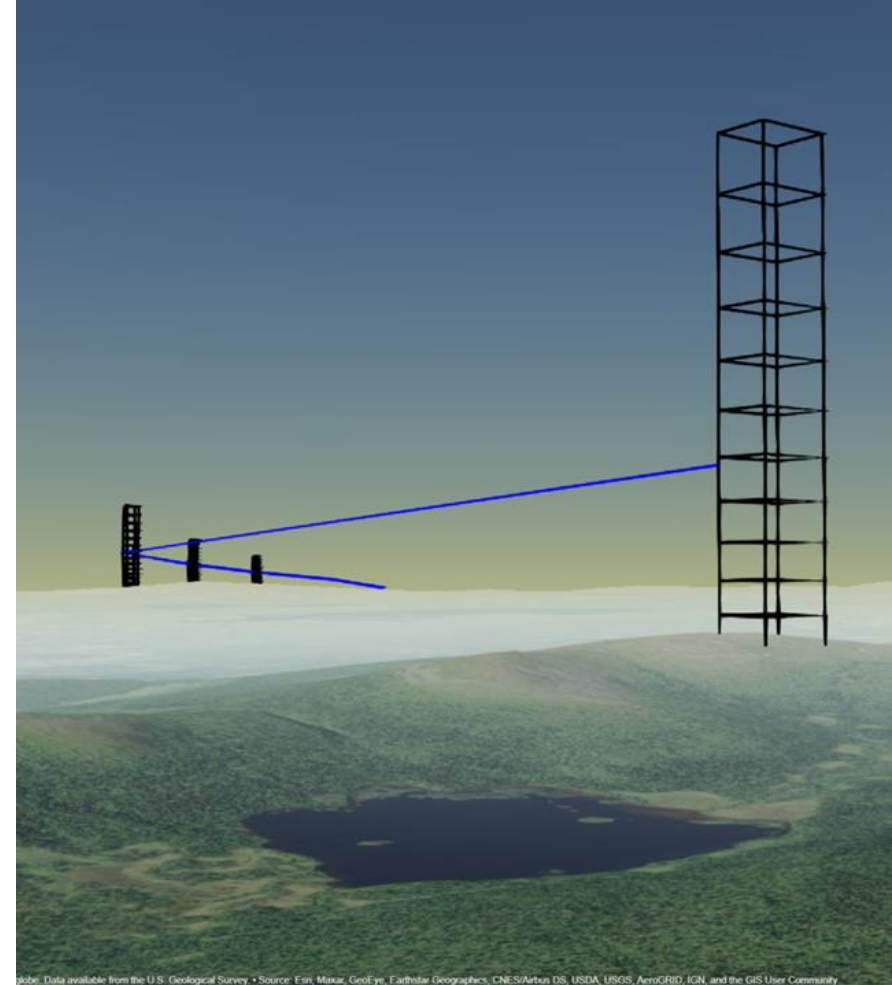


Modelling sub-micron secondary aerosol formation with the ADCHEM-ClusterIn model system

Results over Northern Europe in year 2018

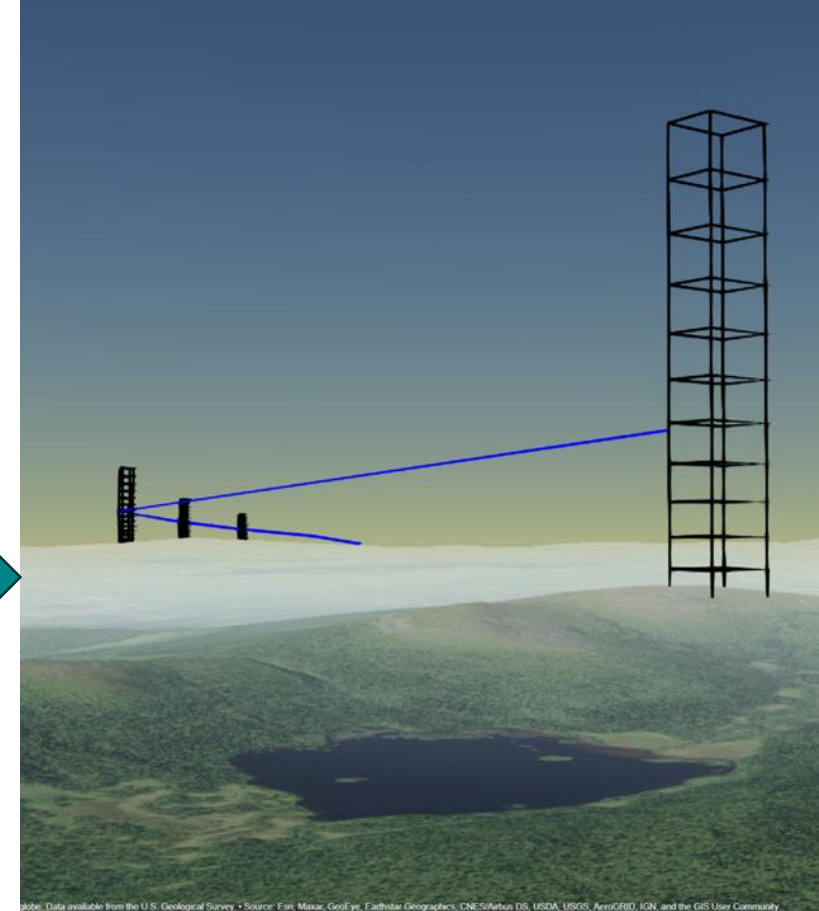
+ preliminary results from the EMEP July 2022 campaign.



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

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-column model, 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
© Author(s) 2011. CC Attribution 3.0 License.

*



Atmospheric
Chemistry
and Physics

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

P. Roldin¹, E. Swietlicki¹, G. Schurgers², A. Arneth^{2,3}, K. E. J. Lehtinen^{4,5}, M. Boy⁶, and M. Kulmala⁶

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. Roldin¹, E. Swietlicki¹, A. Massling^{1,*}, A. Kristensson¹, J. Löndahl¹, A. Eriksson^{1,2}, J. Pagels², and S. Gustafsson³

SCIENTIFIC REPORTS

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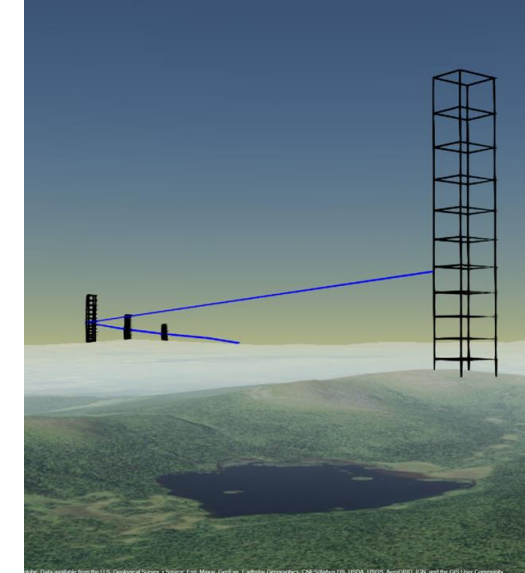
Diesel soot aging in urban plumes within hours under cold dark and humid conditions

Received: 9 May 2017
Accepted: 8 September 2017

A. C. Eriksson^{1,2}, C. Wittborn¹, P. Roldin^{1,3}, M. Sporre⁴, E. Öström^{1,5}, P. Nilsson², J. Martinsson^{1,5}, J. Rissler², E. Z. Nordin², B. Svenningsson¹, J. Pagels² & E. Swietlicki¹

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 monoterpenes**,*** and aromatic compounds****
- The particle size dependent SOA formation involve >1000 organic molecules.



MCM (v3.3.1) Home Browse Export AtChemOnline About Select Mechanism (MCM, CRI) Tutorial

Master Chemical Mechanism (v3.3.1) *

 UNIVERSITY of York

 National Centre for Atmospheric Science
NATURAL ENVIRONMENT RESEARCH COUNCIL



**

ARTICLE

<https://doi.org/10.1038/s41467-019-12339-8> OPEN

The role of highly oxygenated organic molecules in the Boreal aerosol-cloud-climate system

Pontus Roldin^{1*}, Mikael Ehn², Theo Kurtén³, Tinja Olenius⁴, Matti P. Rissanen², Nina Sarnela², Jonas Elm⁵, Pekka Rantala², Liqing Hao⁶, Noora Hyttinen⁷, Liine Heikkinen², Douglas R. Worsnop^{2,8}, Lukas Pichelstorfer^{2,9}, Carlton Xavier², Petri Clusius², Emilie Öström¹, Tuukka Petäjä², Markku Kulmala², Hanna Vehkamäki², Anneli Virtanen⁶, Ilona Riipinen⁴ & Michael Boy²

nature communications

Article

<https://doi.org/10.1038/s41467-023-39066-4>

NO at low concentration can enhance the formation of highly oxygenated biogenic molecules in the atmosphere

Received: 14 October 2022

A list of authors and their affiliations appears at the end of the paper

Accepted: 24 May 2023

nature communications

Article

<https://doi.org/10.1038/s41467-023-40675-2>

Molecular rearrangement of bicyclic peroxy radicals is a key route to aerosol from aromatics

Received: 24 March 2023

Accepted: 7 August 2023

Published online: 17 August 2023

Siddharth Iyer¹, Avinash Kumar¹, Anni Savolainen¹, Shawon Barua¹, Christopher Daub², Lukas Pichelstorfer³, Pontus Roldin^{4,5}, Olga Garmash^{1,6}, Prasenjit Seal¹, Theo Kurtén² & Matti Rissanen^{1,2}

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

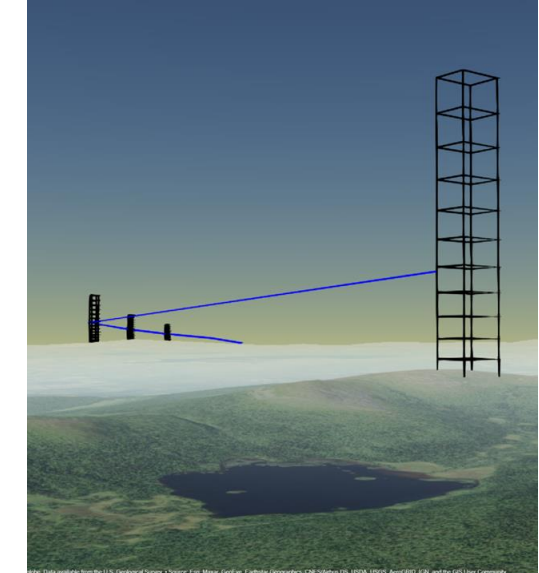
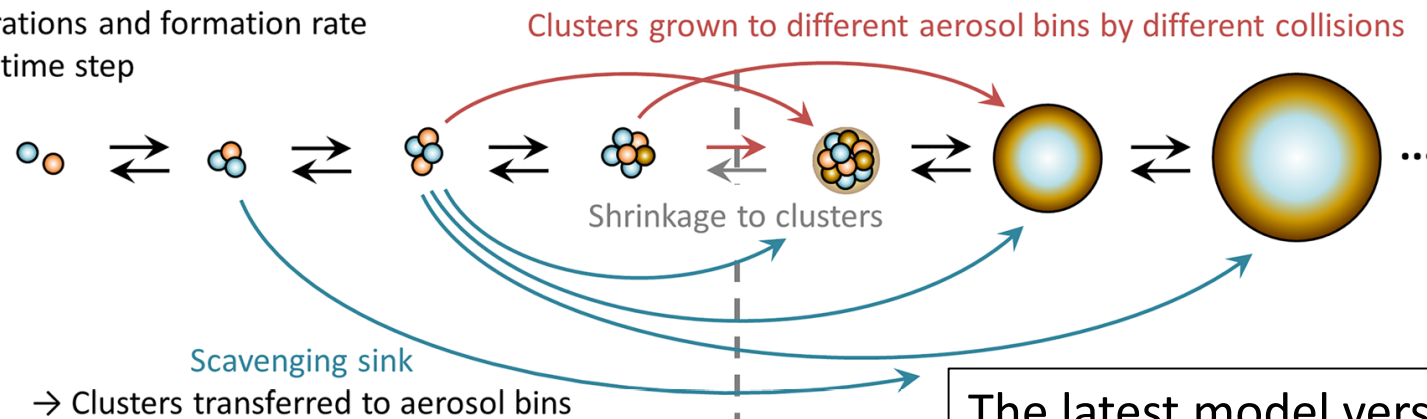
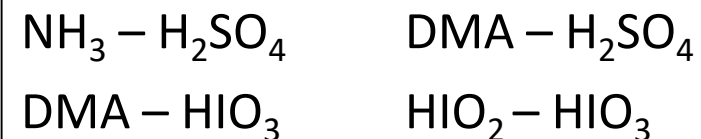


Figure from Olenius and Roldin (2022)*

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



scientific reports

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

Tinja Olenius^{1,2} & Pontus Roldin²

ENVIRONMENTAL Science & Technology

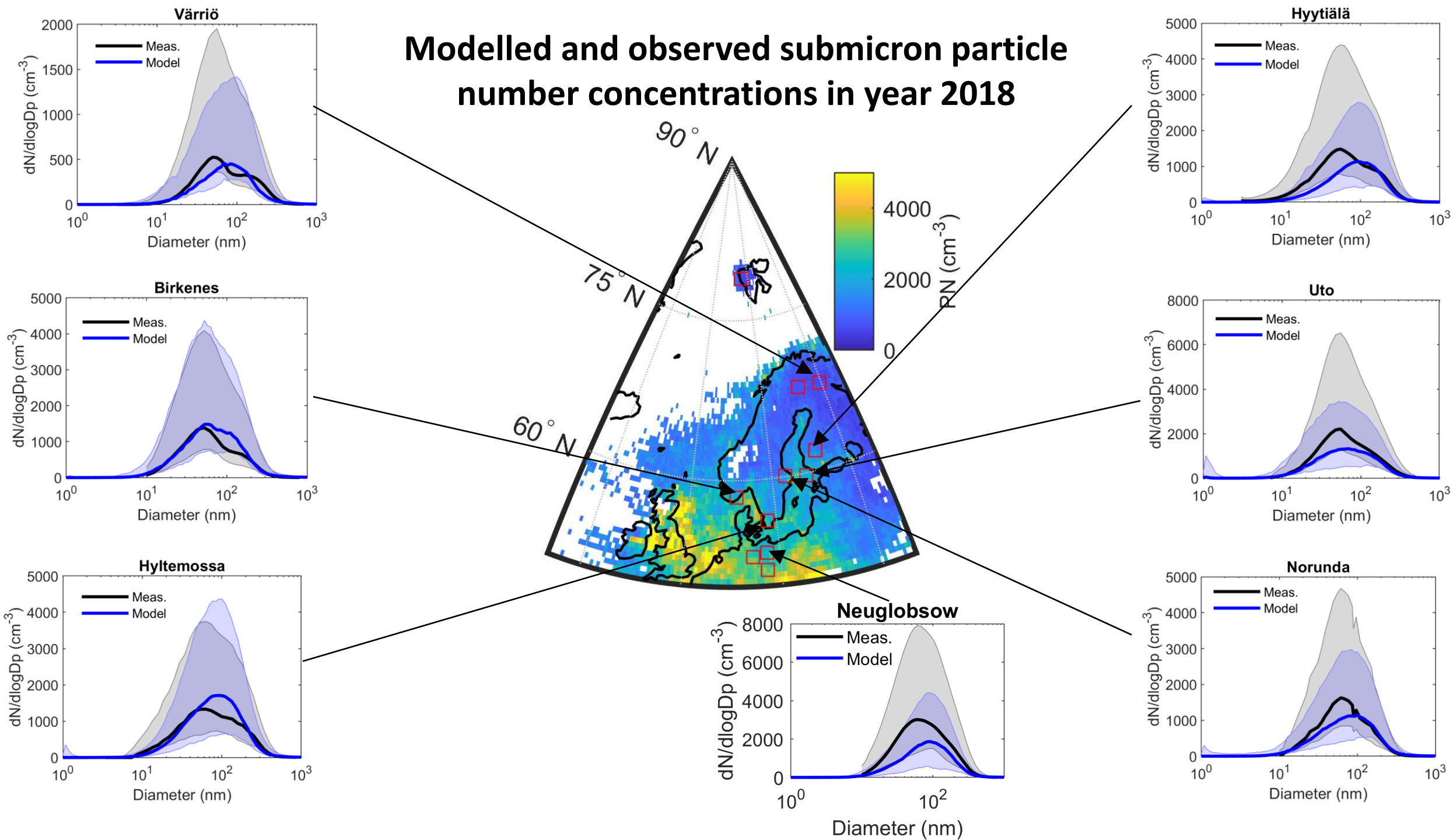
Role of Iodine-Assisted Aerosol Particle Formation in Antarctica

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

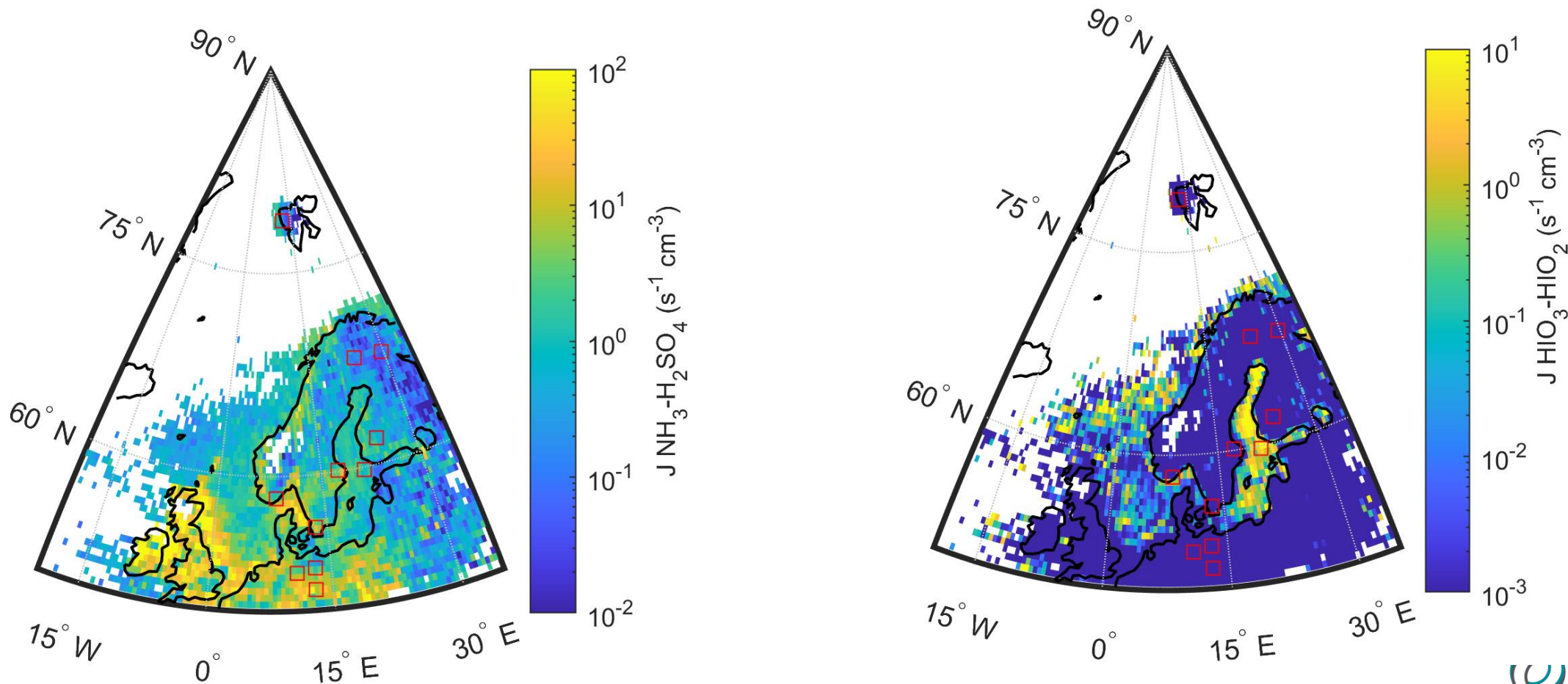
Read Online

Modelled and observed submicron particle number concentrations in year 2018



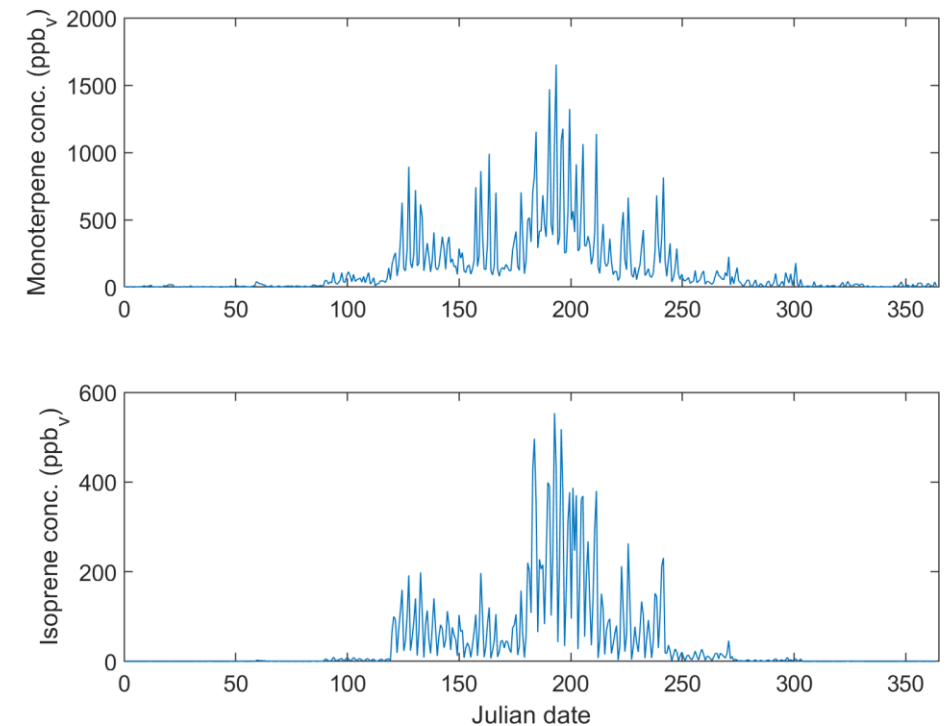
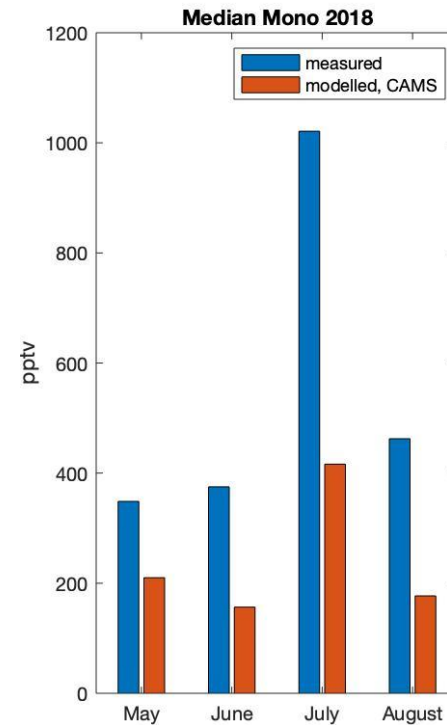
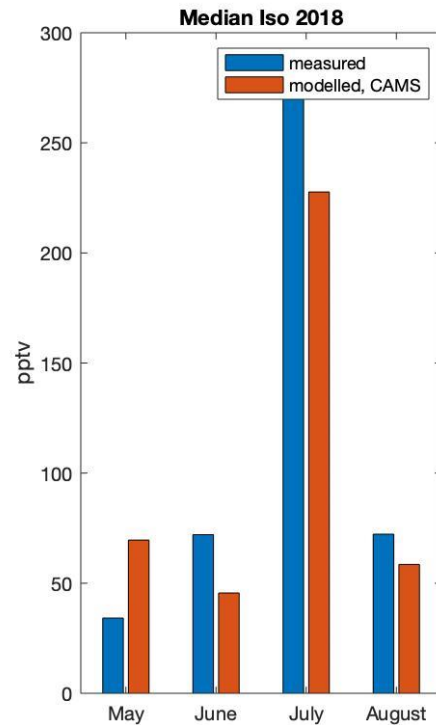
New particle formation in 2018

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



Evaluation of BVOC concentrations using long-term observations

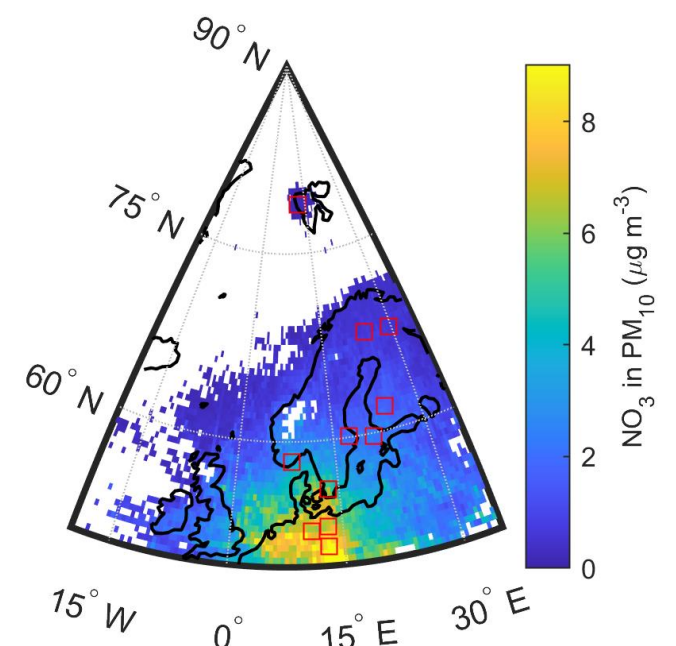
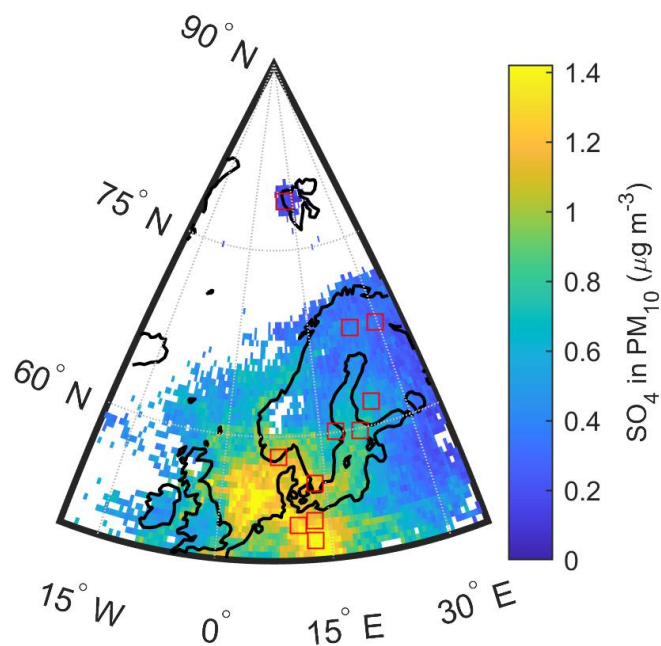
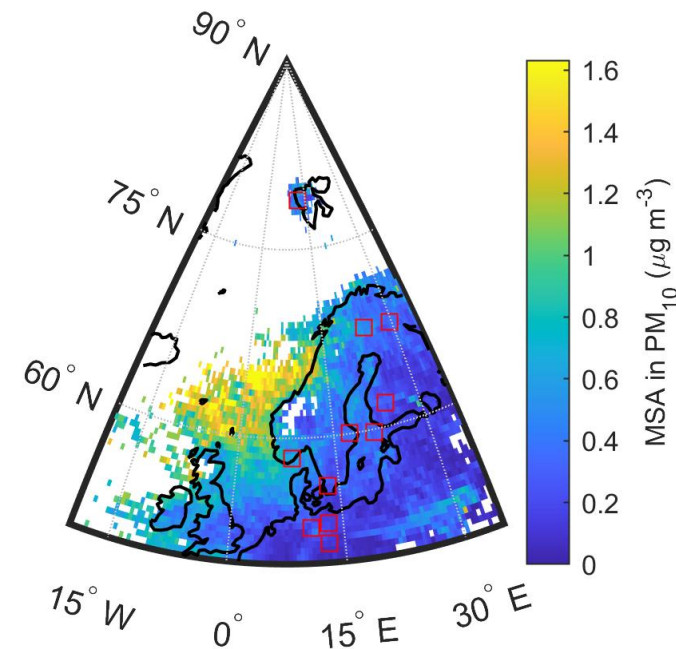
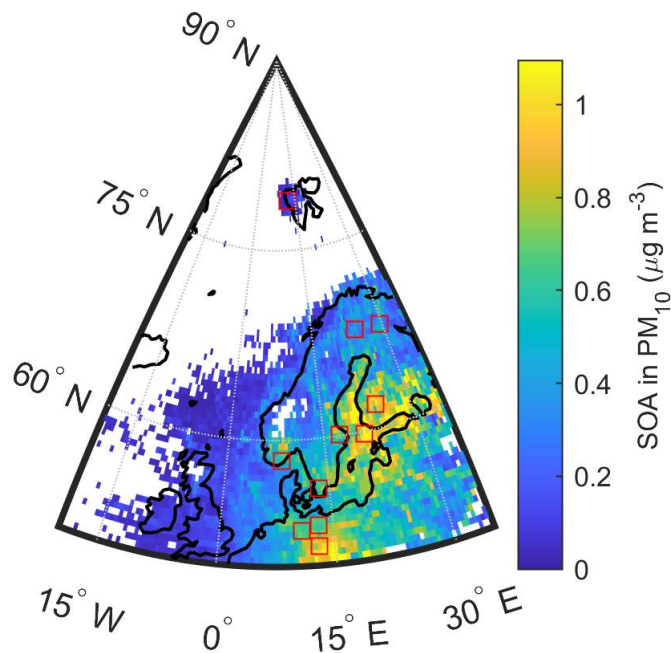
- Evaluation of modelled monoterpene and isoprene concentrations at Hyytiälä, Finland using PTR-MS observations (Master thesis work by Sara Bengtsdotter, Lund Univ.)



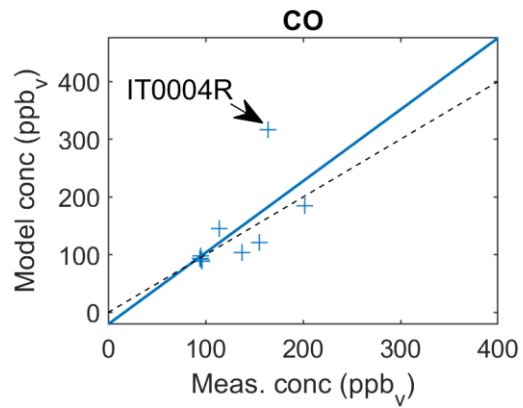
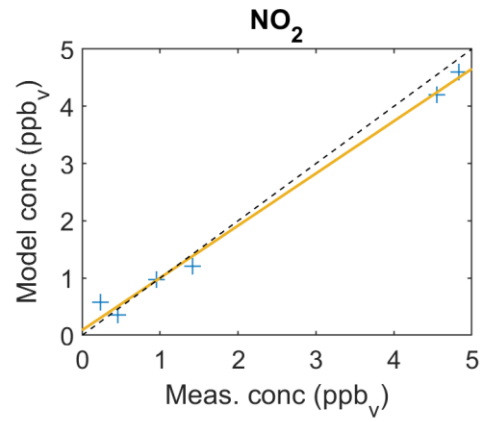
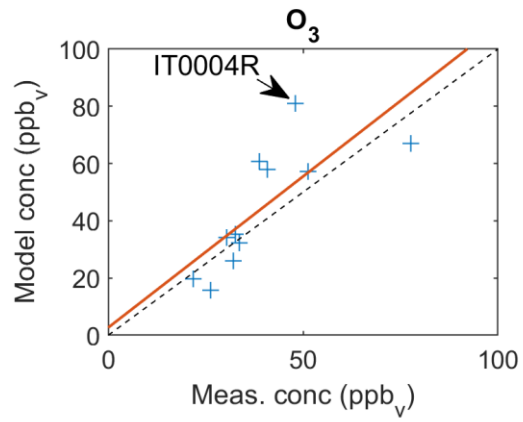
- Outlook - compare modelled and observed (HR PTR-MS) VOC concentrations at the ACTRIS Hyltemossa field station in S. Sweden (VOC observations since 2019)

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.



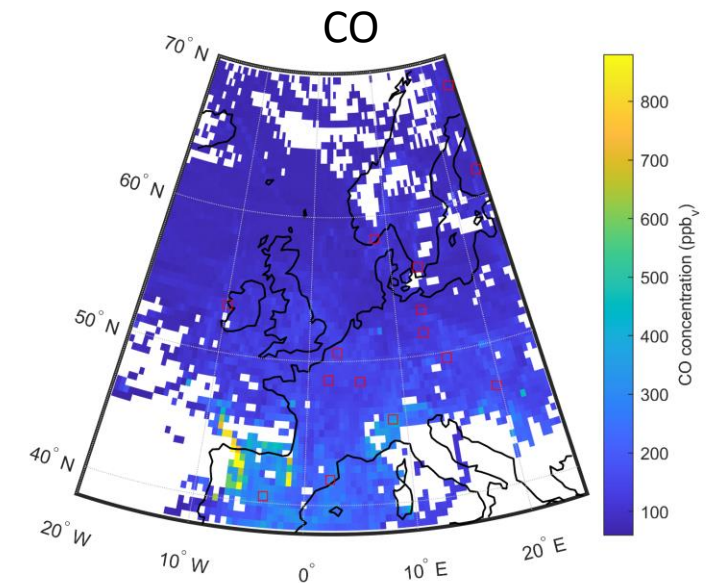
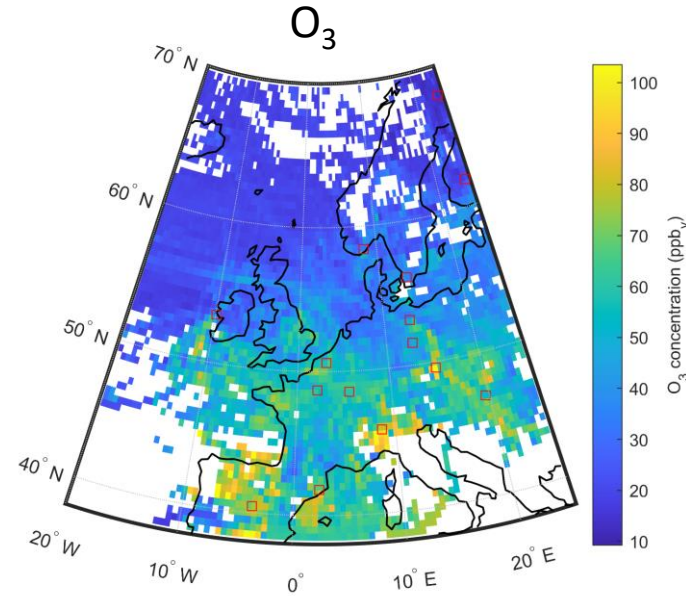
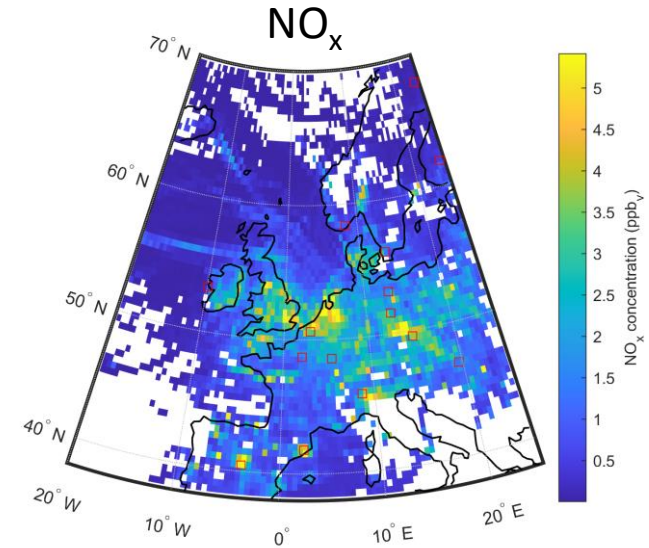
Preliminary model results from the EMEP campaign in July 2022



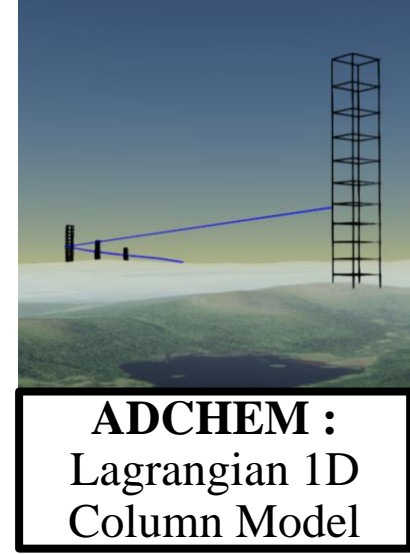
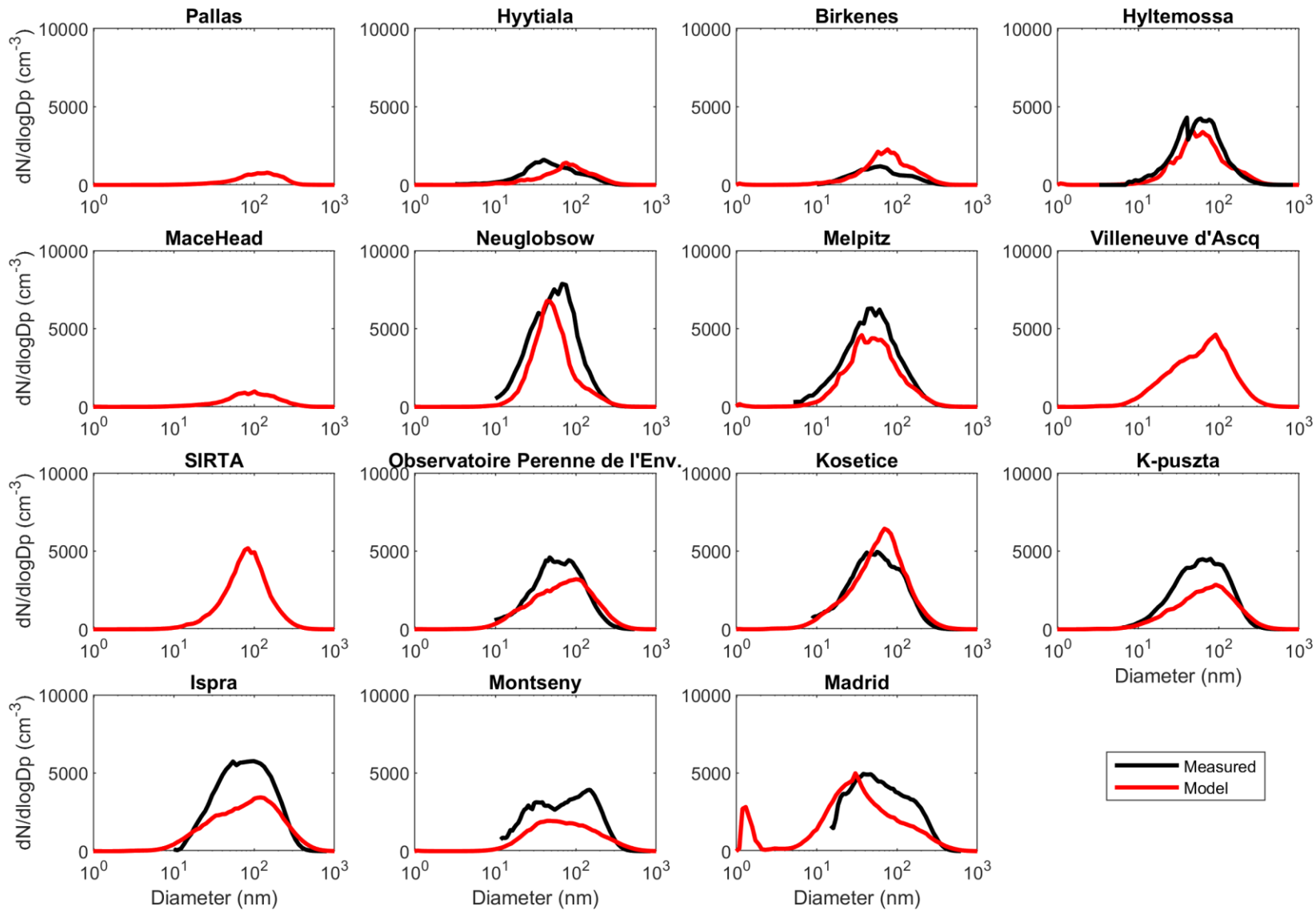
— $y=1.0564x+2.673$, $R=0.762$

— $y=0.913+0.0888x$, $R=0.996$

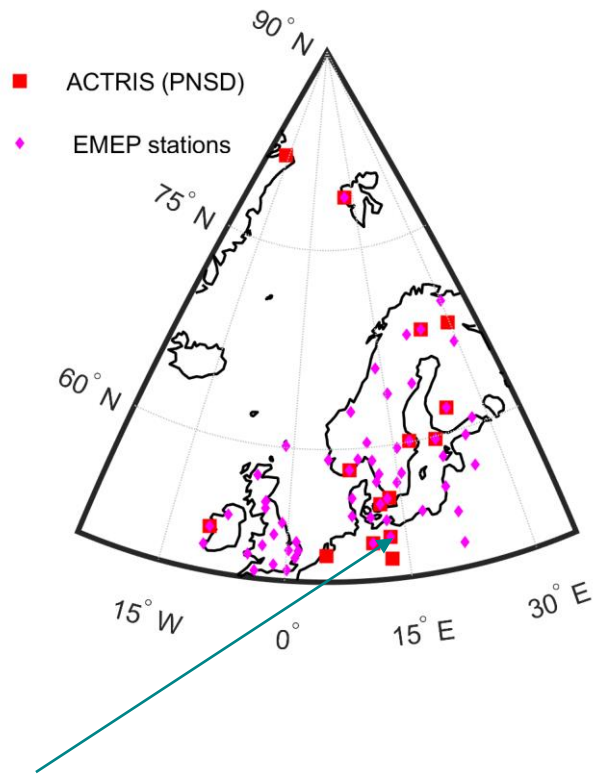
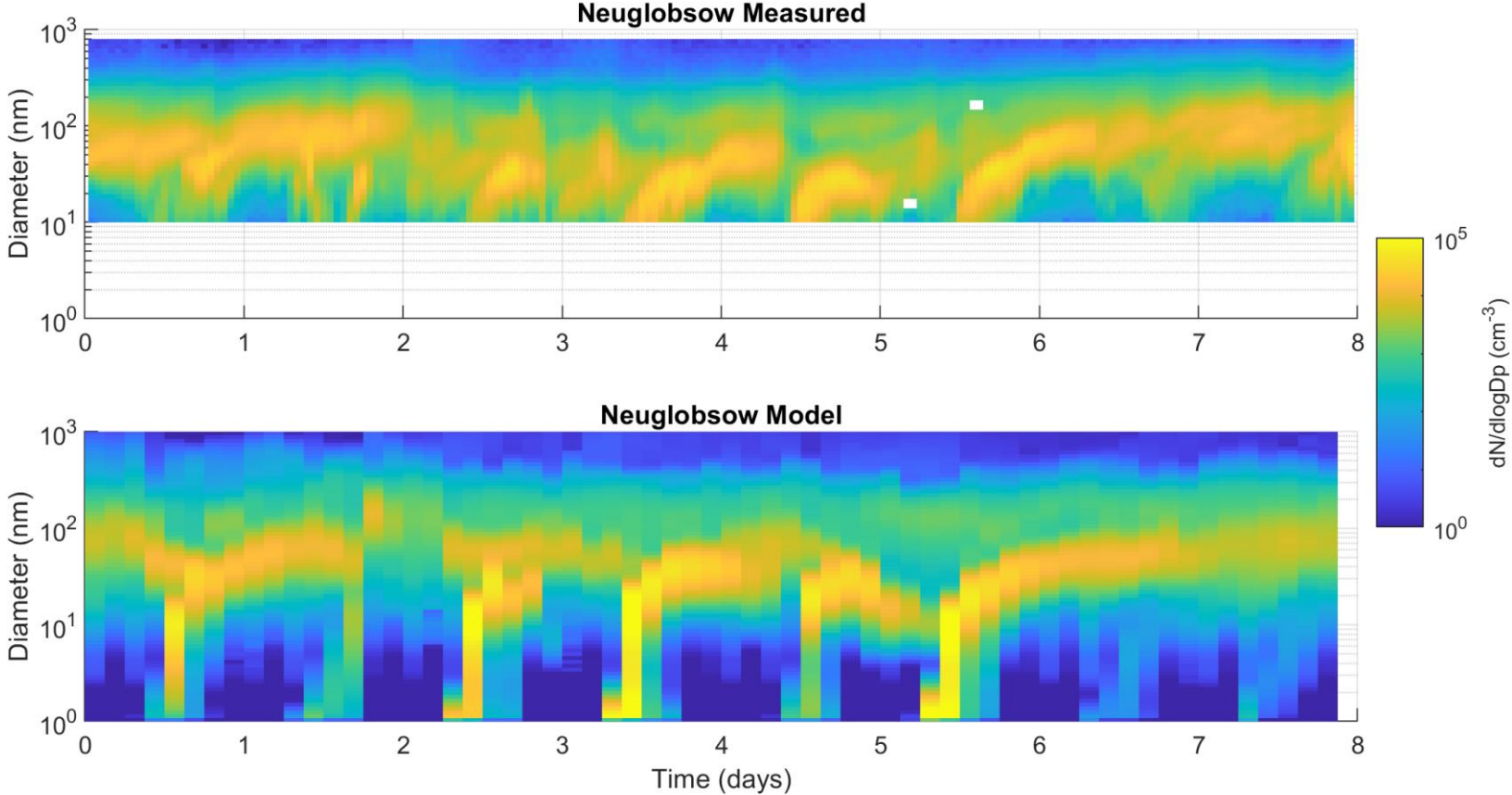
— $y=1.2392x-20.357$, $R=0.650$



Particle number size distributions

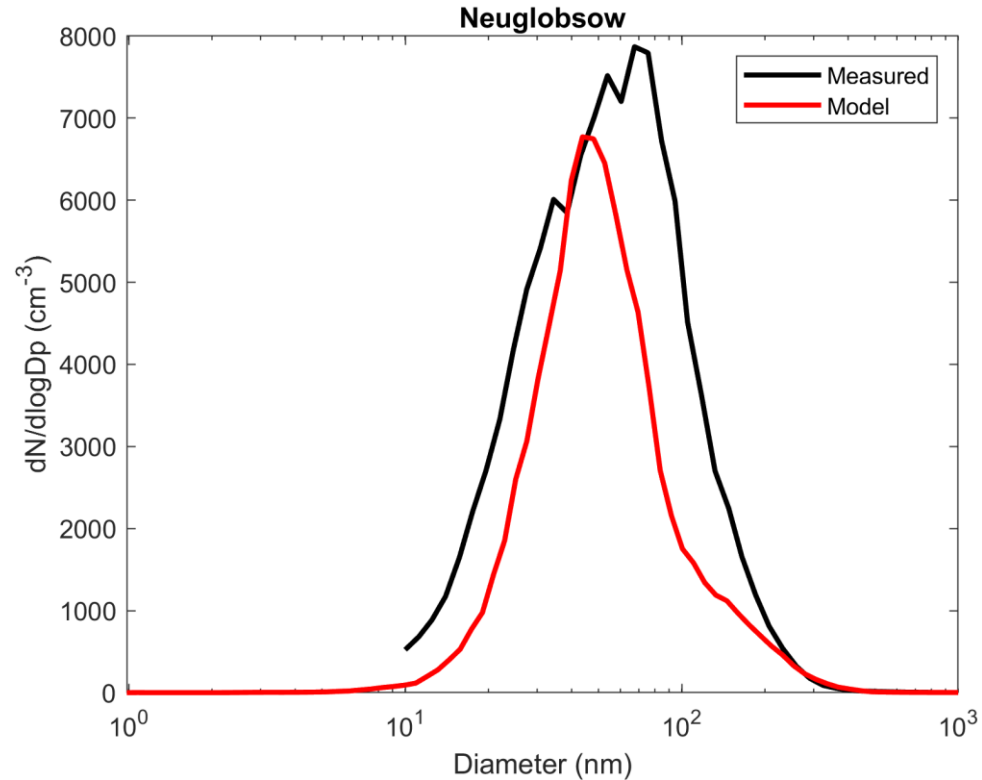


Neuglobsow- New particle formation

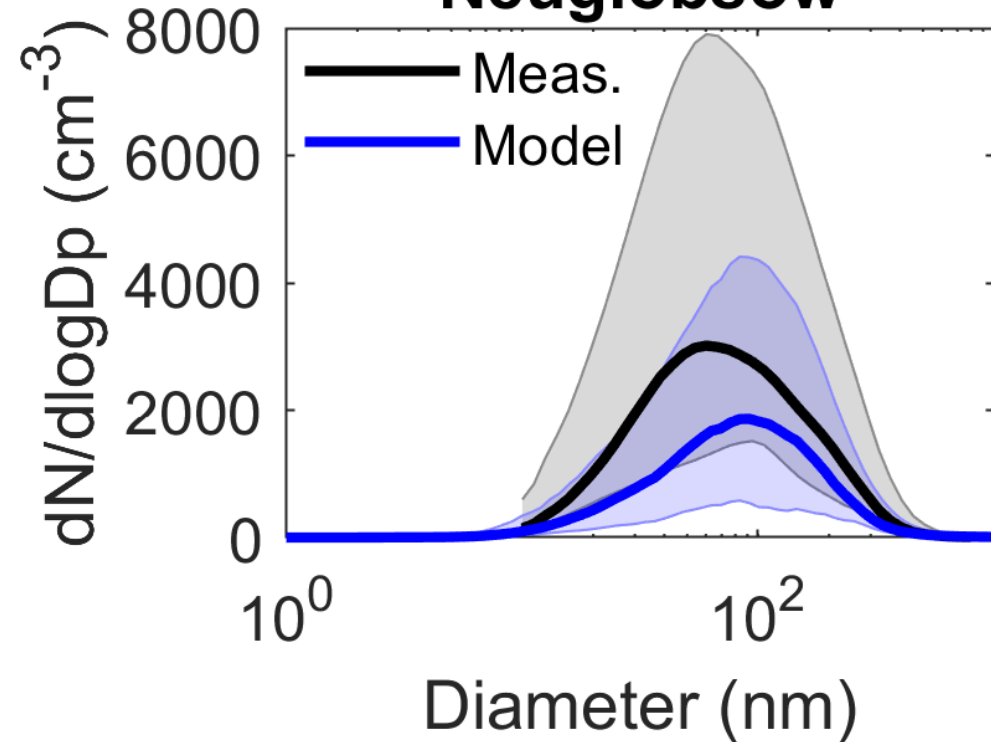


Neuglobsow – Secondary aerosols

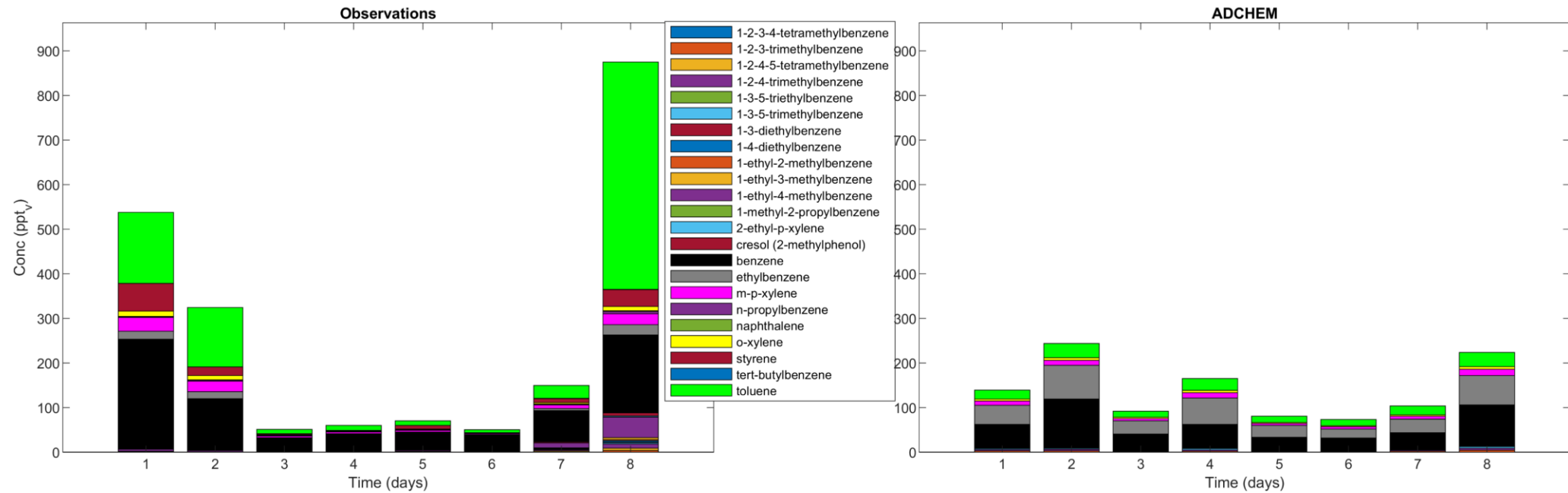
Median PNSD from IMP2022



Median PNSD from 2018 Neuglobsow

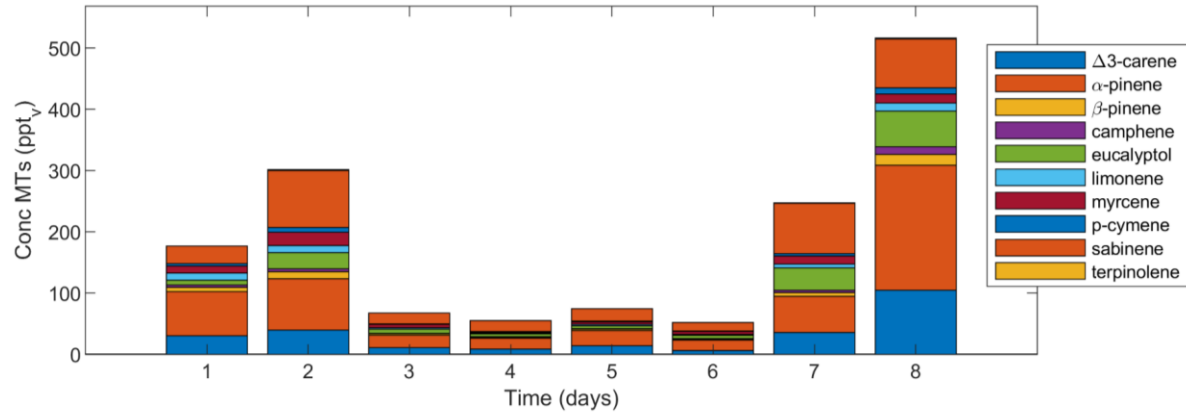


Neuglobsow– aromatic compounds

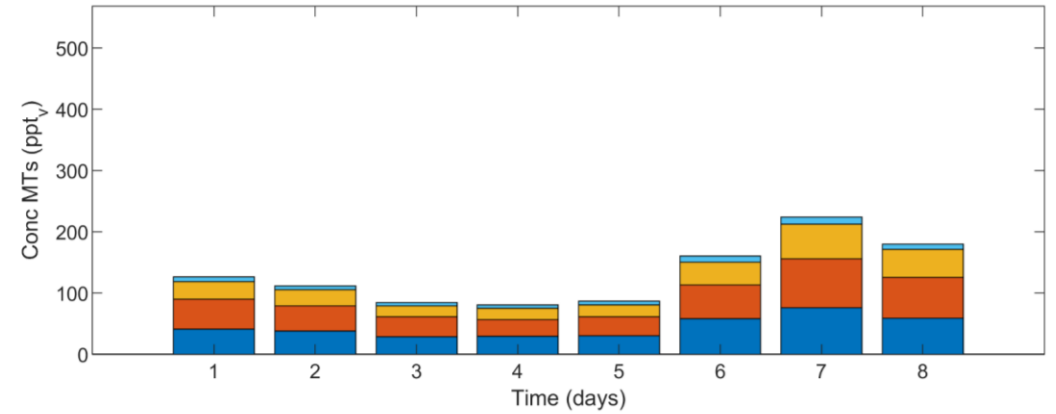


Neuglobsow-monoterpenes

Observations



Modelled



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!

