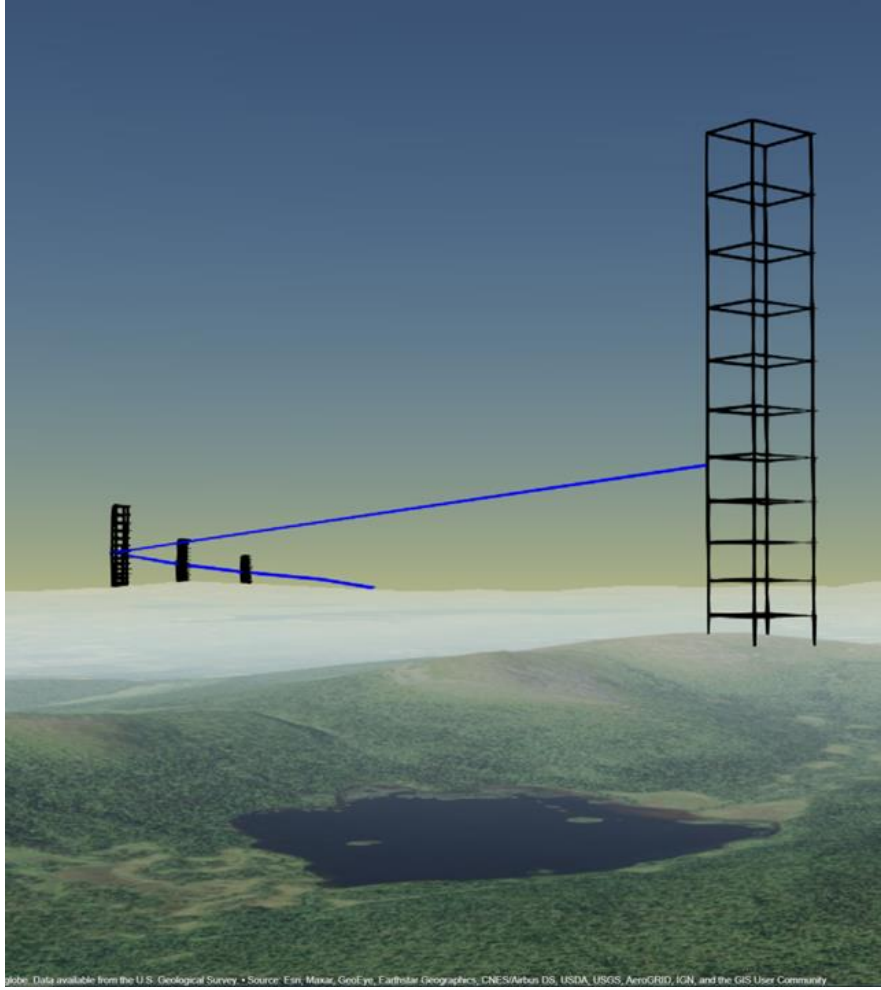
Modelling sub-micron secondary aerosol formation with the ADCHEM-ClusterIn model system

Results over Northern Europe in year 2018

+ preliminary results from the EMEP July 2022 campaign.



Ågot Watne, Pontus Roldin, Michael Priestley, Robin Wollesen de Jonge, Carlton Xavier, August Thomasson, Sara Bengtsdotter and Tinja Olenius.

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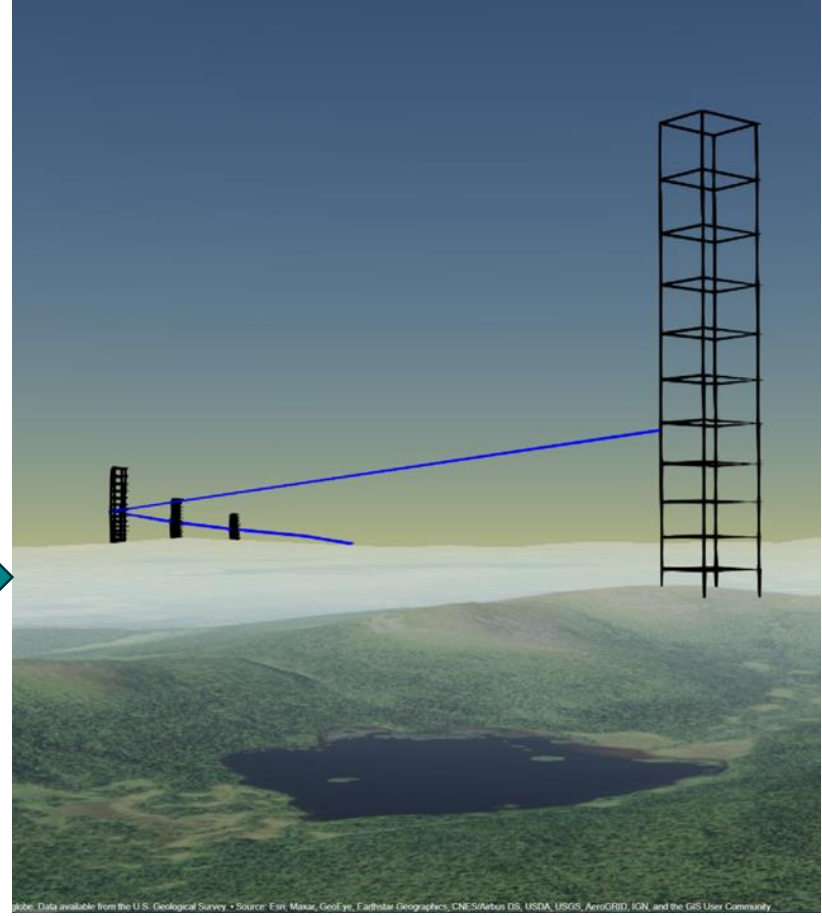
ADCHEM

- A type of semi-Lagrangian chemistry transport model with detailed chemistry and aerosol dynamics*
- Typically run along pre-calculated air mass trajectories (e.g. from HYSPLIT or FLEXPART) that arrive at different measurement stations (receptor locations)
- Mostly run as a 1D-collumn modell, but can also be used as a 2D-model for e.g. urban plume dilution and ageing studies**,***



Atmos. Chem. Phys., 11, 5867–5896, 2011
www.atmos-chem-phys.net/11/5867/2011/
doi:10.5194/acp-11-5867-2011

*

Atmospheric Chemistry and Physics

Development and evaluation of the aerosol dynamics and gas phase chemistry model ADCHEM

P. Roldin[1], E. Swietlicki[1], G. Schurgers[2], A. Arneth[2,3], K. E. J. Lehtinen[4,5], M. Boy[6], and M. Kulmala[6]

Atmos. Chem. Phys., 11, 5897–5915, 2011
www.atmos-chem-phys.net/11/5897/2011/
doi:10.5194/acp-11-5897-2011

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Atmospheric Chemistry and Physics

Aerosol ageing in an urban plume – implication for climate

P. Roldin[1], E. Swietlicki[1], A. Massling[1,*], A. Kristensson[1], J. Löndahl[1], A. Eriksson[1,2], J. Pagels[2], and S. Gustafsson[3]

***

SCIENTIFIC REPORTS

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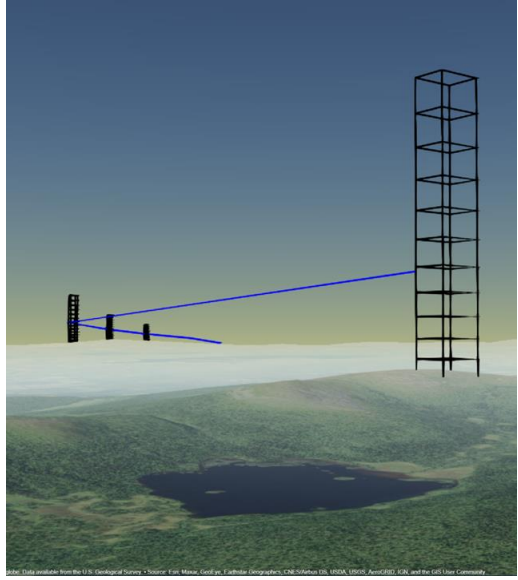
Diesel soot aging in urban plumes within hours under cold dark and humid conditions

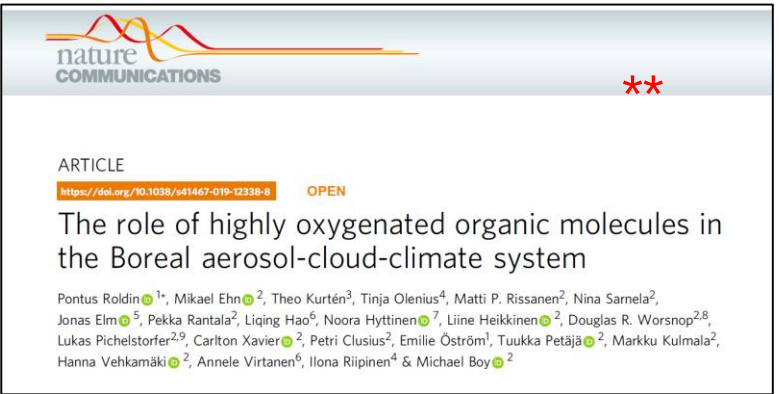
Received: 9 May 2017
Accepted: 8 September 2017

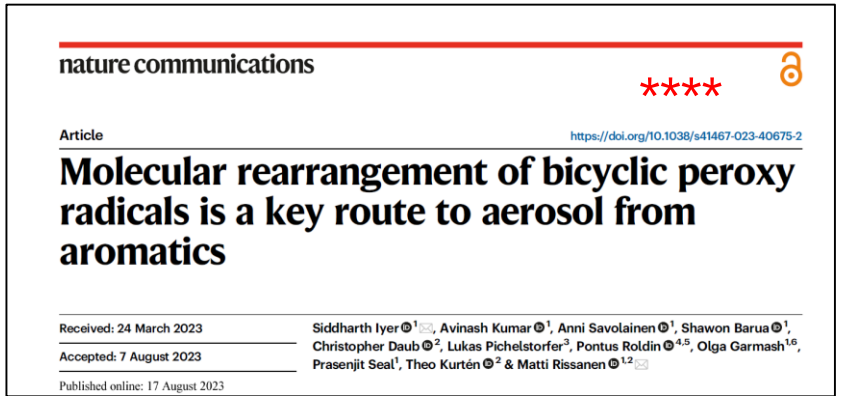
A. C. Eriksson[1,2], C. Wittbom[1], P. Roldin[1,3], M. Sporre[4], E. Öström[1,5], P. Nilsson[2], J. Martinsson[1,5], J. Rissler[2], E. Z. Nordin[2], B. Svenningsson[1], J. Pagels[2] & E. Swietlicki[1]

Representation of secondary organic aerosol (SOA) formation in ADCHEM

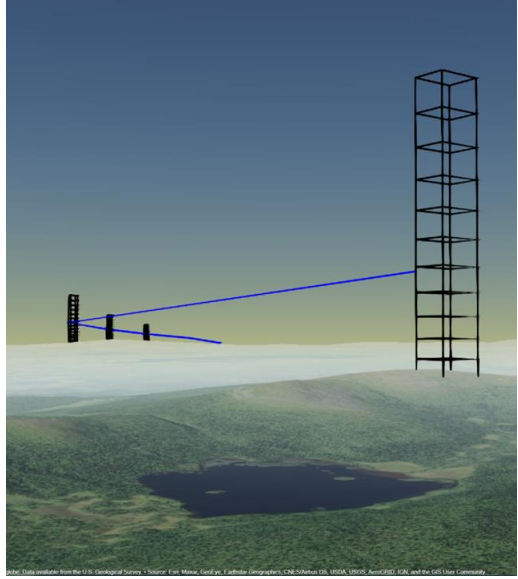


- ADCHEM-ClusterIn simulates the gas-phase chemistry and secondary organic aerosol formation using a detailed chemical mechanism based on the Master Chemical Mechanism* and the Peroxy Radical Autoxidation Mechanism (PRAM) for HOM formation from monoterpens**,*** and aromatic compounds****
- The particle size dependent SOA formation involve >1000 organic molecules.





Representation of atmospheric new particle formation (NPF) in ADCHEM



Gas–cluster–aerosol dynamics processes in ADCHEM-ClusterIn

Time evolution of vapor and cluster concentrations and formation rate for each time step

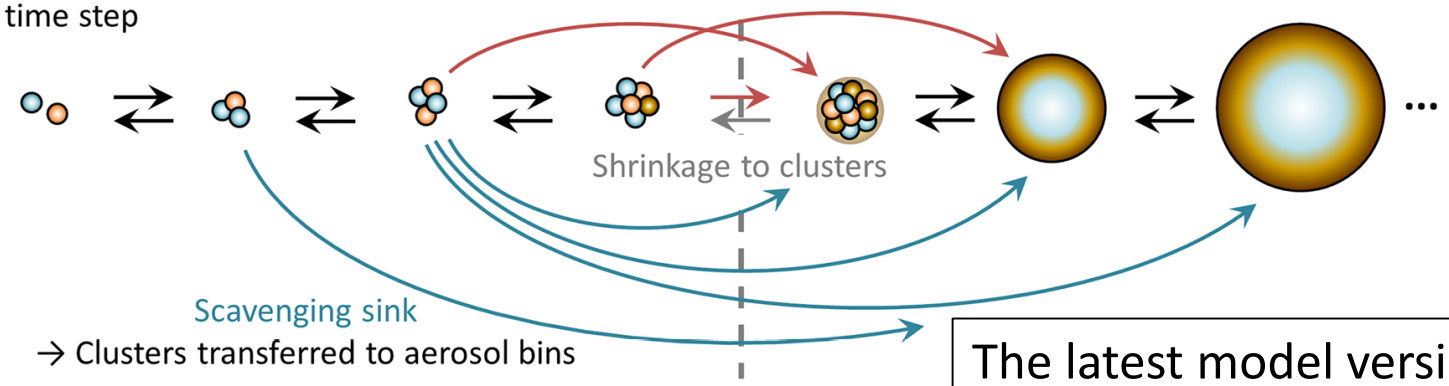
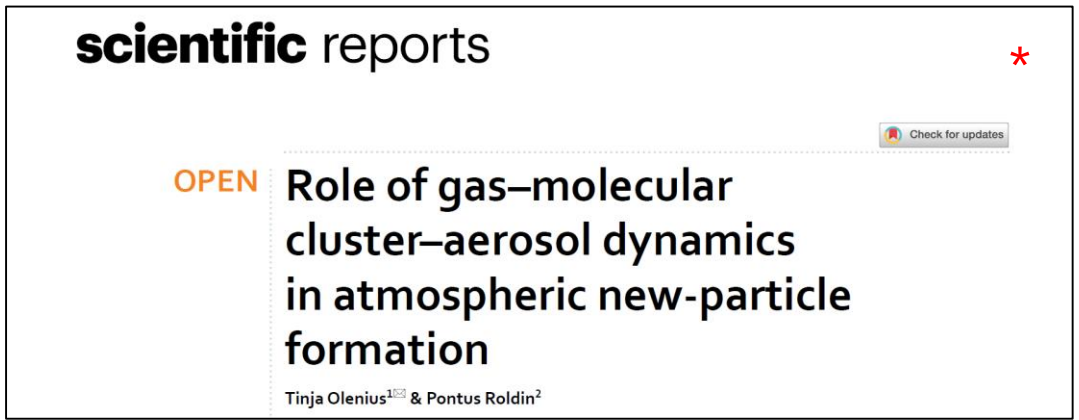


*Figure from Olenius and Roldin (2022)**

The latest model version** considers ion-mediated NPF involving 4 mechanisms:

$NH_3 – H_2SO_4$ DMA – H_2SO_4

DMA – HIO_3 $HIO_2 – HIO_3$



scientific reports *

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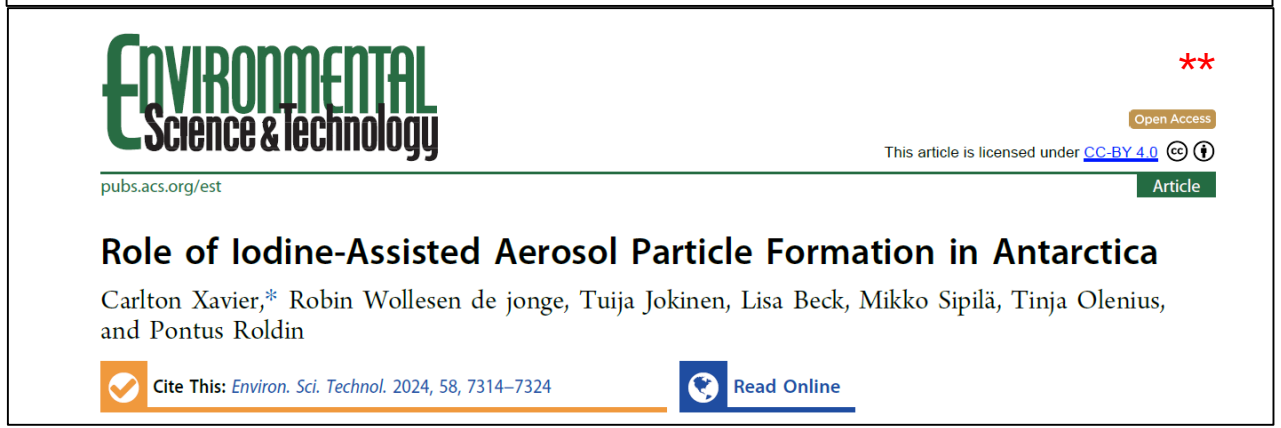
Role of gas–molecular cluster–aerosol dynamics in atmospheric new-particle formation

Tinja Olenius[1] & Pontus Roldin[2]



Environmental Science & Technology **

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Article

Role of Iodine-Assisted Aerosol Particle Formation in Antarctica

Carlton Xavier,* Robin Wollesen de jonge, Tuija Jokinen, Lisa Beck, Mikko Sipilä, Tinja Olenius, and Pontus Roldin

Cite This: *Environ. Sci. Technol.* 2024, 58, 7314–7324

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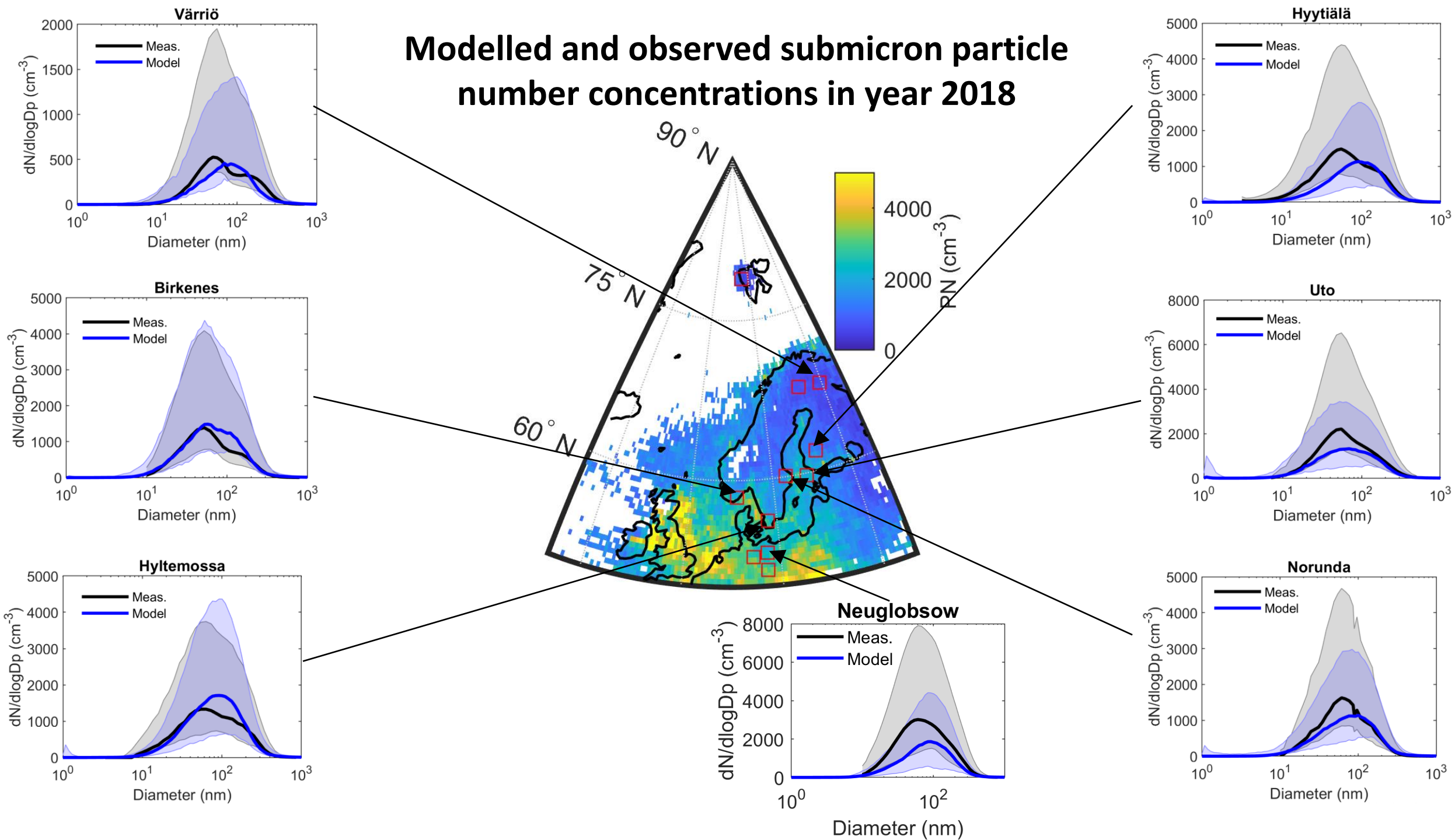
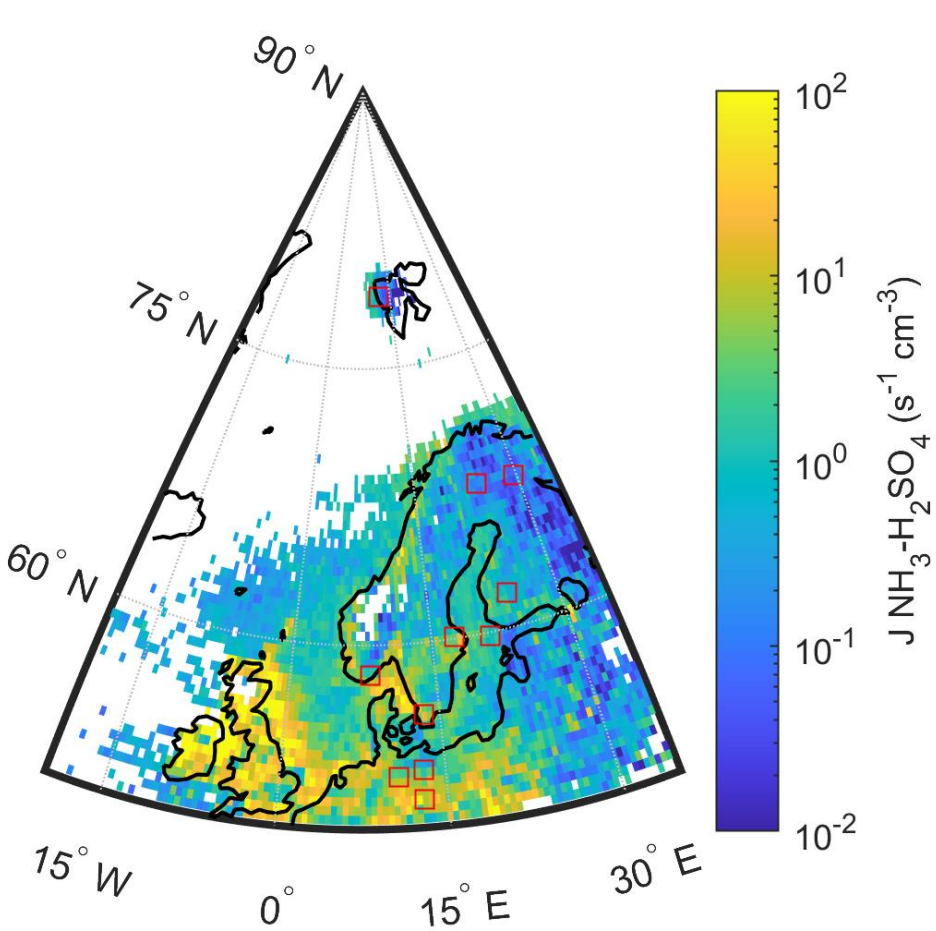
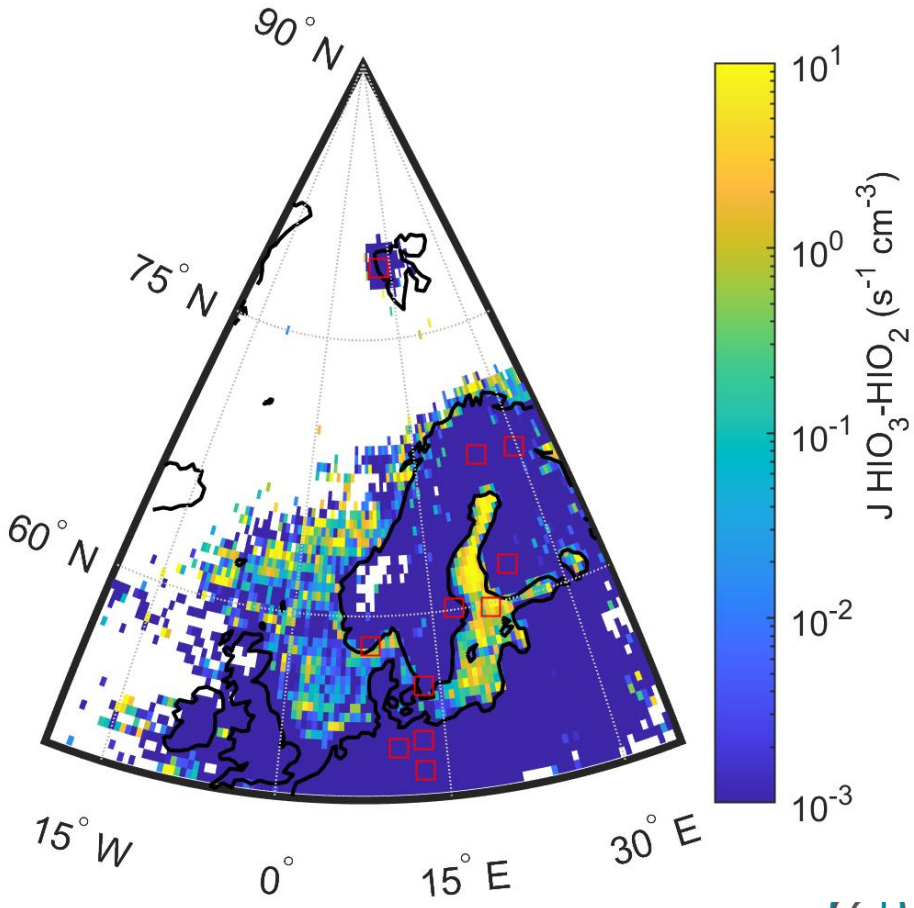
Modelled and observed submicron particle number concentrations in year 2018



New particle formation in 2018

90-percentile NPF rates ammonia-sulfuric acid and iodine oxides





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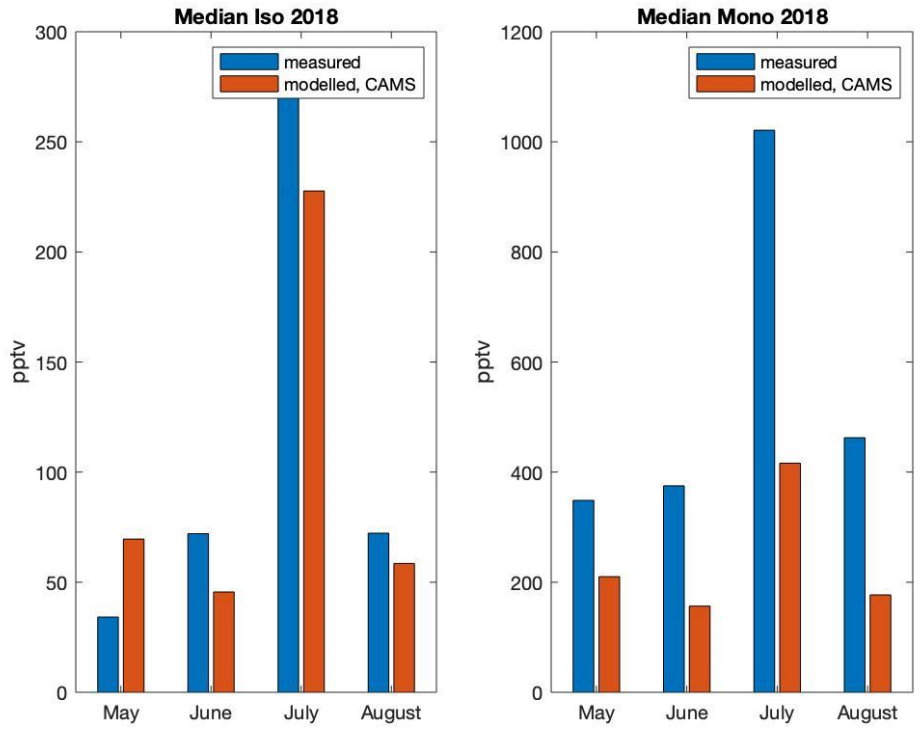
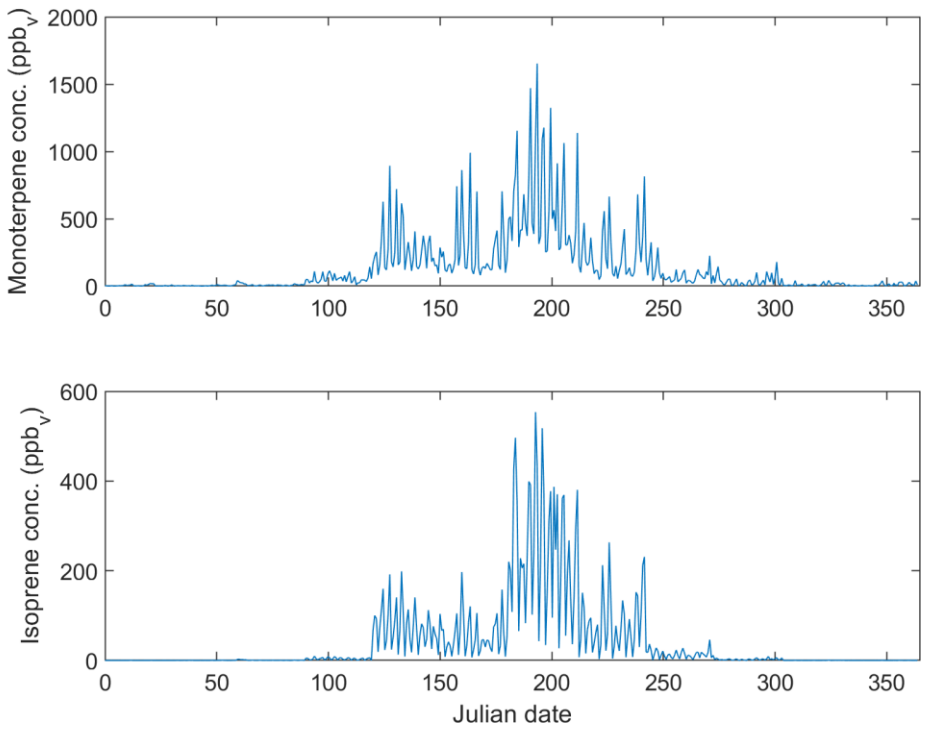
Evaluation of BVOC concentrations using long-term observations

- Evaluation of modelled monoterpene and isoprene concentrations at Hyytiälä, Finland using PTR-MS observations (Master thesis work by Sara Bengtsdotter, Lund Univ.)





- Outlook - compare modelled and observed (HR PTR-MS) VOC concentrations at the ACTRIS Hyltemossa field station in S. Sweden (VOC observations since 2019)

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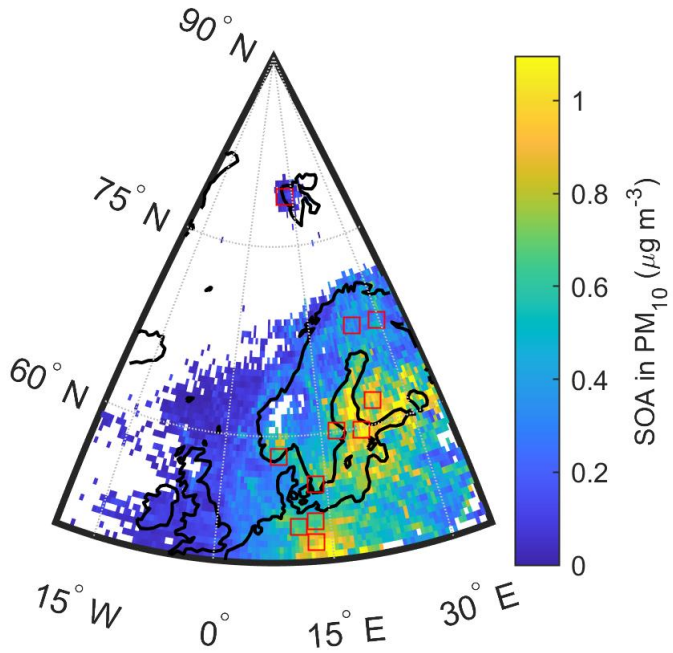
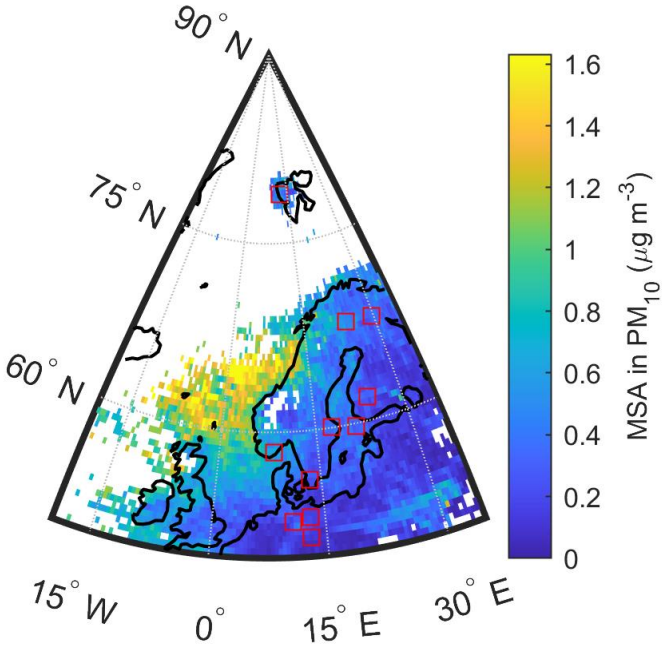
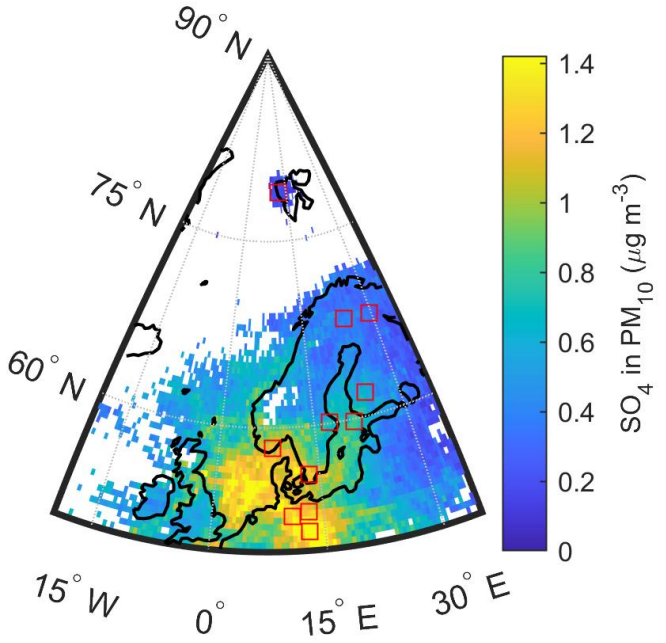
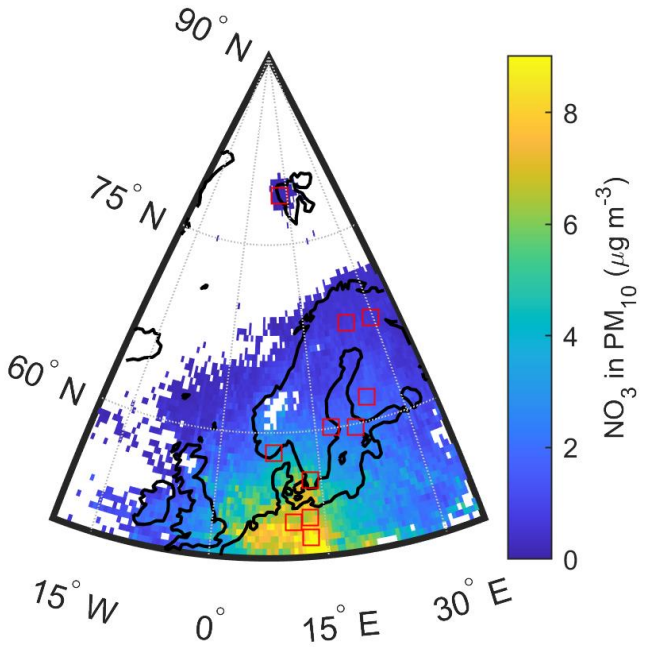
Secondary aerosol concentrations in 2018



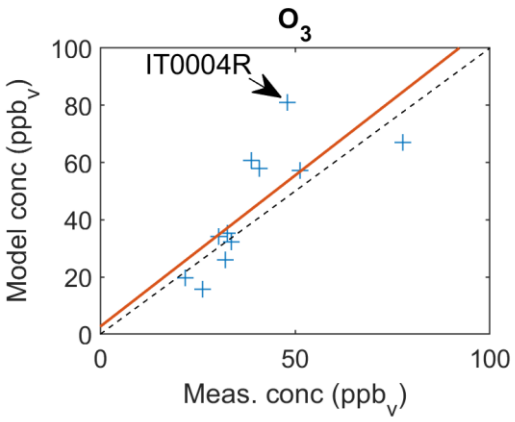


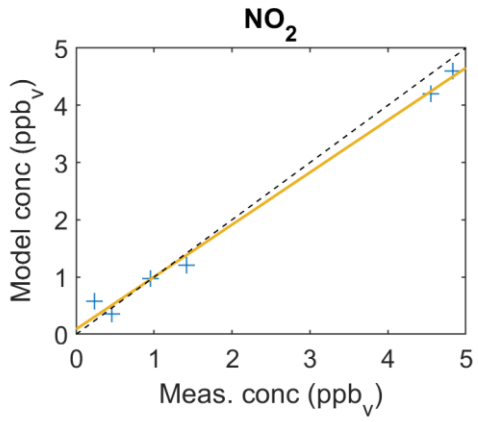
- Although the BSOA formation mechanisms is ADCHEM can be considered state-of-the-art the modelled monoterpene concentrations are underestimated with a factor of ~2 in 2018 (Hyytiälä).
- The present model version most likely underestimates the anthropogenic secondary organic aerosol formation. Ongoing work to improve the anthropogenic SOA formation in the Horizon Europe project PAREMPI: https://parempi.eu/
- Dimethyl sulfide (DMS) emissions an important source of MSA and SO_4 aerosol mass outside the coast of Norway.

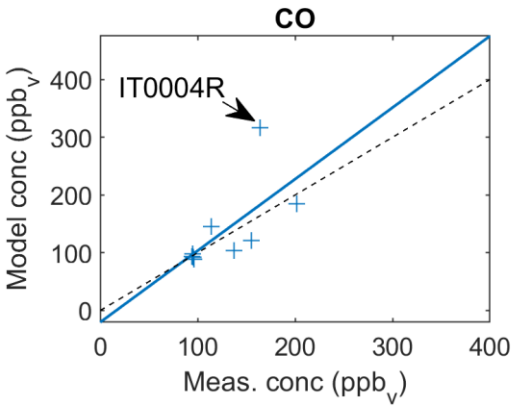




Preliminary model results from the EMEP campaign in July 2022



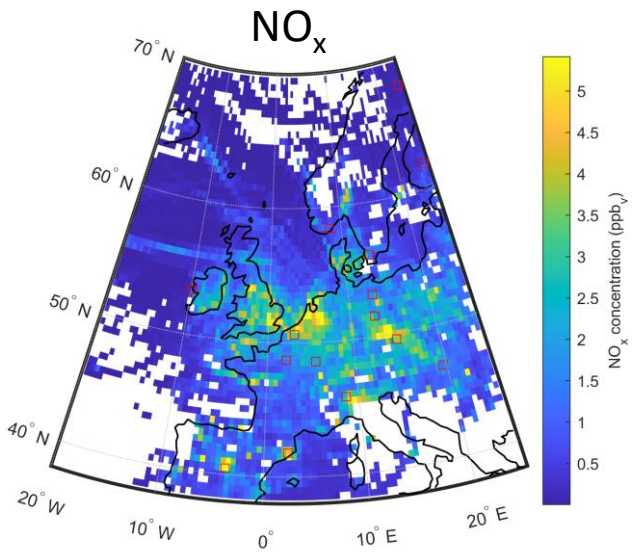


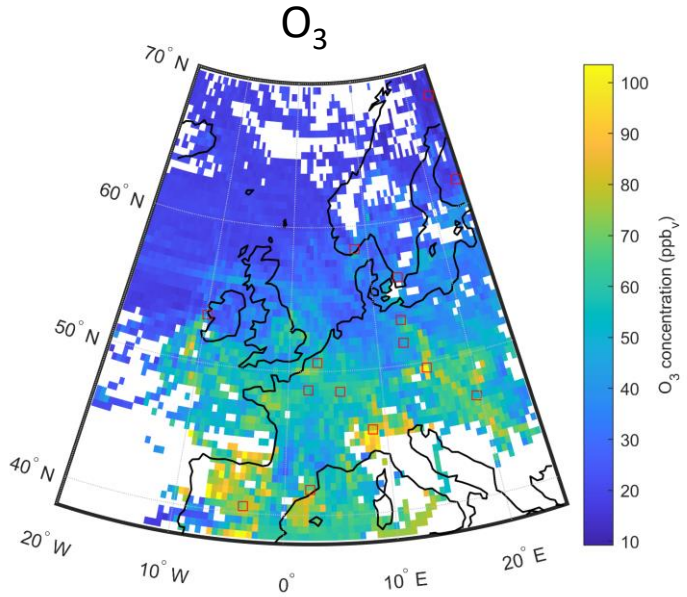


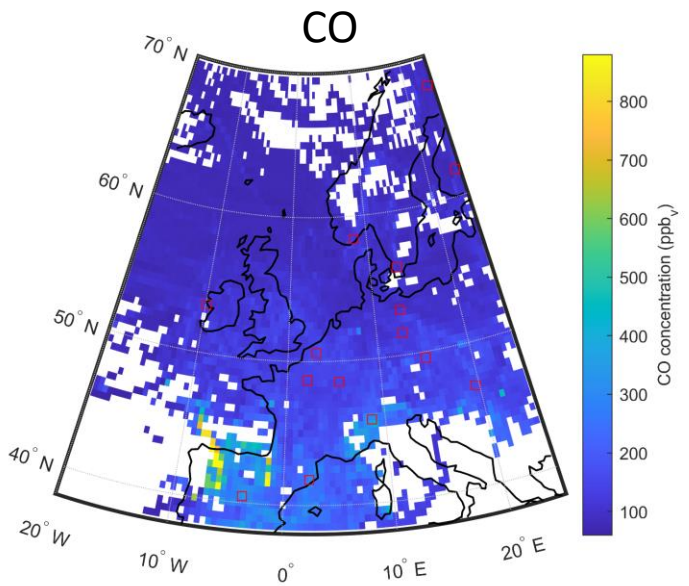
y=1.0564x+2.673, R=0.762

y=0.913+0.0888, R=0.996

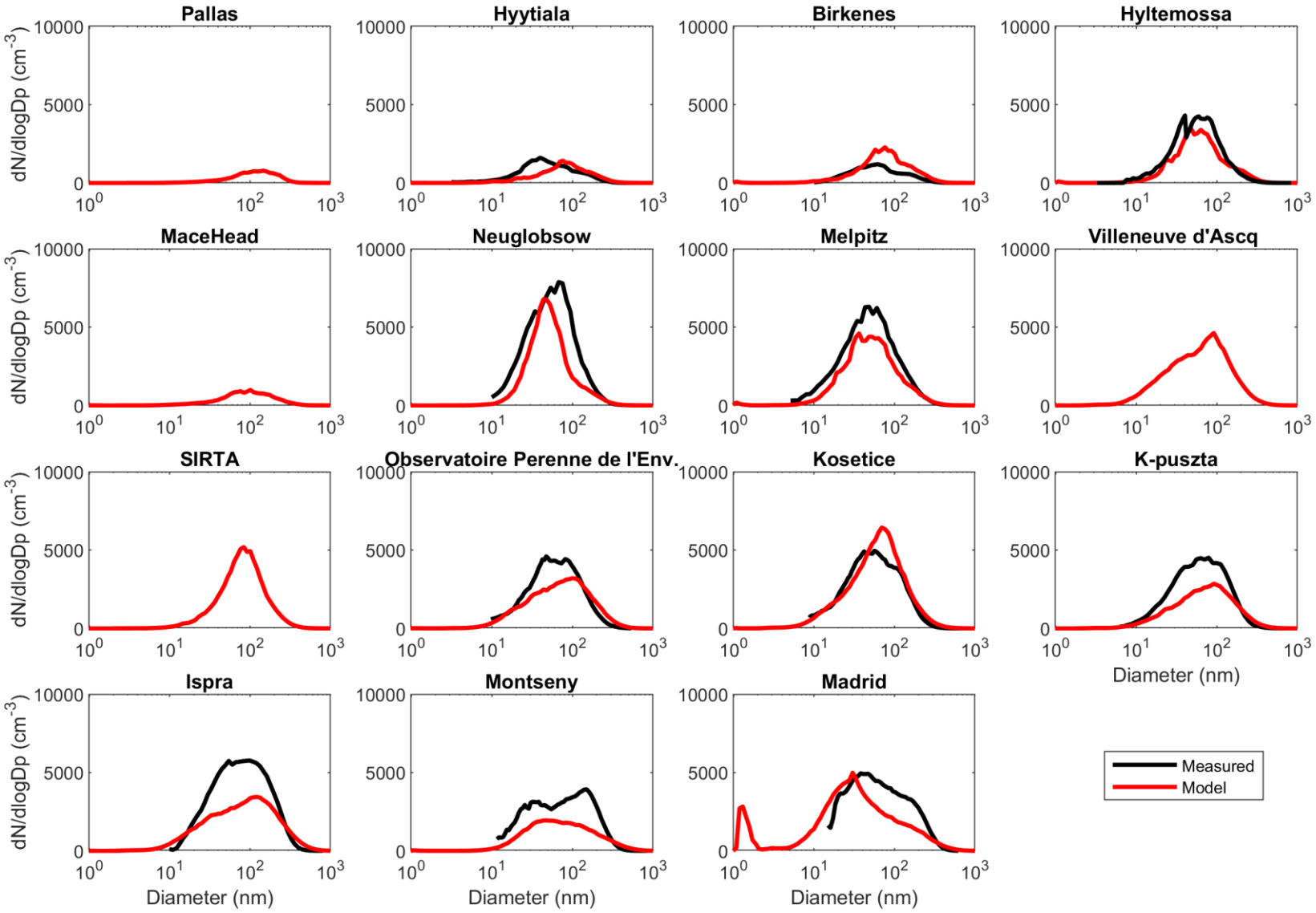
y=1.2392x-20.357, R=0.650

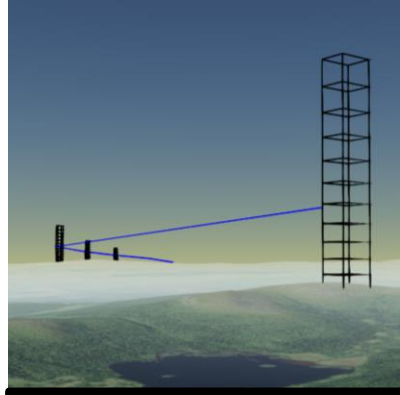






Particle number size distributions





ADCHEM :
Lagrangian 1D Column Model

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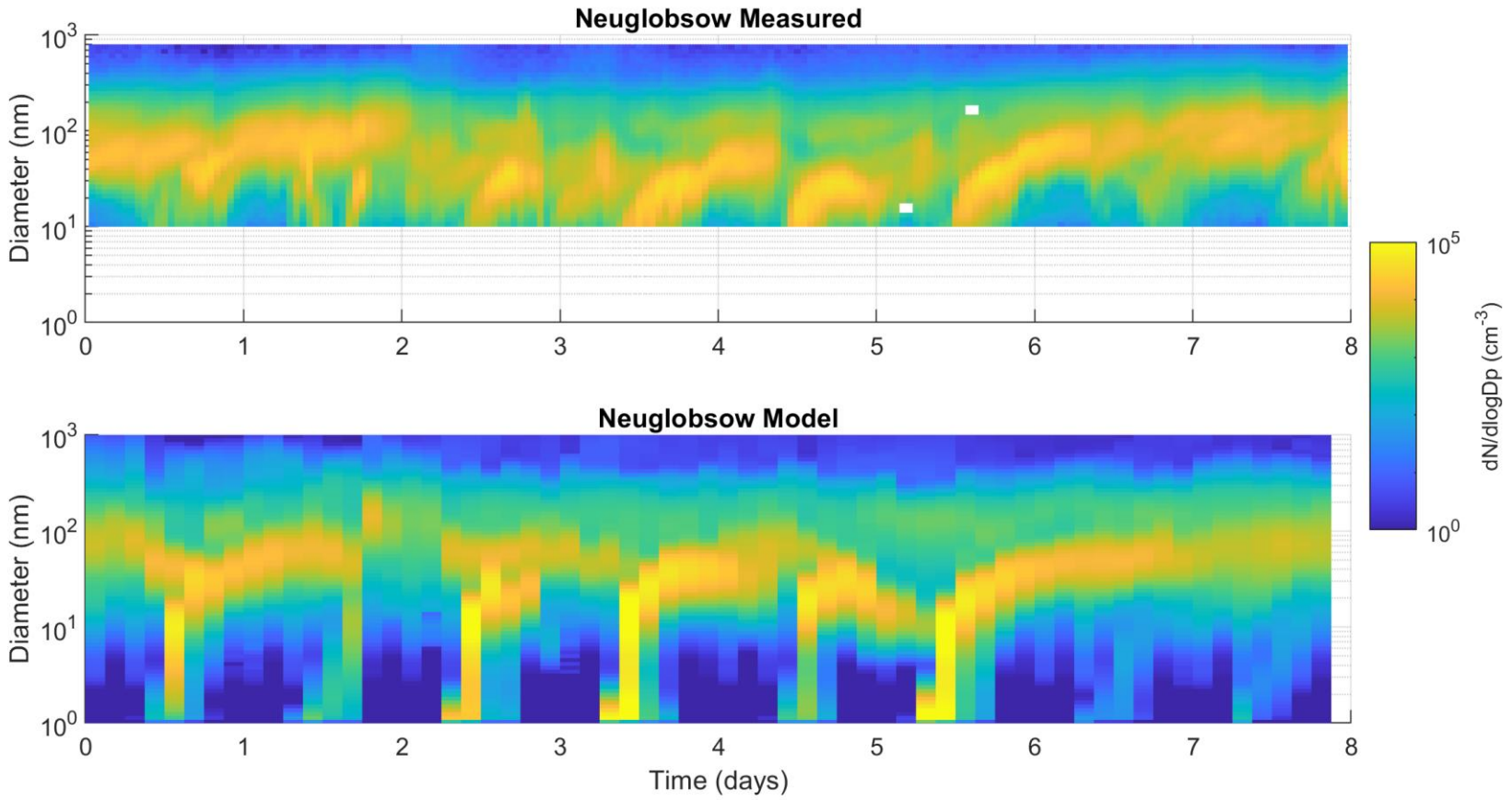
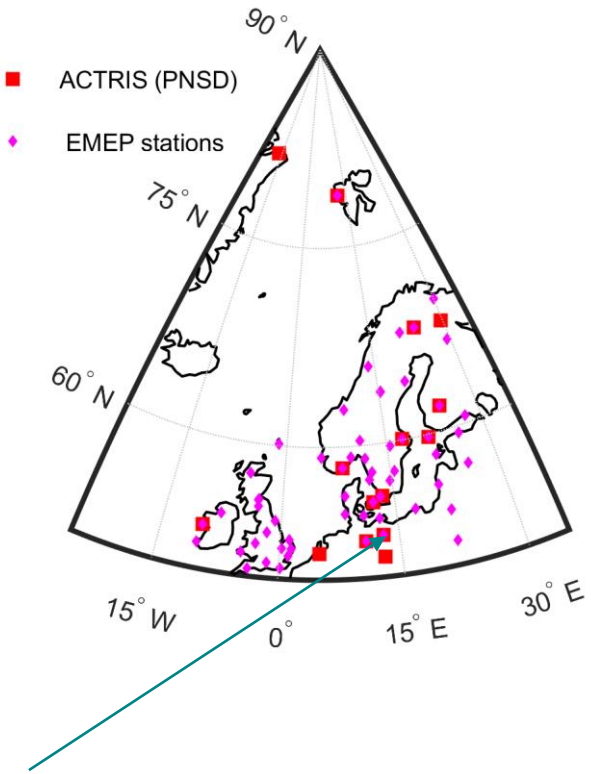
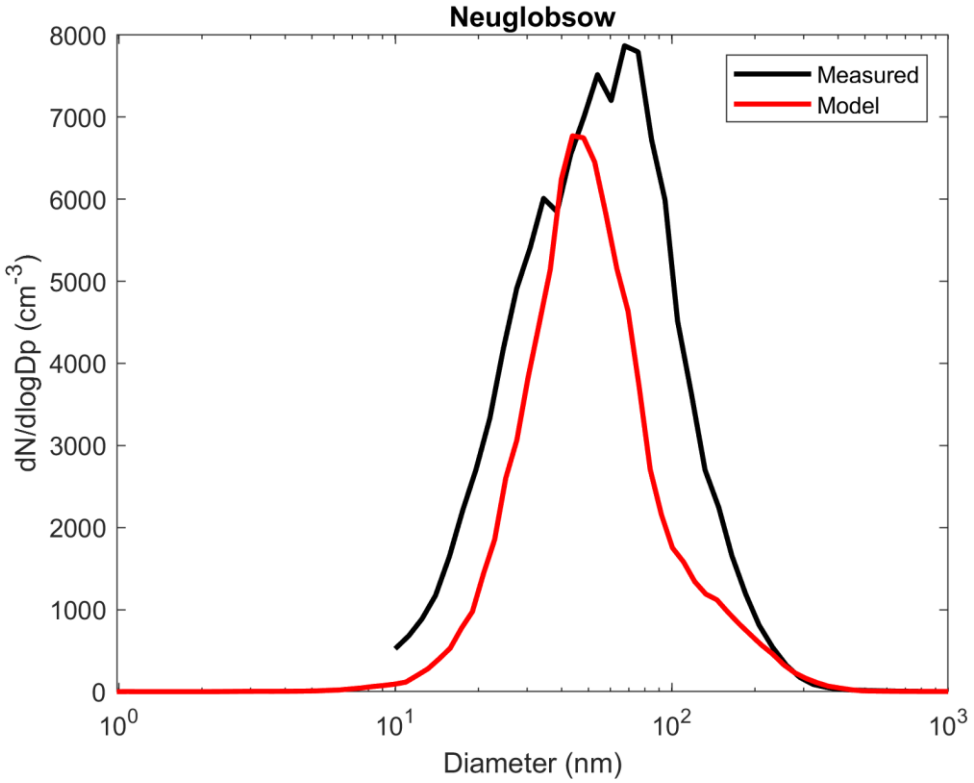
Neuglobsow- New particle formation



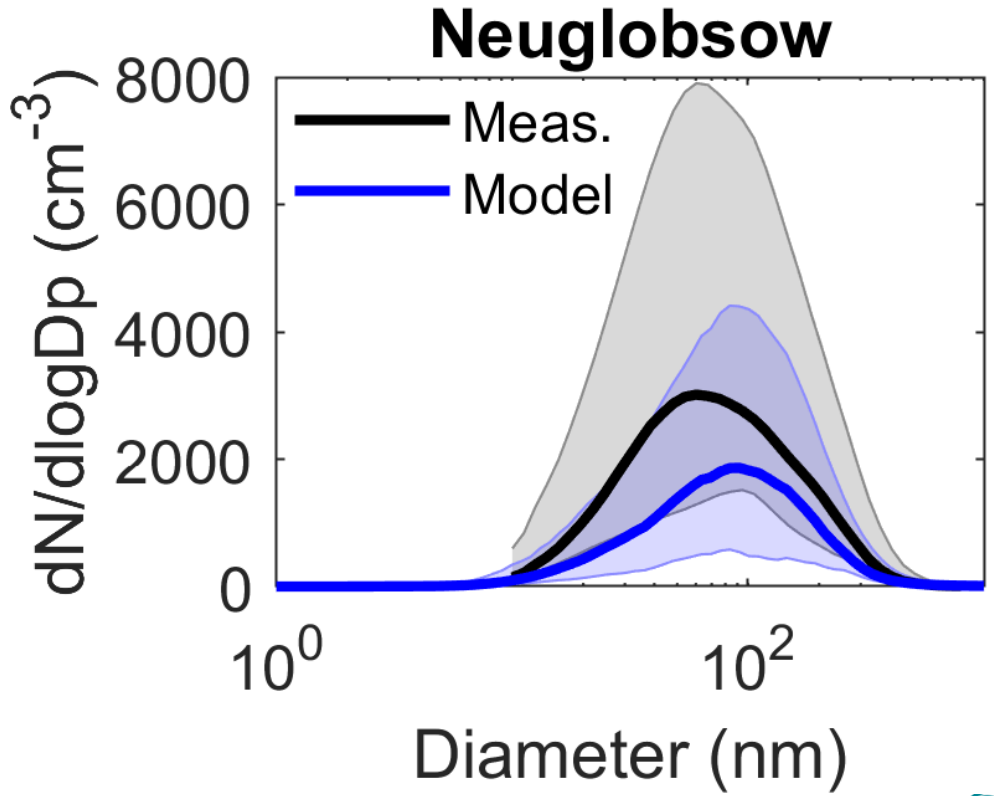


Neuglobsow – Secondary aerosols

Median PNSD from IMP2022



Median PNSD from 2018



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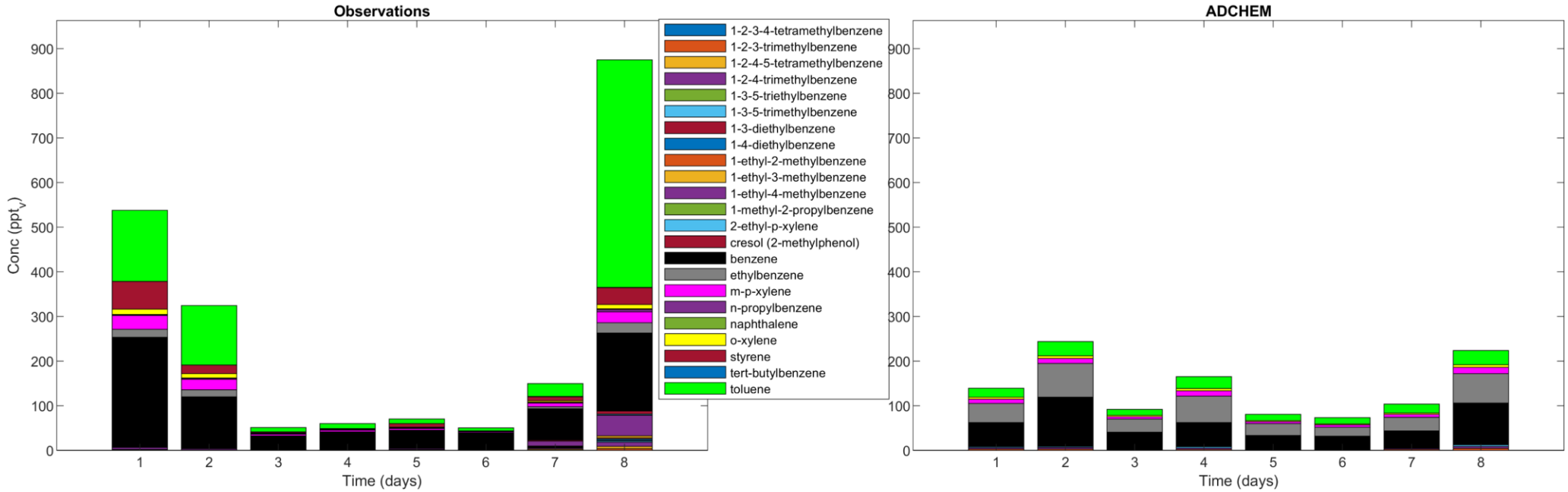
Neuglobsow– aromatic compounds



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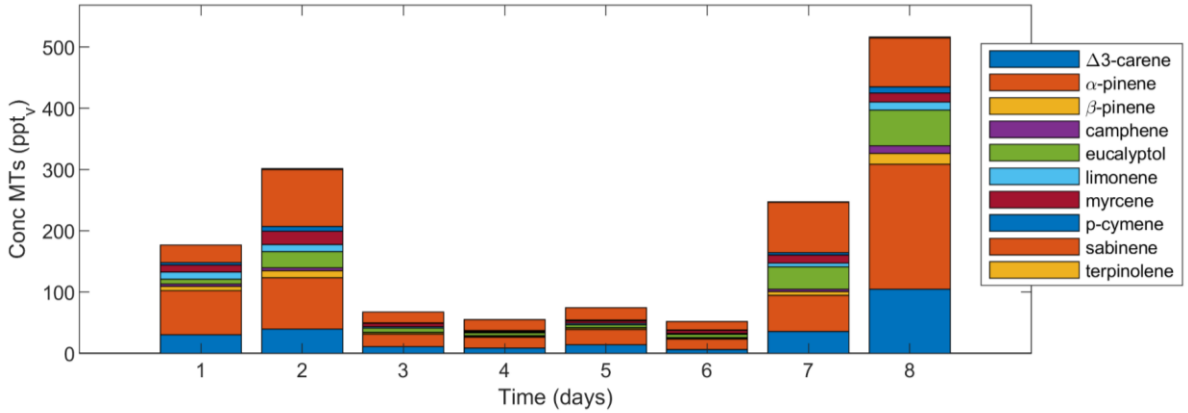
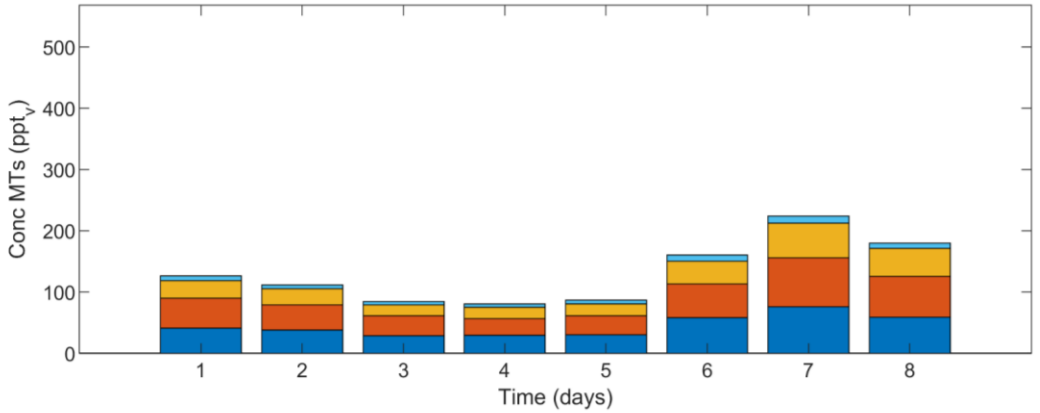
Neuglobsow-monoterpenes

Observations



Modelled



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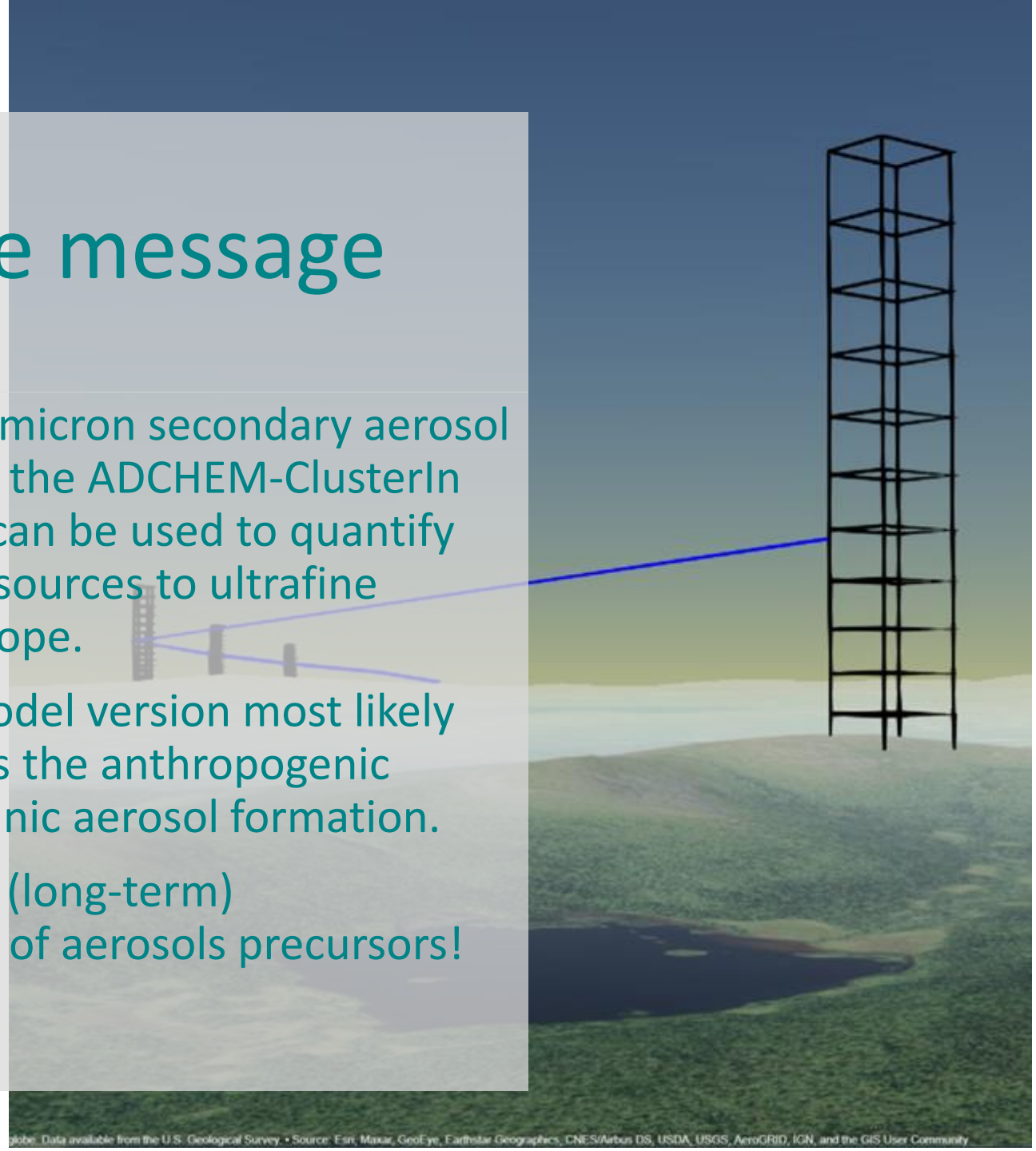
Take home message

- Modelling sub-micron secondary aerosol formation with the ADCHEM-ClusterIn model system can be used to quantify processes and sources to ultrafine particles in Europe.
- The present model version most likely underestimates the anthropogenic secondary organic aerosol formation.
- We need more (long-term) measurements of aerosols precursors!



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