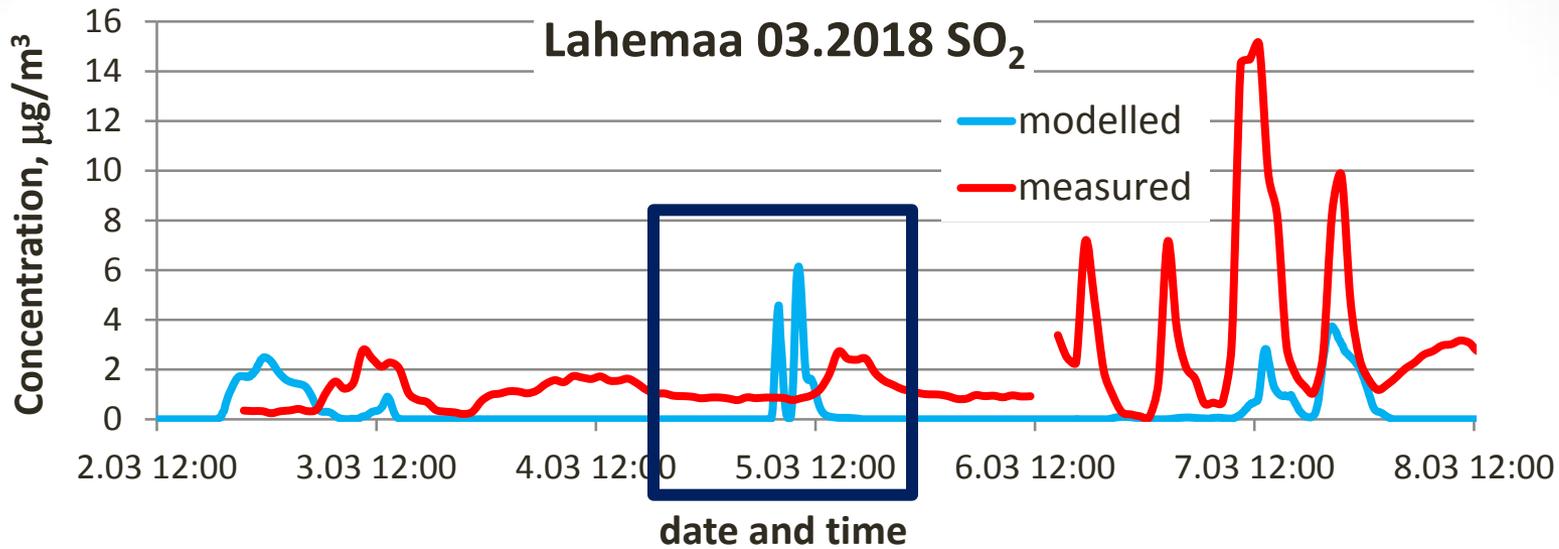
³Institute of Forestry and Rural Engineering, Estonian University of Life Sciences, Tartu, Estonia

Context

SO₂ concentration 10Z05MAR2018, z = 12.5 m



Context

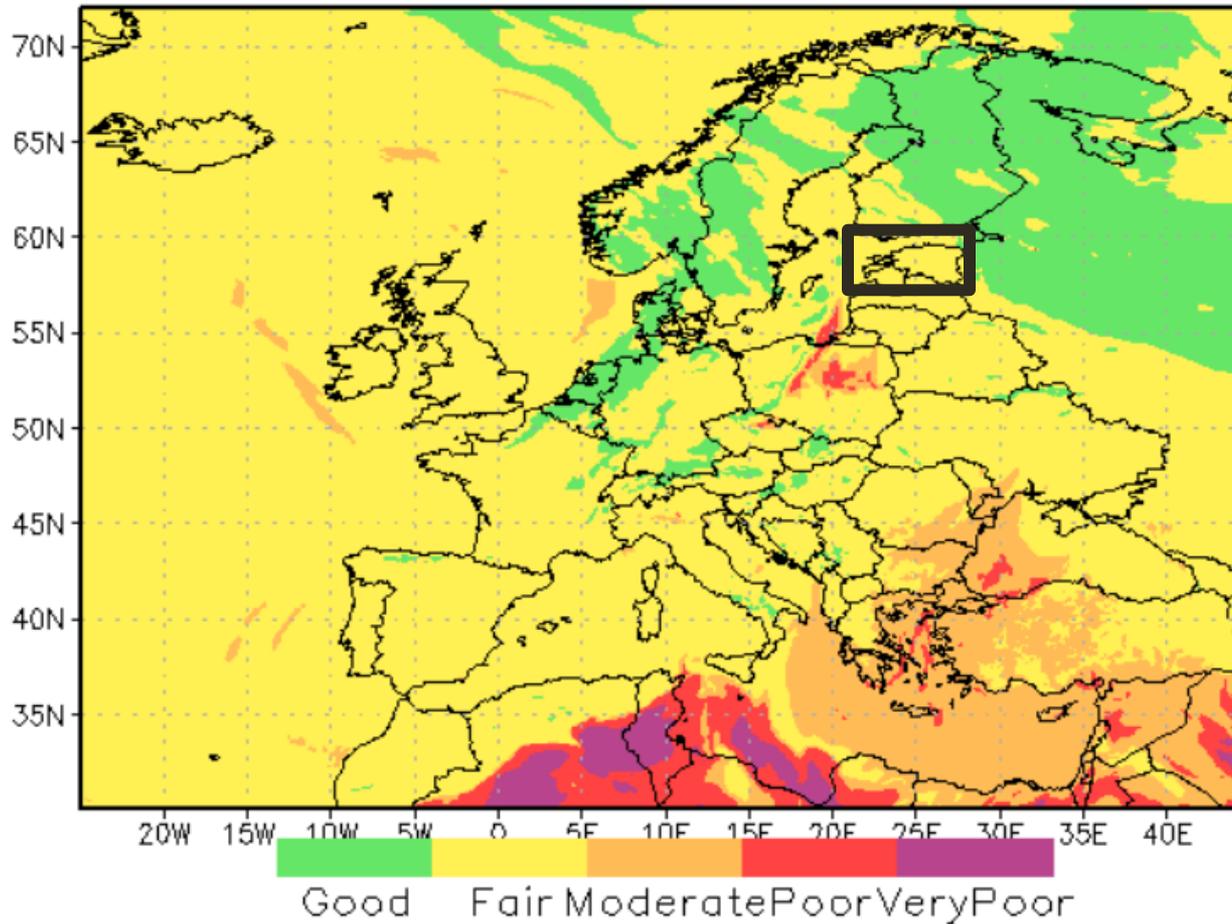


Context

Forecast for AQI. Last analysis time: 20220926 00



AQI

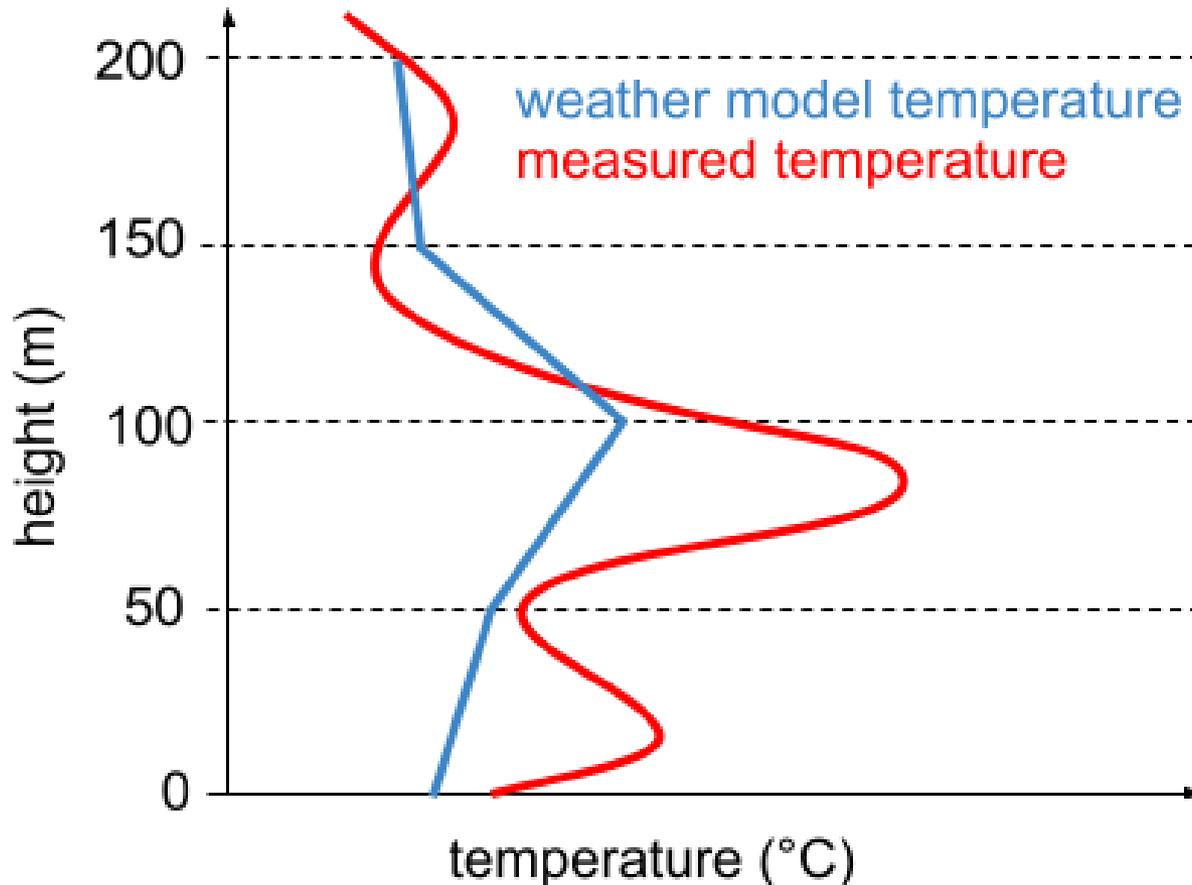


Air Quality Index forecasted for upcoming lunch break by SILAM.
Source: <https://silam.fmi.fi/aqforecast.html> (scientific use only)

Limitation of models: thermal inversion.

Cause of limitation: input from weather model.

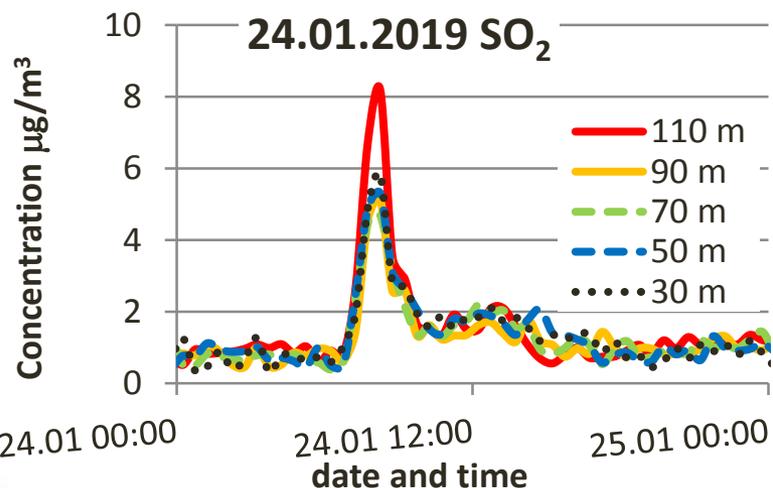
SILAM restates the boundary-layer parameters.



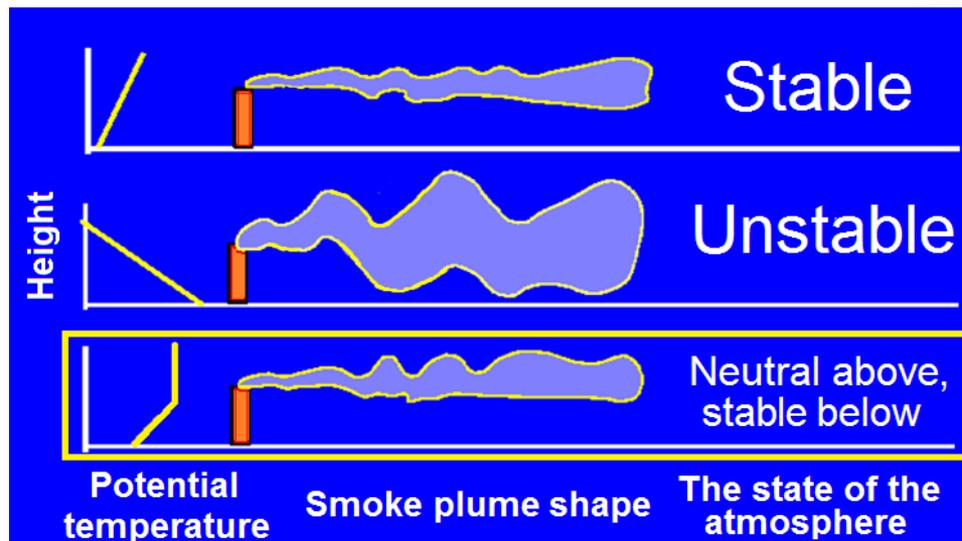
Illustrative **model-predicted** and **measured** temperature vertical profiles. Approximate weather model levels are on the vertical axis.

Rationale

- Aim of study: how well does SILAM perform?
- How predicts thermal inversion, concentrations?
- How and why deviates from measurements?
- Studied trace gases: SO_2 , NO_x . Peaks, origin.
- Good opportunity to compare model with measurements.



SO_2 concentration peak measured at SMEAR Estonia mast. Different colors indicate various mast heights.



Dispersion of smoke plume from a tall stack during different states of atmosphere.

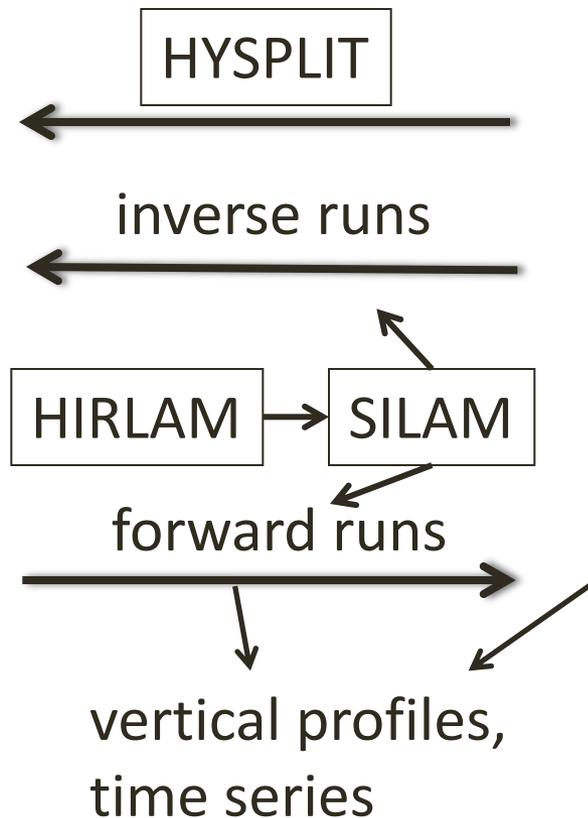
Methods

- Period 2016-2020
- Model comparison with measurements at mast location

Sources: industries of North-East Estonia. Known: SO_2 , NO_x emissions (tons per year).



Photo: Marko Kaasik.



Receptor: SMEAR Estonia Järvelja measuring mast.
Measured: SO_2 , NO_x concentration ($\mu\text{g}/\text{m}^3$), temperature ($^{\circ}\text{C}$).



Photo: Marko Kaasik.

Used data sources



Järvselja mast marked in **red**, lower masts in **blue** (used to estimate inversion geographical extent) and initially chosen industrial pollution sources (stacks) in **yellow**. In the calculations only sources with emission more than 1 g/s were used.

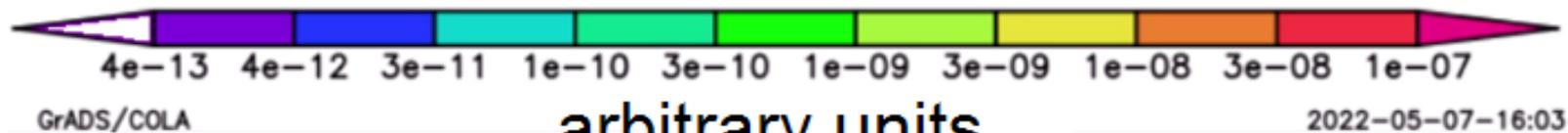
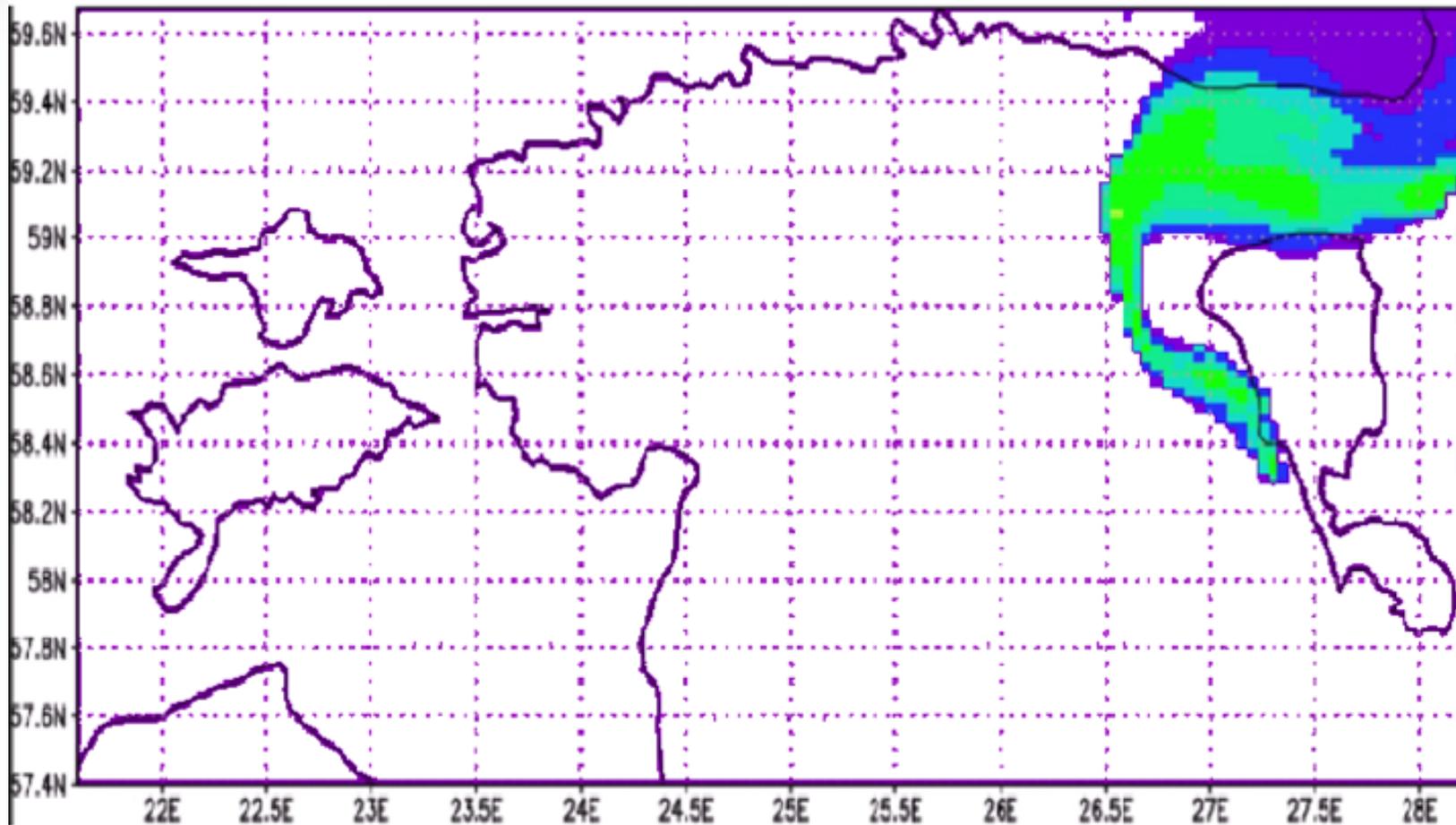
Simulation setup

- Weather model HIRLAM input:
- Meteo timestep: 1 hour
- 0–6 hour forecasts

- SILAM: 10 min timestep
- SO₂, NO_x yearly emissions, as passive tracers
- Stack heights 70 to 250 m, distance from mast 110 to 150 km
- grid about 2.8x2.8 km (resolution 0.025° latitude, 0.05° longitude)
- 11 vertical levels at 10, **30, 50, 70, 90, 110**, 160, 300, 600, 1400, 3000 m (layer midpoints).

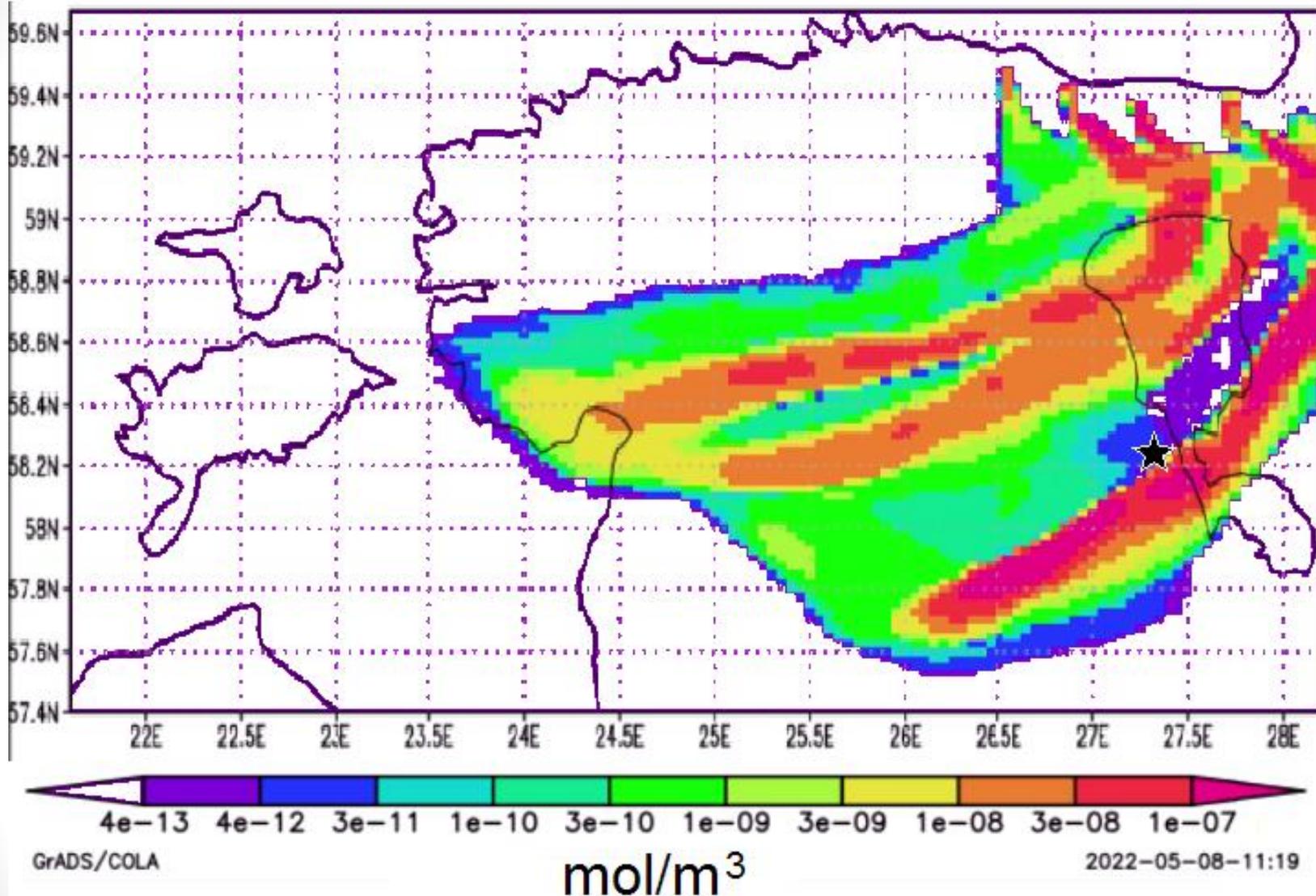
- Järvselja mast heights: **30, 50, 70, 90, 110** m

Inverse run SO₂ lev=10 m , 01:30Z 28 AUG 2017



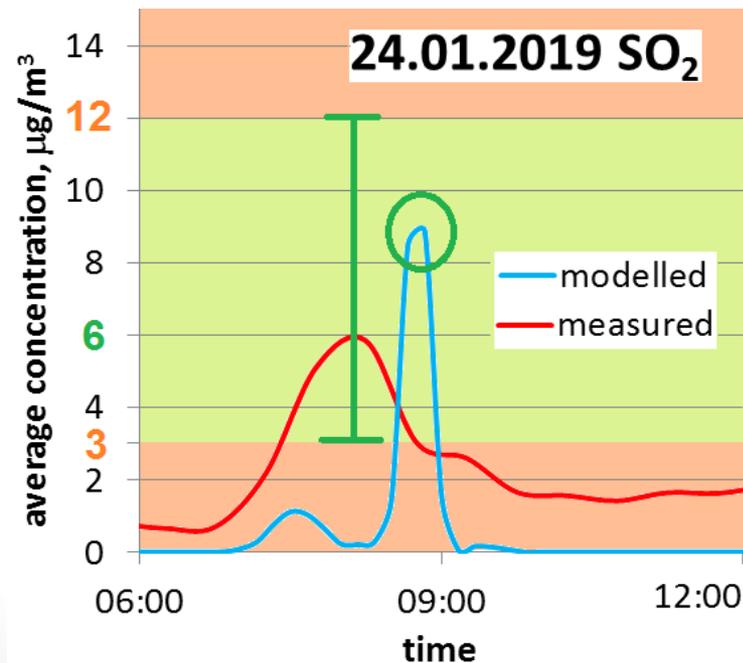
Sensitivity distribution calculated by SILAM to check measured trace gas origin.
Sensitivity source is at 110 m, where higher SO₂ concentrations were measured.

Forward run SO₂ lev=10 m, 01:30Z 28 AUG 2017

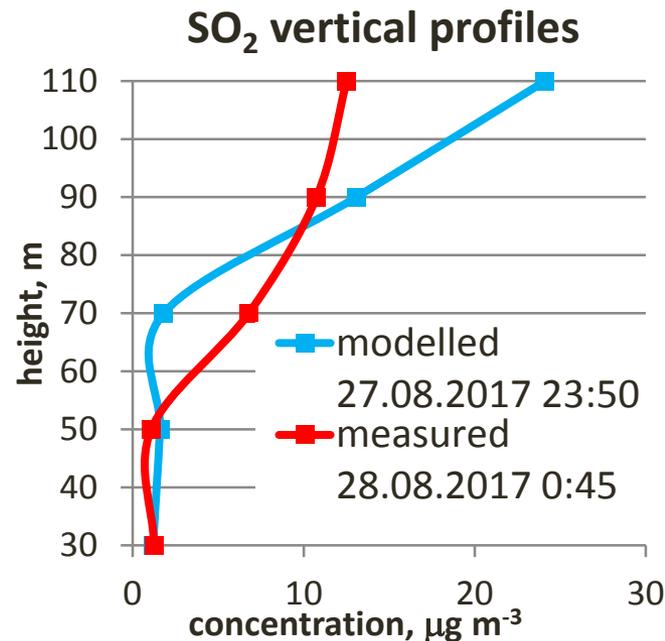


Source-oriented forward run. Stack height and diameter, gas temperature and initial vertical velocity are taken into account. Järvselja is marked with black star.

- Fraction in factor two (FA2) calculated for SO₂ and NO_x peak maxima, vertical profiles compared qualitatively
- Time series, vertical profiles
- Concentration, (potential) temperature



Modelled peak maximum should not differ more than two times from the measured peak maximum.



Illustrative comparison of vertical profiles at mast heights.

Järvselja mast

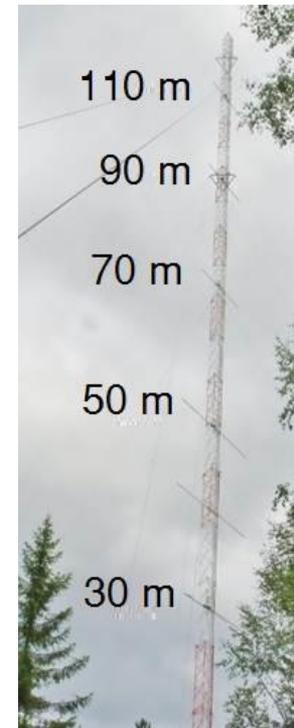
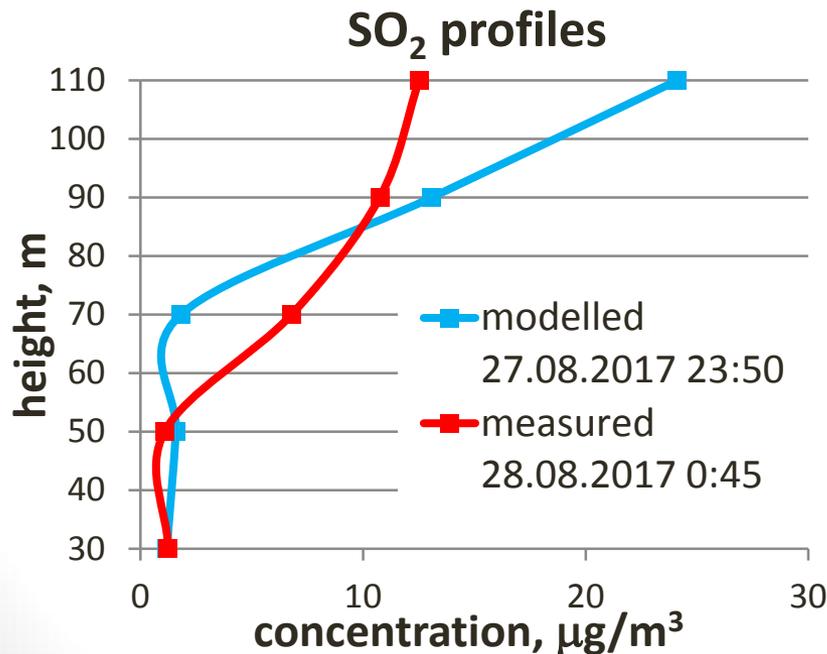


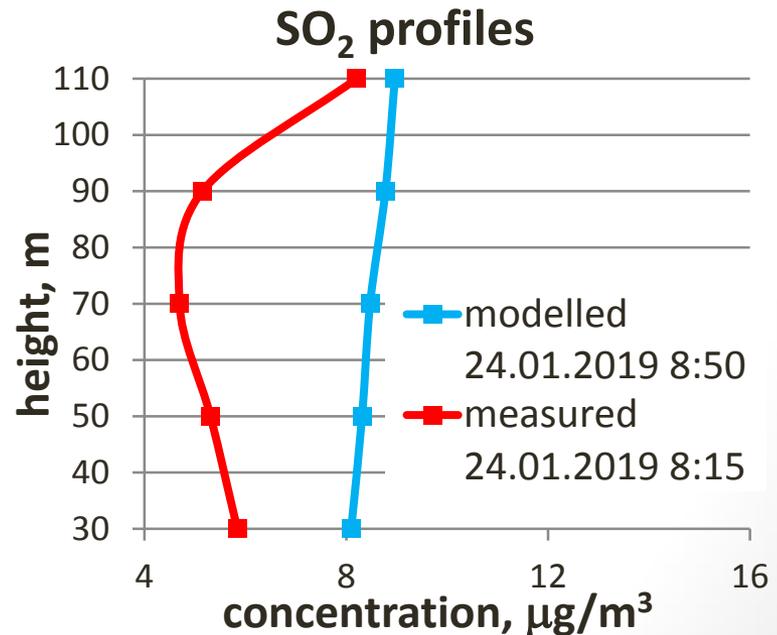
Photo: Marko Kaasik

- Peak (maximum) arrives at Järvselja with a shift in time.
- Peak duration is on average 3 hours shorter.

	SO ₂	NO _x
Number of concentration peaks	10	9
Concentration well assessed	5/10	1/9
Was the peak during a weak inversion? (below 1 °C)	3/5	1/1
Concentration underestimated	5/10	6/9
Concentration profile well estimated	3/10	5/9

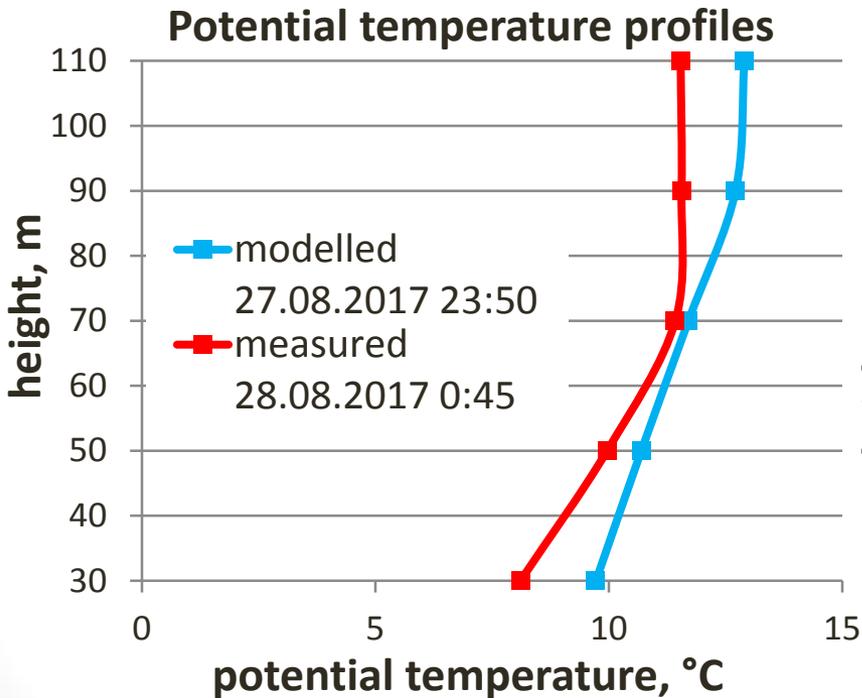


Well estimated profile.

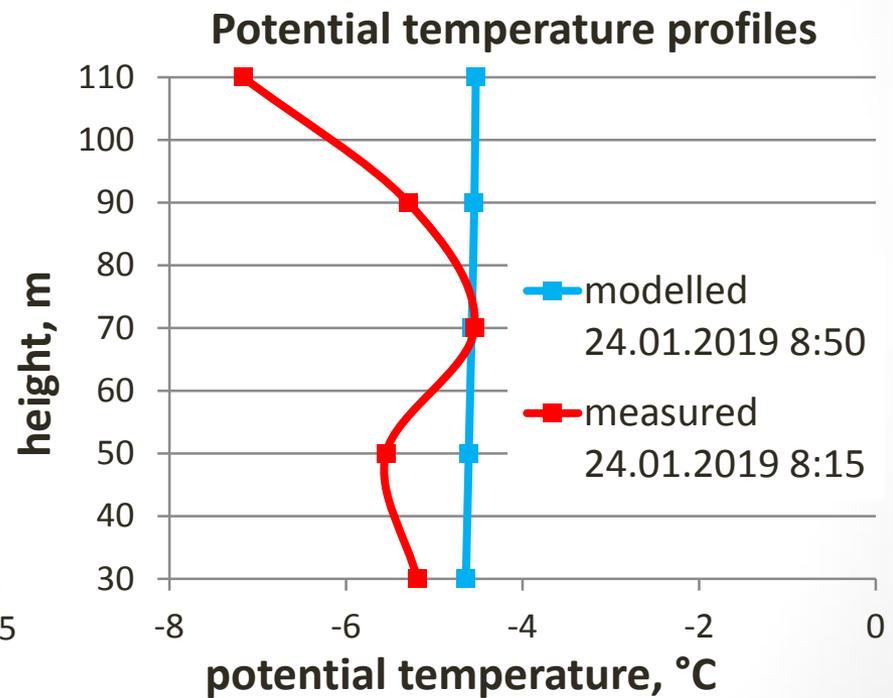


Poorly estimated profile.

	Potential temperature
Number of events	12
Were profiles possible to compare?	9/12
Profile well assessed	5/9
All peak profiles during the event well assessed	3/5



Well estimated profile.



Poorly estimated profile.

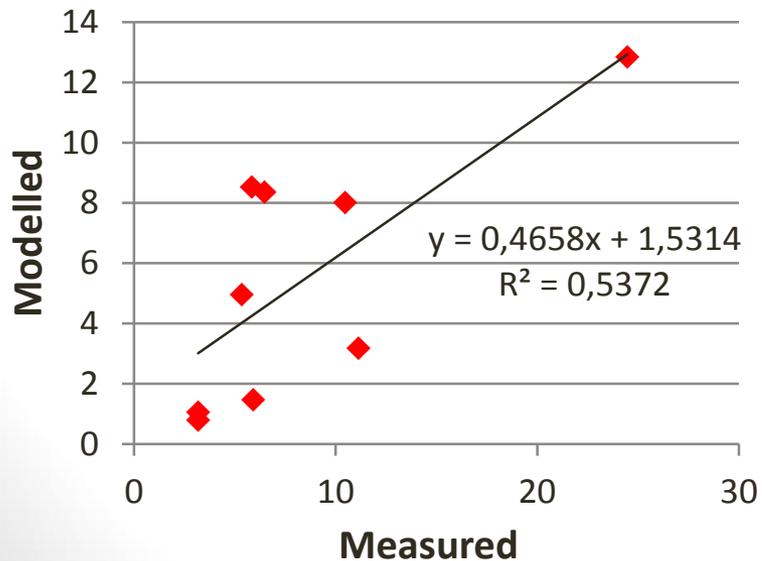
- Inversion strength between 30-70 m up to 3 °C underestimated.

Discussion

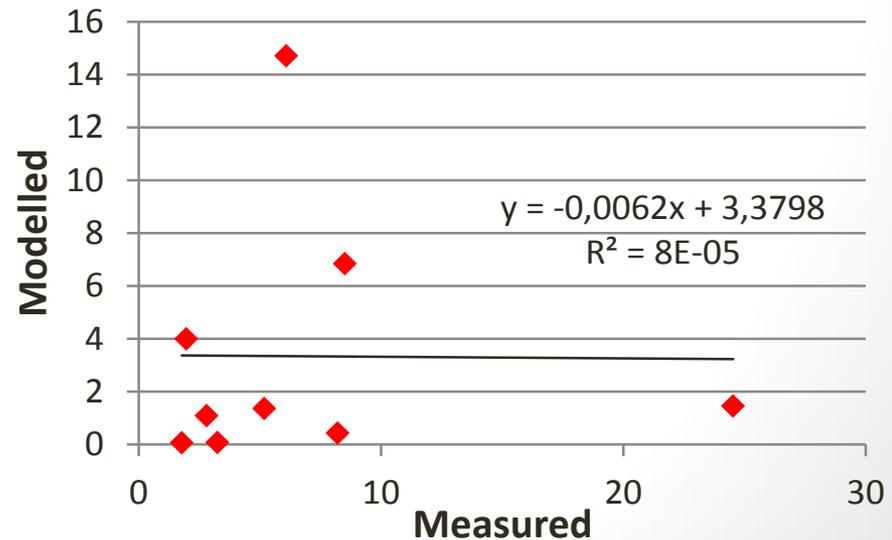
Effect – possible cause

- Peaks underestimated – vertical dispersion underestimated (low confidence)
- Uncertainty in modelled concentrations – emission data
- Peak maxima arrive with shift in time – probably weather model
- Shorter peak duration – horizontal dispersion underestimated
- Inversion strength underestimated – parametrization of the surface layer

Intercomparison for SO₂



Intercomparison for NO_x



Conclusions

Based on FA2, SILAM assesses peak concentrations fairly less than half of the cases. Peaks of SO_2 are assessed better than NO_x .

Peak concentrations and peak durations are mostly underestimated, this may indicate underestimation of, respectively, vertical and horizontal dispersion during inversions.

SILAM tends to underestimate inversion strength between 30 and 70 m. Therefore surface layer parametrisation in SILAM should be looked into.

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Thank you!

Acknowledgements



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tuleviku heaks

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Thank you!