WP3: Improving modelling and emission inventories for policy assessment using advanced observation-based methodologies

WP Leads: Maria Kanakidou, Augustin Colette,

Task Leads: Leena Järvi, Marc Guevara, Jeroen Kuenen, **Spyros Pandis**, Hilde Fagerli

FORTH, INERIS, BSC, METNO, UHEL, TNO, NOA, KNMI, FMI, CNRS

RI-URBANS (101036245)

September 2025

WP3 : Specific Objectives

- Better quantification of emissions of gaseous and particulate pollutants at spatio-temporal scales relevant to urban areas;
- Disentangling the urban, regional and LRT contributions to urban pollutants;
- Coupling urban and regional scales;
- Innovative modelling of the source contribution of ROS, non-exhaust vehicle PM emissions, nanoparticles, BC, secondary PM, PM and O_3 precursors, such as VOCs, NOx;
- Optimizing the use of new observations

WP3 Tasks

Tasks ↓ Month →	2	9	20	28	30	36	40	48
3.1 Characterization of urban dispersion using advanced observations-based methodologies and modelling (Lead: Leena Järvi, UHEL; Marc Guevara, BSC; Inv.: CNRS, FMI, KNMI).					D, M			
3.2 Enhancing quality and completeness of emissions inventories (Lead: Jeroen Kuenen, TNO, Marc Guevara, BSC, Inv.: NOA).		D	M	D,M				
3.3 Extending AQ modelling to health and policy relevant indicators down to urban scale (Lead: Spyros Pandis, FORTH; Augustin Colette, INERIS; Inv.: FMI, MET Norway, TNO, CNRS).			M		D			
3.4 Implement novel AQ indicators in tools supporting policy decision making to improve citizen health (Lead: Hilde Fagerli, METNO; Maria Kanakidou, FORTH; Inv.: INERIS, NOA, FMI, CNRS, TNO).			M			D		
3.5 WP3 synergy to support SPs 2 and 3 for modelling novel health and policy relevant indicators and emission inventories (Lead: Maria Kanakidou, FORTH; Augustin Colette, INERIS; Inv.: BSC, METNO, UHEL, TNO, NOA, FMI, CNRS).							D	

M02-M30

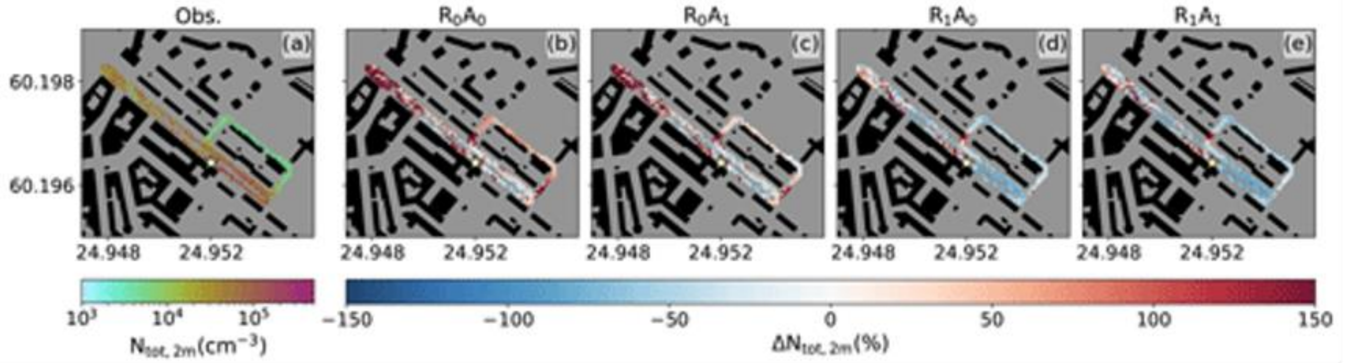
Task 3.1 Characterization of urban dispersion using advanced observations-based methodologies and modelling

UHEL: LES Modelling

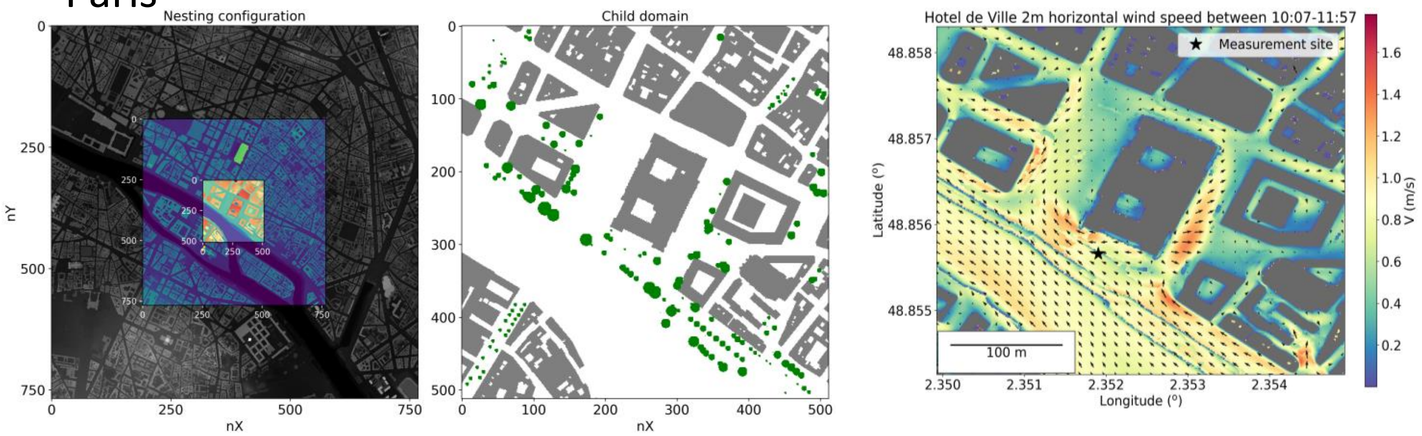
Examining the **relevant processes needed to conduct realistic turbulence and air quality simulations within urban settings** in Helsinki by studying the impact of the **inclusion of radiation interaction and aerosol particle dynamics** into a high-resolution LES using the PALM model system 6.0.

Street scale **model comparison (CFD, PALM, MUNICH) exercise in Paris**

Helsinki



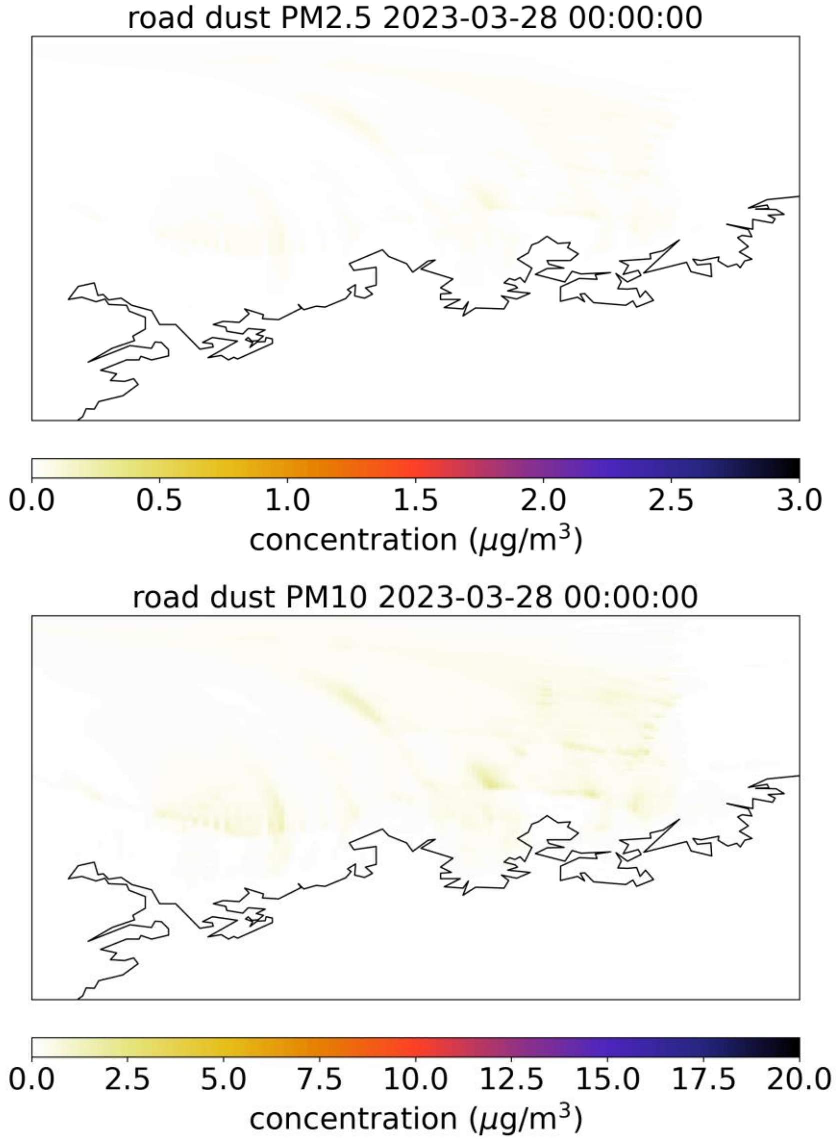
Paris



By Jani Strömberg

FMI: road-dust / Urban SILAM

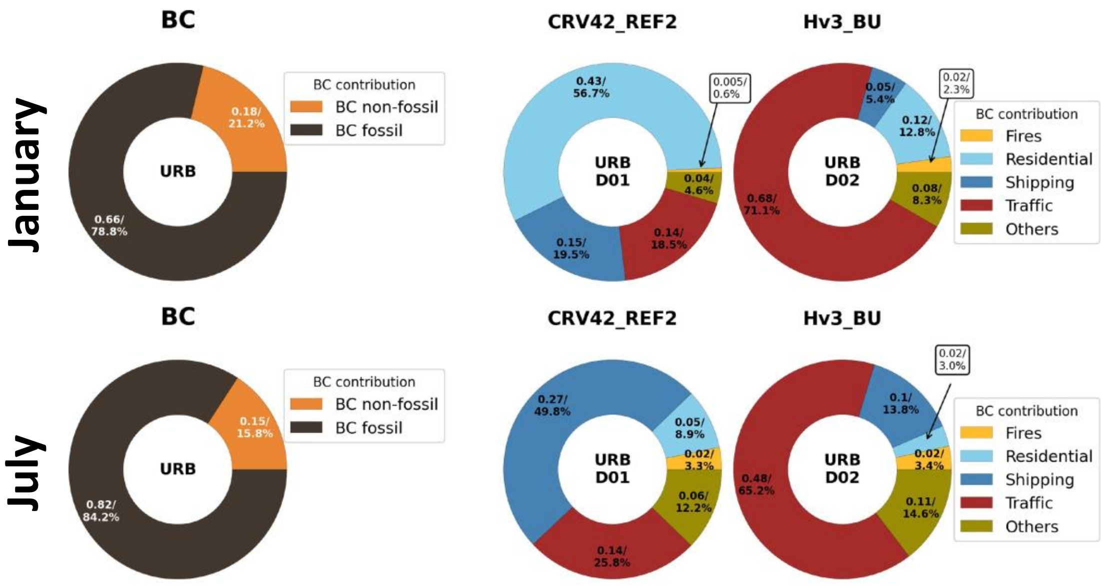
- Urban SILAM application: Helsinki PM composition is strongly controlled by road resuspended dust (esp. springtime Helsinki is among the most-dusty cities in Europe)
- **New road dust model has been developed**
- Applicable also outside Finland
- Runs: 3 years for Helsinki, 200 m
  1 year Europe, 10 km



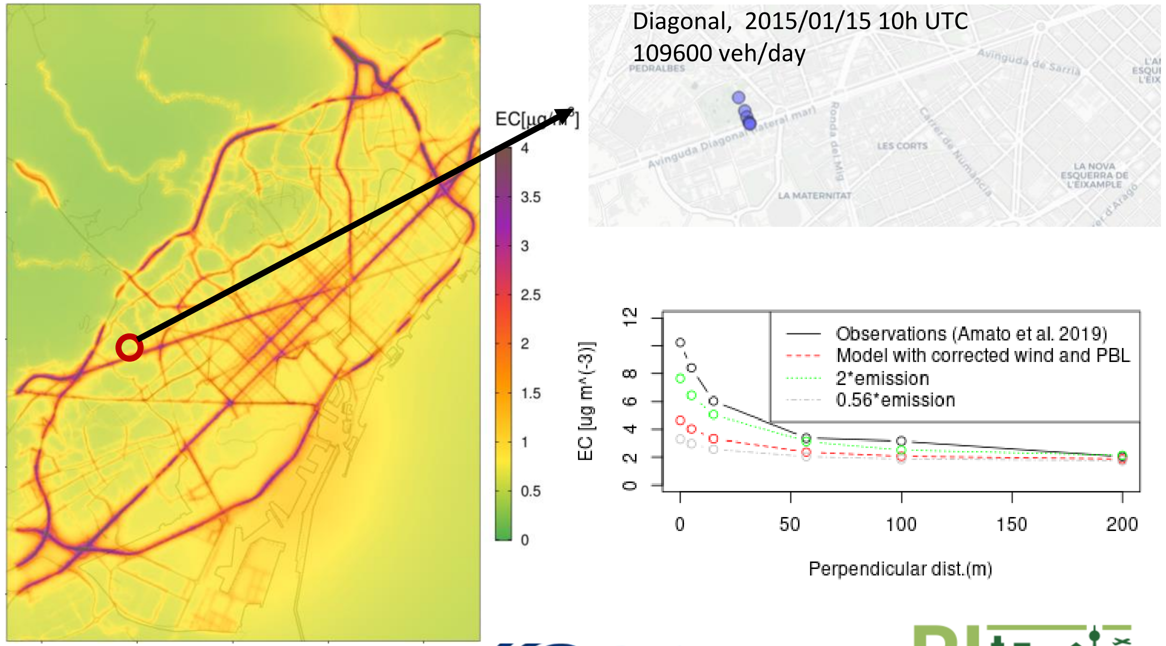
BSC: Traffic black carbon

- Assessing urban background and urban traffic black carbon levels combining mesoscale and urban scale modelling

Uncertainties in source apportionment of urban background BC



Uncertainties in the reproduction of urban traffic BC horizontal profiles

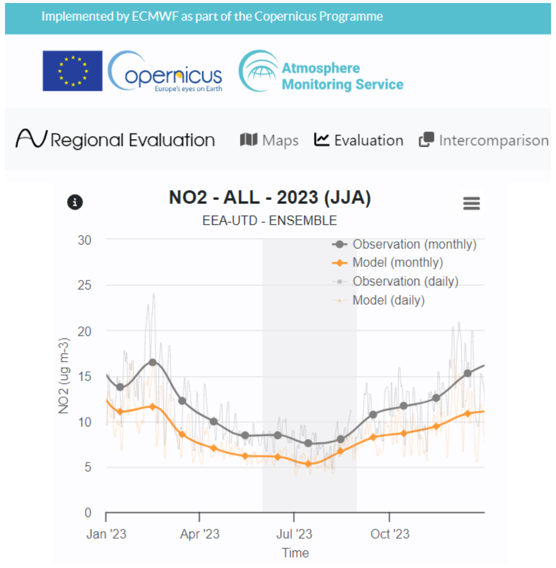


RI-URBANS (101036245)

September 2025

KNMI/CNRS: NO_2 vertical profiling evaluation in CAMS

CAMS Regional AQ Models suffer from systematic low bias for NO_2, long attributed to resolution



Progress in joint assimilation of TROPOMI (S5P, soon S4) and surface AQMN

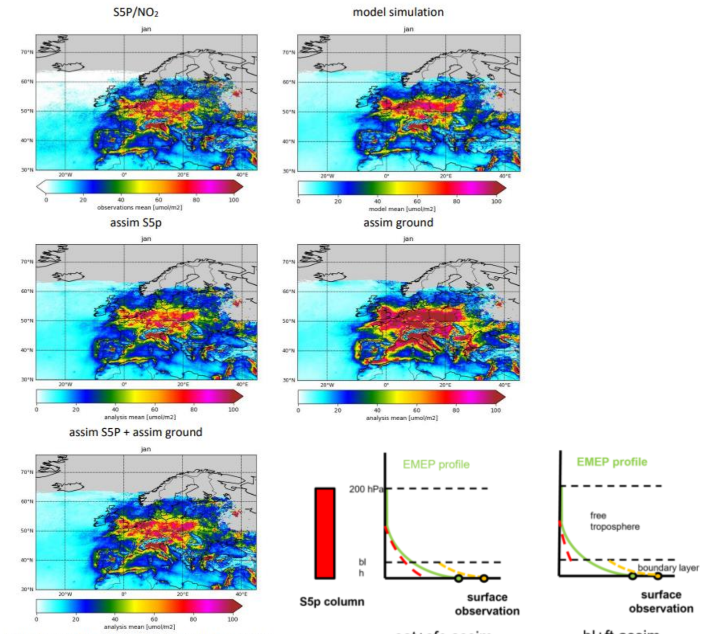
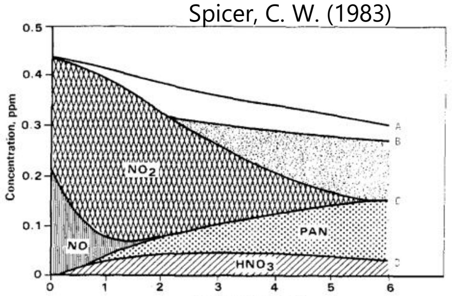
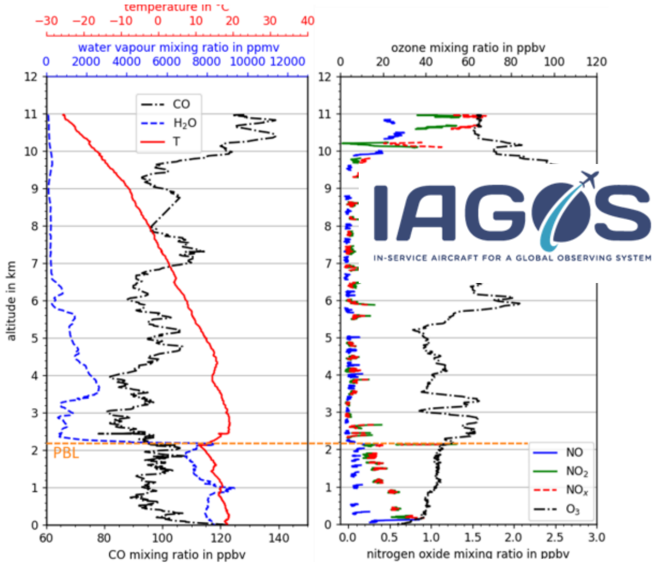


Figure 41 –S5P NO_2 observations and simulations averag

High quality in-situ data are instrumental for CAMS QA/QC:

- IAGOS NOx Profiles
- ACTRIS-grade NO2



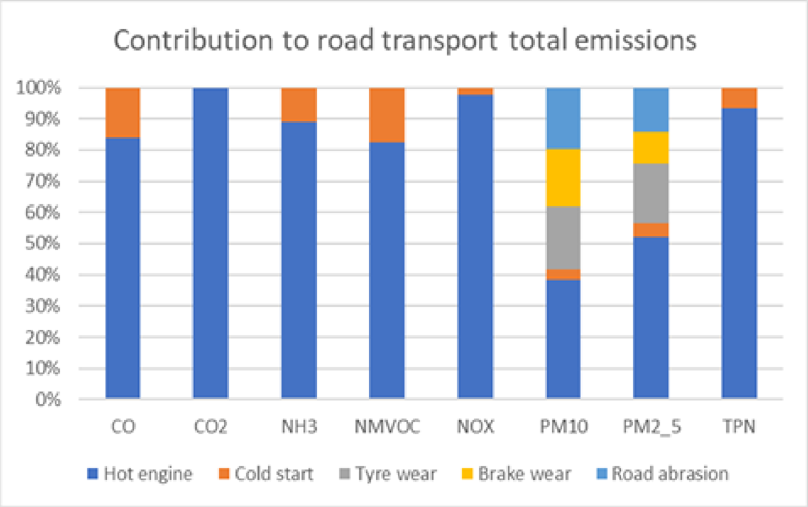


ACTRIS
Exploring the Atmosphere

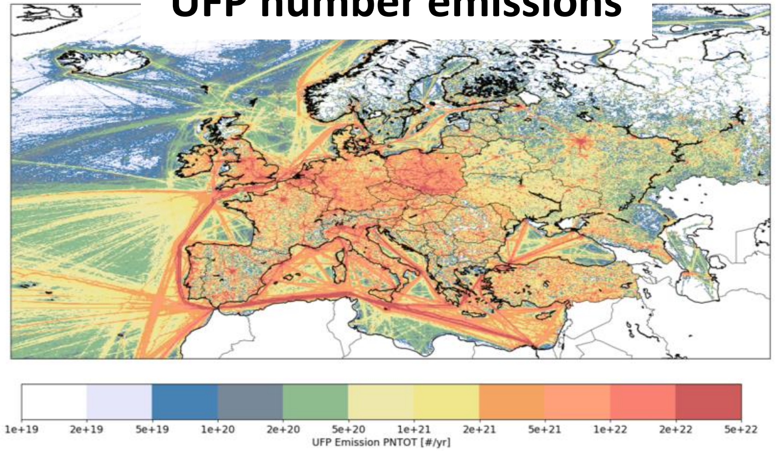
M02-M28

Task 3.2 Updates to EU emission estimates

- **Updated UFP (TPN) emissions** (based on new literature)
- Specific updated calculations for non-exhaust contributors to PM mass based on EMEP/EEA Guidebook approach
- Explicit accounting of cold start emissions, 95% allocated to urban areas
- **Fully updated spatial distribution map for Europe and pilot cities**
- Open Street Map for location of all roads
- Open Transport Map (Jedlička et al., 2016) for intensities
- Random forest model used based on multiple predictors (e.g. land use, administrative units, road characteristics as in OSM, etc.) to assess intensities for missing roads



UFP number emissions



Enhancing Urban Emission Inventories

- Multi-scale modelling down to street-level to capture pollutant dispersion.
- A framework cross-checking of methodologies was developed and applied to assess urban emissions and air quality and examine the improvements finer scale simulations can bring in specific case studies made in Barcelona (Spain), Paris (France), Turku (Finland), Helsinki (Finland) and Rotterdam (the Netherlands).
- Differences were found between top-down and bottom-up inventories.
- A model evaluation toolbox (D16) was proposed for routine evaluation within the Copernicus Atmosphere Monitoring Service (CAMS).

Refining CAMS-REG Inventories

- A methodology was created to downscale CAMS-REG emissions to 1 km² resolution using open-access spatial datasets (deliverable D17 (D3.2)).
- This enabled high resolution mapping of sectoral emissions like industrial, transport, and residential emissions.
- The first inventory for ultrafine particles (UFPs) and non-exhaust vehicle emissions was developed (Deliverable D18 (D3.3)).
- A relevant service tool (ST15: First UFP-PNSD and non-exhaust vehicle PM EU emission) was developed.

Done in Task 3.2

M02-M30

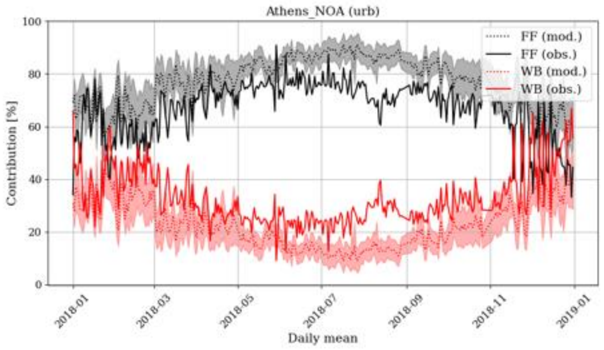
Task 3.3: Extending AQ modelling to health and policy relevant indicators down to urban scale

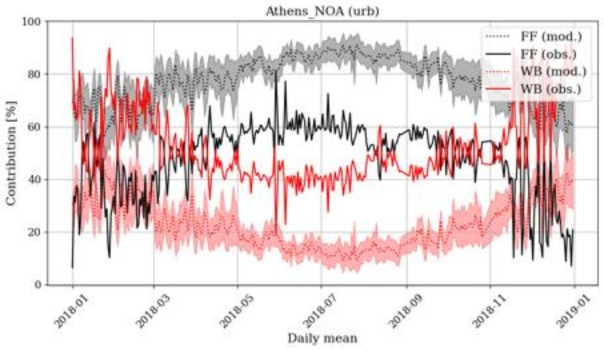
INERIS/CSIC: eBC Evaluation & QC

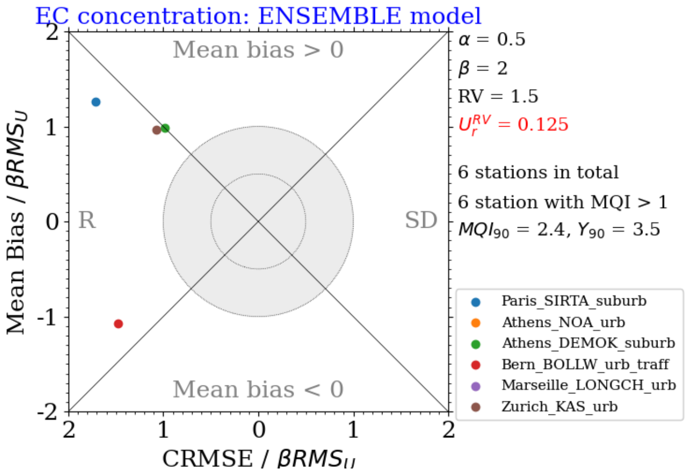
- Improved uptake of eBC observation estimates from WP1 and WP4 Pilots:
  - robust eBC/EC/BC
  - source apportionment sf/lf

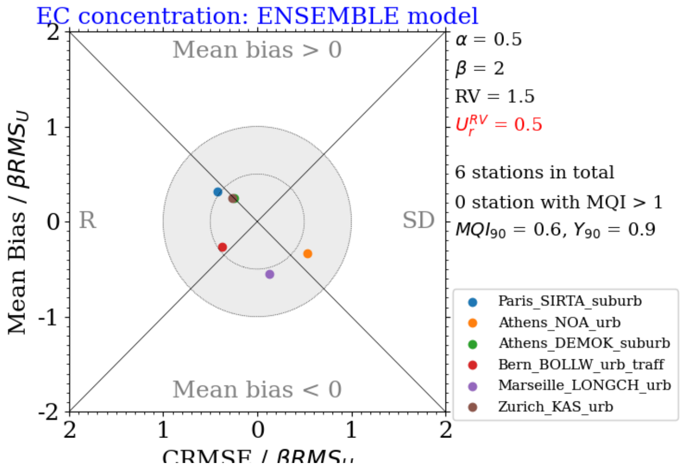
- Confronted against the 11-member CAMS operational ensembles

- Using the FAIRMODE recommended target plots accounting for observation uncertainties



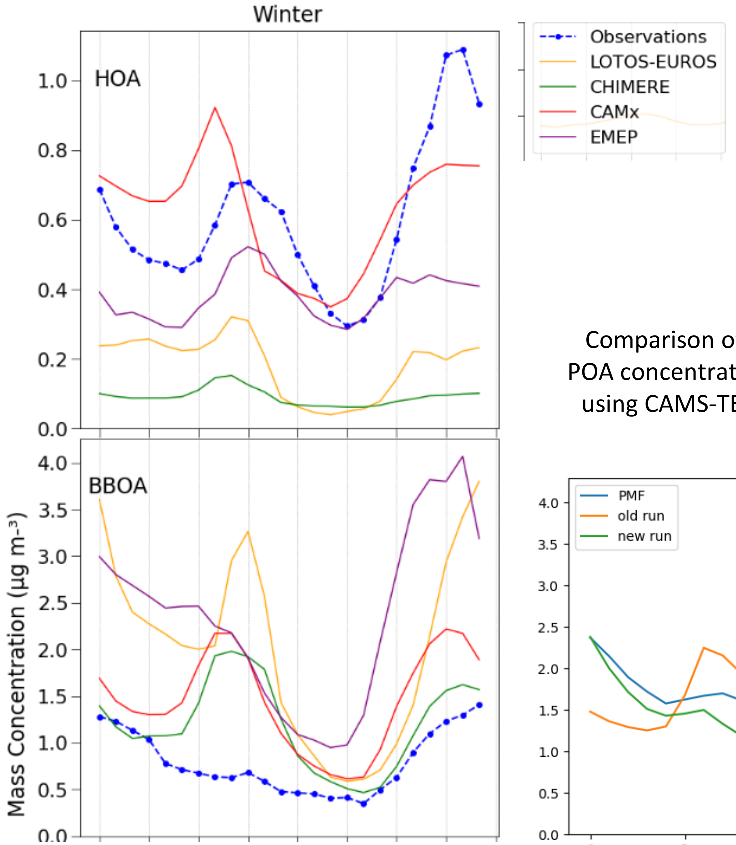






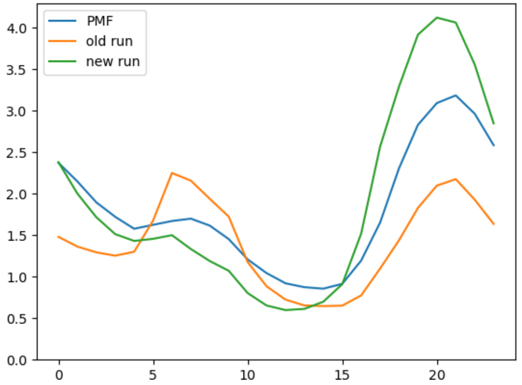
INERIS/METNO/TNO/PSI: OA Evaluation & QC

Comparison of results of 4 CTMs (CHIMERE, EMEP, LOTOS-EUROS, CAMx) with PMF estimations of HOA, BBOA and OOA (ACSM at RI-Urbans Pilot sites)



- Other results
  - Proof of concept for Near-Real Time evaluation of modelled organic aerosol in relation with dominant emission sources
  - Important building block for NRT QA/QC of Source apportionment products, which constitute a key policy support diagnostic

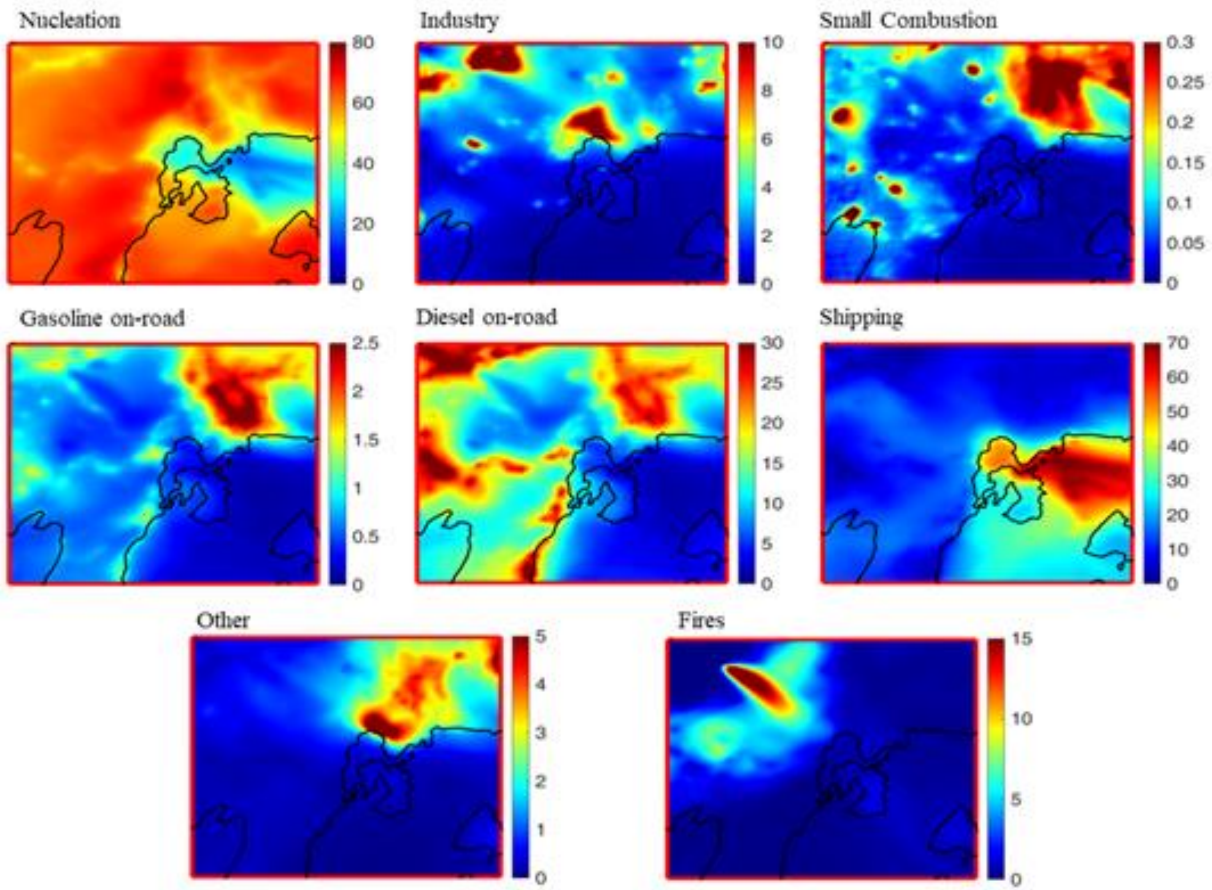
Comparison of CHIMERE diurnal profile of POA concentrations with PMF. New run after using CAMS-TEMPO and adding aging with NO_3 radicals.



FORTH: Development of UFP nested SA modeling

Model development

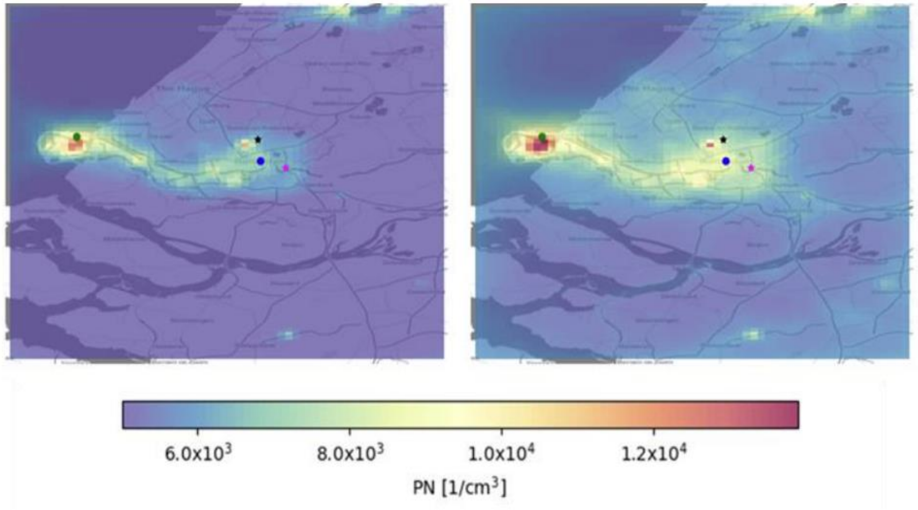
1. Developed a S/A concept for UFP for use in PMCAMx-UF
2. Extended PSAT to be applicable to nested modeling framework for $PM_{2.5}$ mass
3. High resolution applications – using low cost sensors

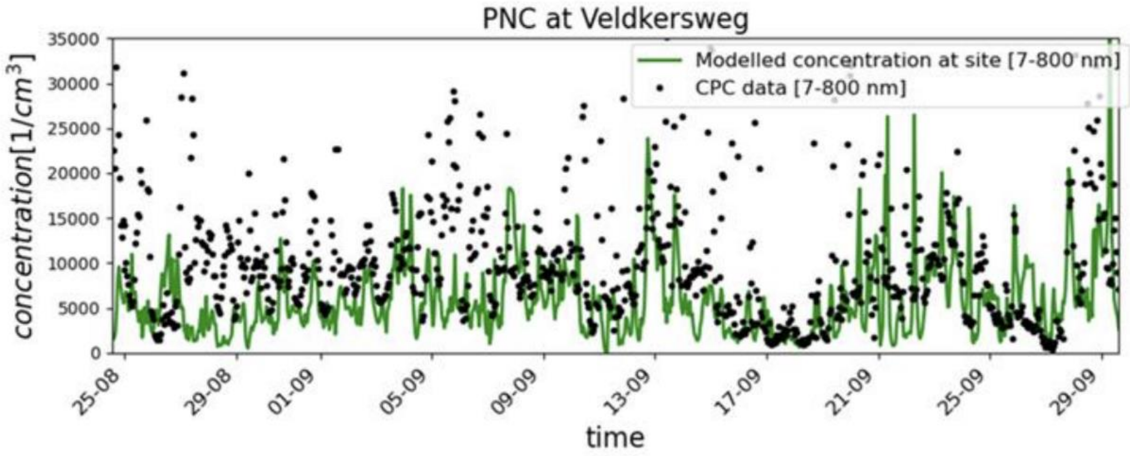


Predicted source contributions as ***percentage of the total*** ***N_{10}*** *over Athens (1x1 km^2) for the summer of 2019 using PMCAMx-UF with three nested domains*

TNO: UFP modelling LOTOS-EUROS

Annual mean concentrations for UFP (left) and PN (right) for 2022 in the Rijnmond area around Rotterdam.





UFP modeling and evaluation with LOTOS-EUROS over city of Rotterdam using the RI-urbans UFP emissions from Task 3.2 and Pilot Site data

UFP Modeling Framework

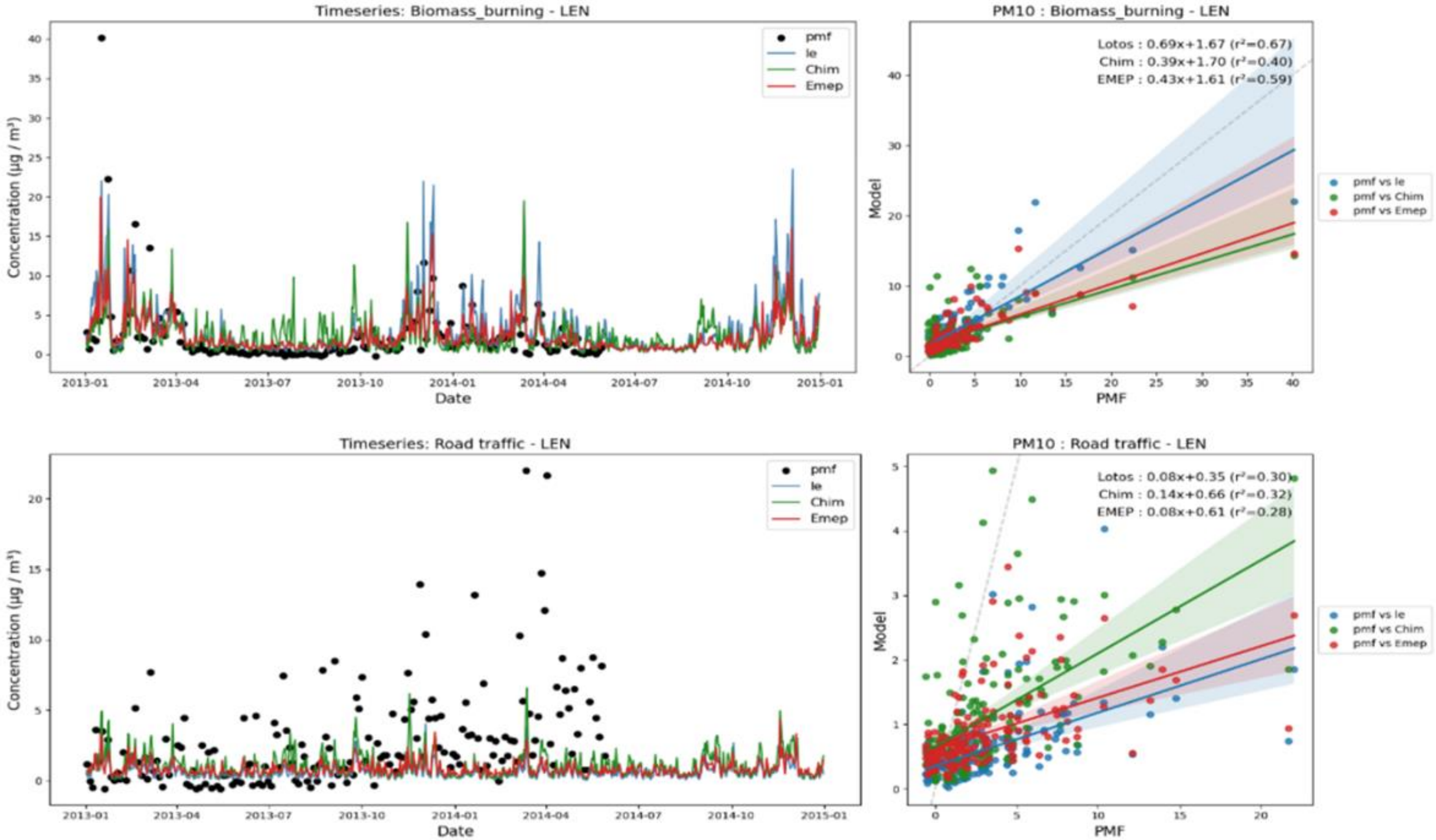
- A multi-scale framework was developed to predict UFP concentrations and size distributions across Europe in parallel with the $PM_{2.5}$ modeling.
- A few models are now able to simulate particle number concentrations (PNC) and UFP concentrations.
- Spatial, seasonal and sectoral source contributions to UFP were identified.
- This modeling supports site selection, exposure assessment, and mitigation planning.
- A guidance on deterministic modeling (ST12) has been released and a service tool (ST16) on multiscale modeling of UFP- particle number size distribution (PNSD) has been provided.

CNRS-LISA/TNO/METNO: Modelled OP intercomparison

Multi-Model Comparison with measurements

- CHIMERE, LOTOS-EUROS, EMEP
- Observations provided by WP2 (IGE & PSI, CSIC, EMPA, and NABEL)

Comparison of source matching from three models with PMF data



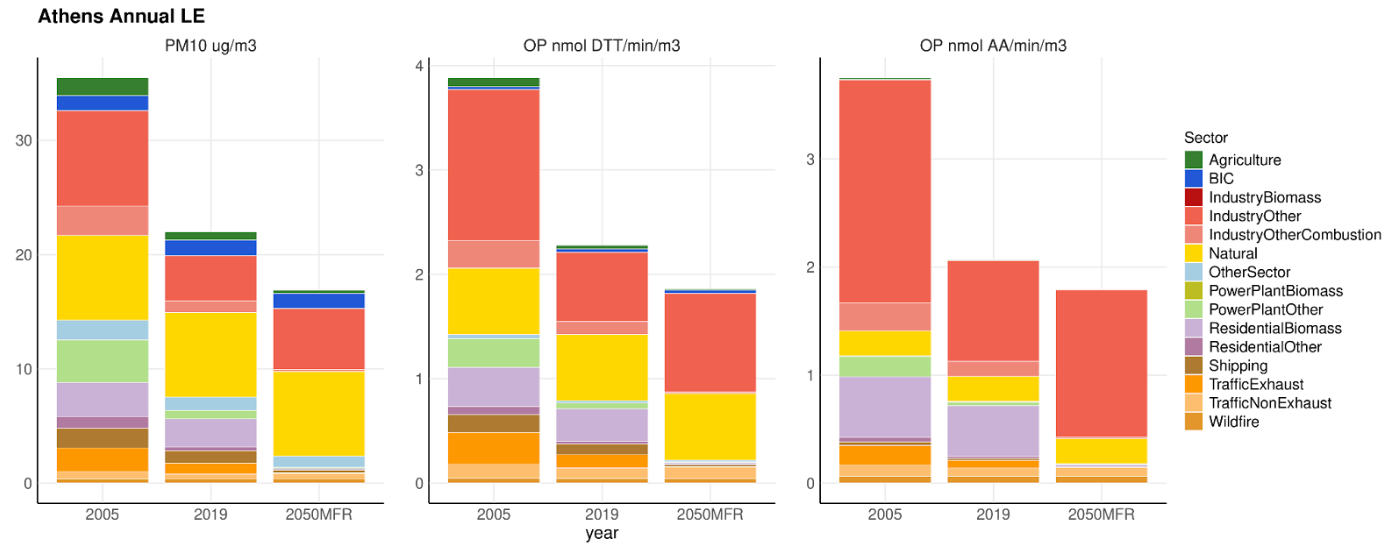
M20-M36

T3.4. Implement novel AQ indicators in tools supporting policy decision making to improve citizen health

T3.4. & Task 3.5 synergy to support SPs 2 and 3 for modelling novel health and policy relevant indicators and emission inventories

TNO/METNO/INERIS 2005-2050 Evolution of source attribution of PM and OP for policy purposes

- A multi-model exercise was set-up involving the EMEP, CHIMERE and LOTOS-EUROS chemistry transport models and their source attribution tools
  - Different SA methods were used (brute force, local fraction, surrogate modelling and tagging)
  - Source sector contributions to PM_{10} in 2005, 2019 and for future 2050 scenario
- **Illustrative** findings for Athens:
  - Continued downward trend of traffic exhaust.
  - The residential has not changed much between 2005 & 2019
  - The industrial sector will remain important in 2050, even more so in terms of OP

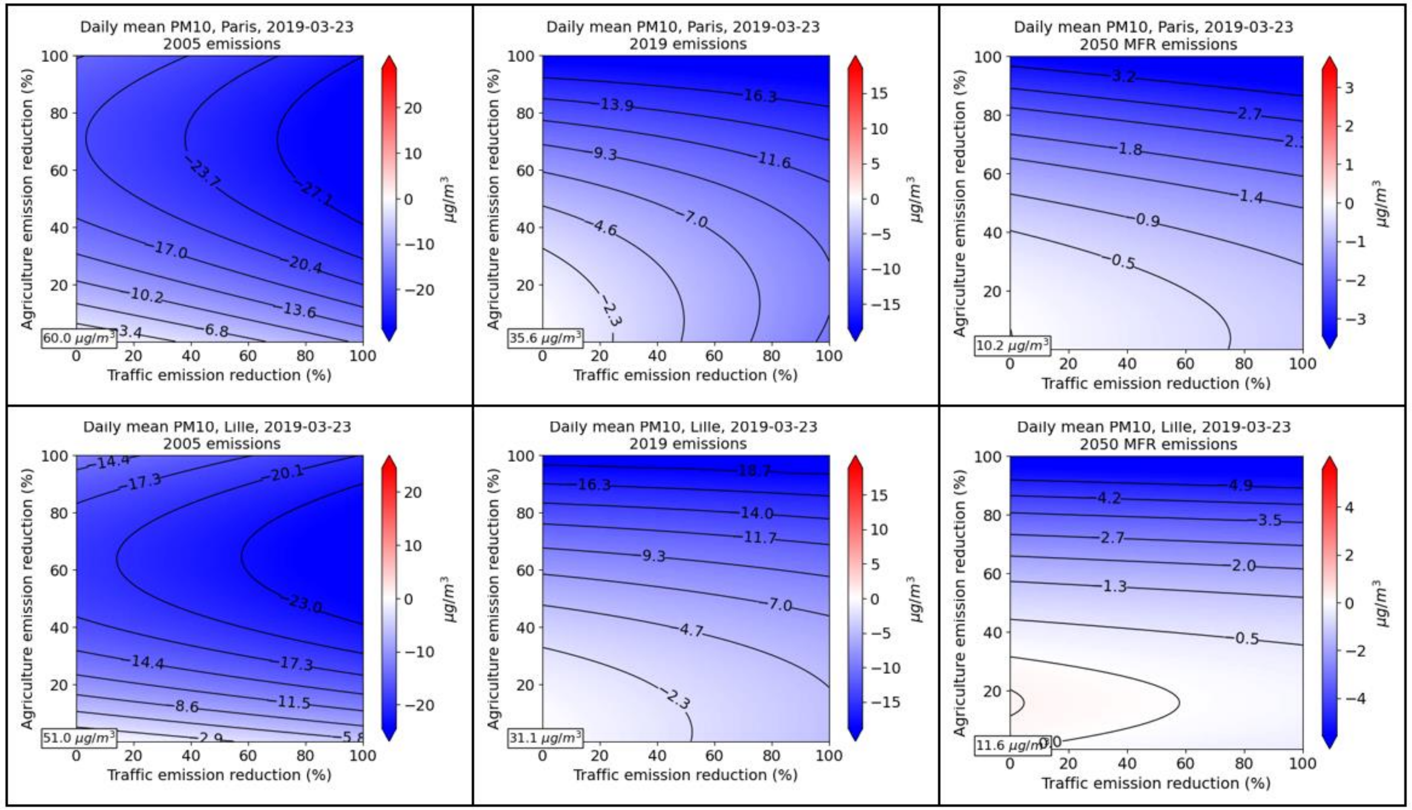


PM_{10} and OPDTT and OPAA source contributions for Athens for the years 2005, 2019 and 2050 CLE/MFR from LOTOS-EUROS model

INERIS: 2005-2050 Evolution of chemical regimes

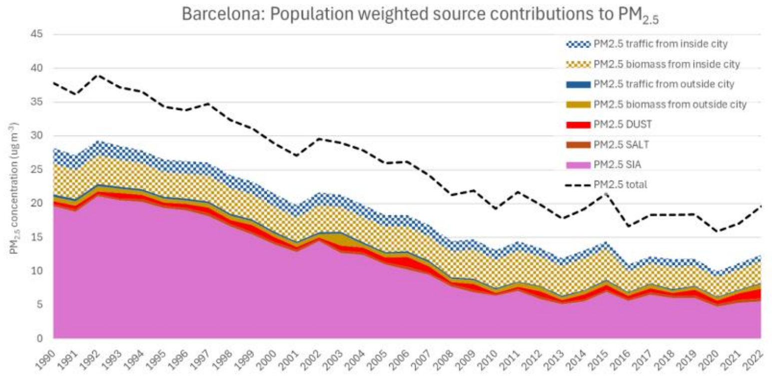
- Chemical Regimes Assessed with a machine learning surrogate emulator based on CHIMERE (CAMS Air Control Toolbox)

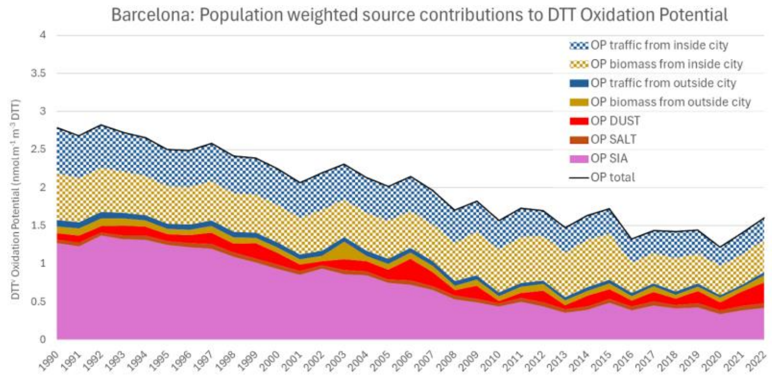
- Illustrative of the change in PM & ozone formation regime when using 2005/2019/2050 emission

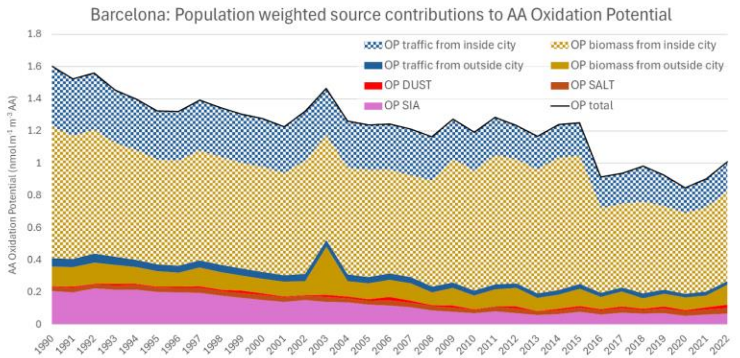


METNO: OP and $PM_{2.5}$: trends & city contribution

- The newly developed SA&OP metrics are tested at local (city) level since it is critical for decision making, as well as long term trends to assess policy effectiveness
- **The in-city source contribution for OP is considerably higher than for $PM_{2.5}$.**
- On average, over the 10 cities, we find city contributions to the $PM_{2.5}$ population weighted concentrations to be 16%.
- In contrast the population weighted city contributions to OP are found to be 42% and 60% for OP DTT^{v} and OP AA^{v} respectively.
- Thus, OP exposure can be significantly reduced via emission reduction measures inside the cities themselves

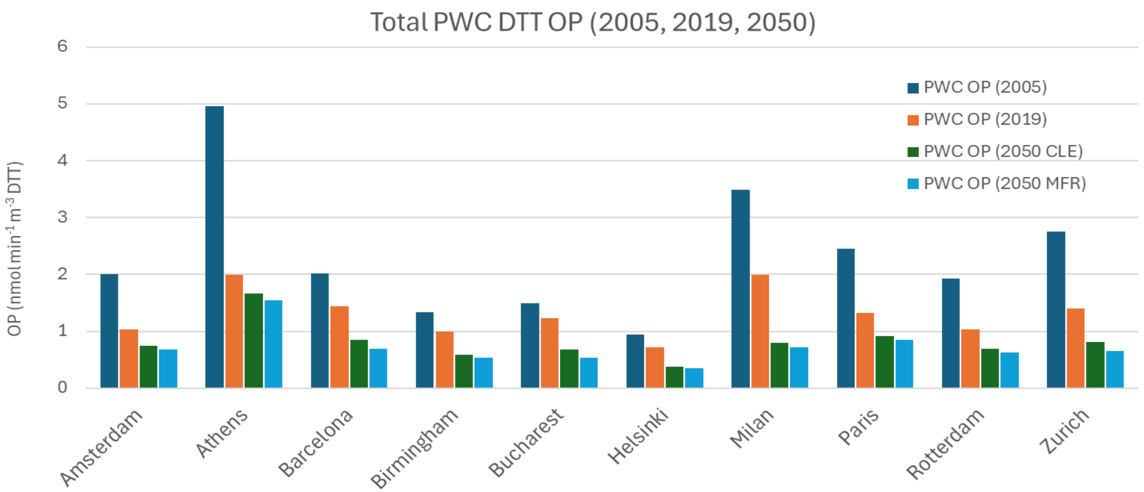




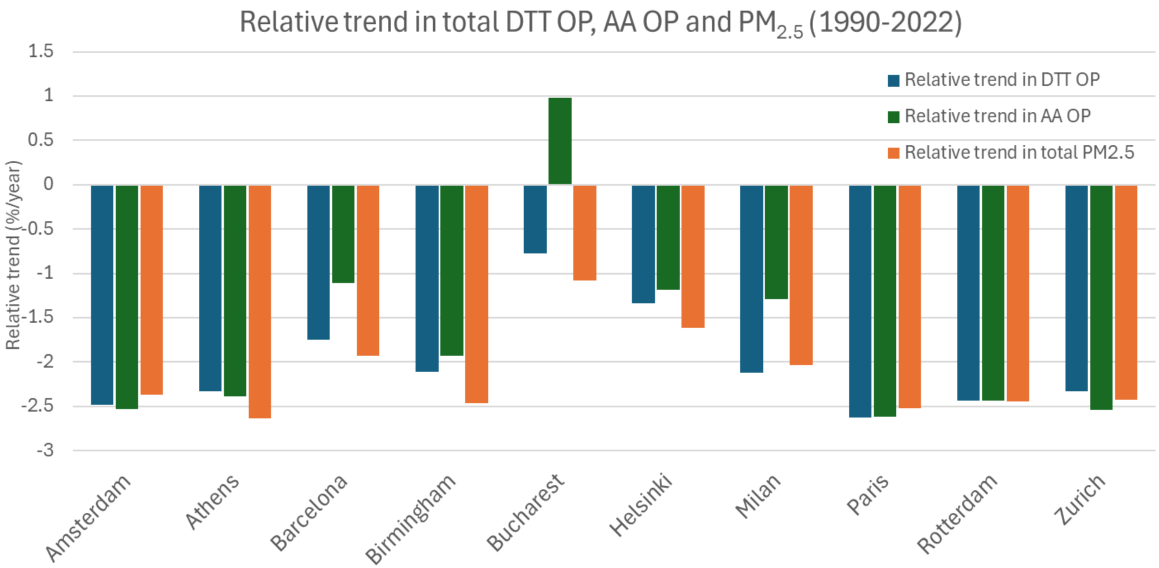


Health indicators - Intercity comparisons, trends and city contributions - uEMEP

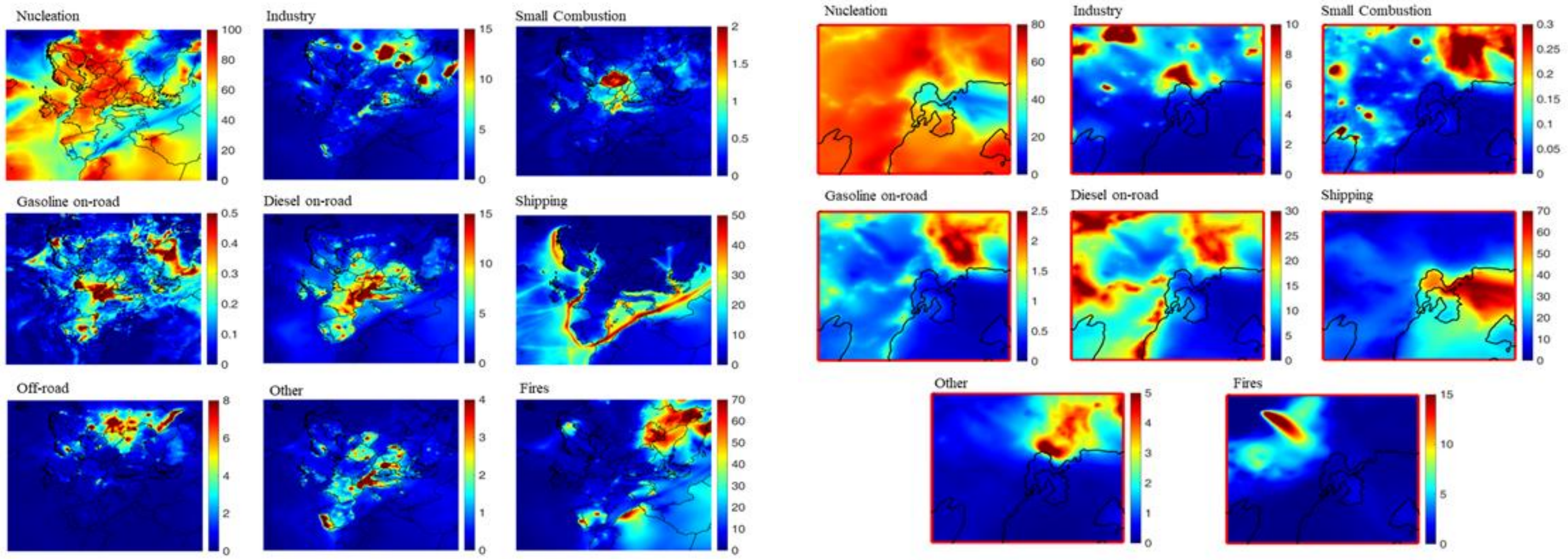
- Population weighted concentrations (PWC) of OP DTT$^{\nu}$ for the 10 target cities calculated with EMEP/uEMEP for the years 2005, 2019 and 2050



- Relative linear trend, relative to 1990, in total OP DTTν, OP AAν and PM2.5 for the period 1990-2022 for the ten target cities



FORTH: UFP source attribution



*Predicted source contributions as **percentage of the total N_{10}** over Europe (36 x 36 km^2) and over Athens (1x1 km^2) for the summer of 2019 using PMCAMx-UF with three nested domains.*

Service tools: Uptake of Regional Modelling Developments in SP3

- **ST12:** Deterministic multiscale urban modelling of UFP (WP3/WP4)
- **ST15:** Emission inventories for regional and urban scale modelling applications (WP3)
- **ST16:** UFP-PNSD multiscale modelling (WP3)
- **D5.4** STs for modelling novel urban air diagnostics and evaluation of regional AQ models over urban areas (WP3/WP5)

European Commission

Joint Research Centre

FAIRMODE

Brought forward to National Competent Authorities for Air Quality Modelling in support of the implementation of the Directives

- Presentation at FAIRMODE Plenary Meeting (March 2025)
- Cited in Technical Support Document on the use of Modelling in AAQD 2024/2881

WP3 : Deliverables

- **D3.1:** Framework to cross-check methodologies to assess urban emissions (UHEL, R/PU, M30)
- **D3.2**: Methodology to improve European urban emission inventories (NOA, R/PU, M09)
- **D3.3**: High resolution annual sectoral emissions for main pollutants, nanoparticles and non-exhaust contributors (TNO, OTHER/PU, M28)
- **D3.4**: High resolution mapping over European urban areas (INERIS, OTHER/PU, M30)
- **D3.5**: Assessment of the modelling system supporting policy implementation (METNO, R/PU, M39)
- **D3.6**: Pan-European report on modelling health indicators, variabilities, sources, uncertainties, and roadmap in support of the pilots (FORTH, R/PU, M41)

Milestones

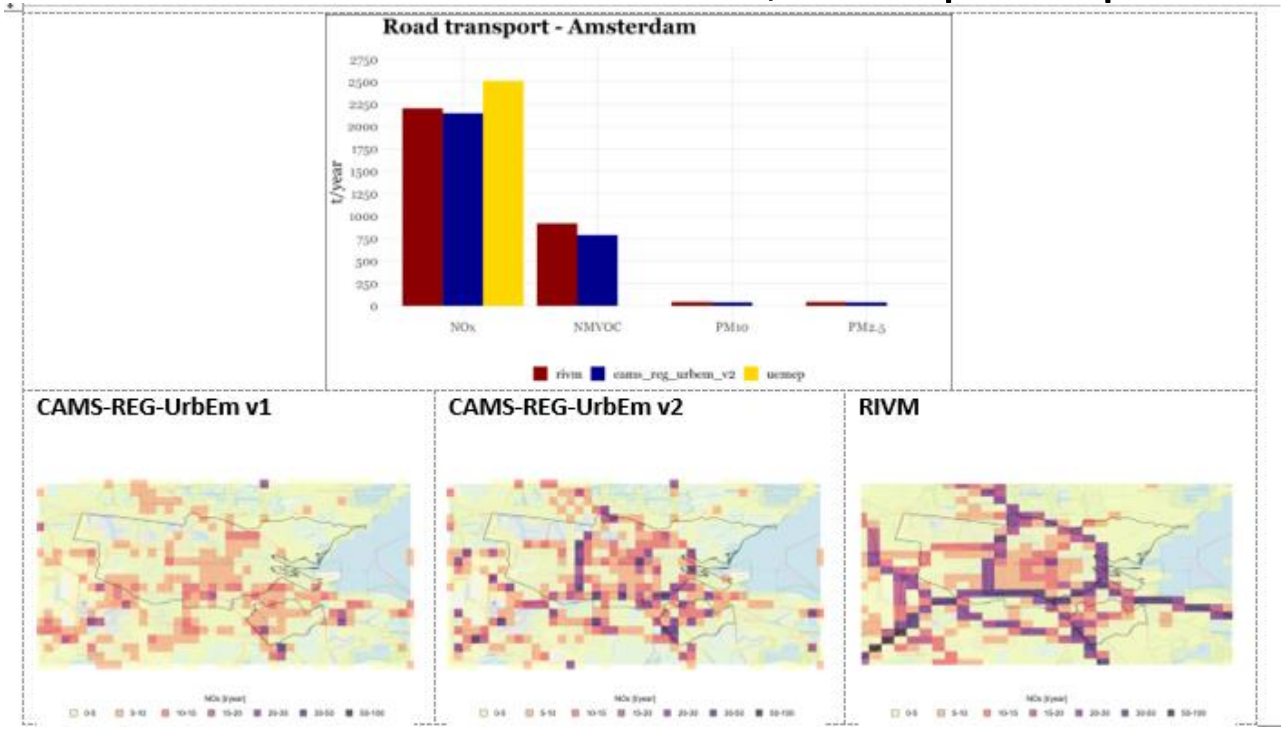
- MS12: Validation of regional models' vertical profiles including diagnostics relevant to urban air - **KNMI M36** - vertical profiles validated.
- MS13: Dataset on PM ultrafine and non-exhaust sectoral emissions distribution over Europe and pilot cities **TNO M12** *first dataset available for consortium use*
- MS14: Top-down and bottom-up estimation of city scale emission inventories **BSC M24** *emission inventories compared*
- MS15: Improved modelling tools integrating regional and urban scales **FORTH M18** *first design available*
- MS16: Definition of metrics for subgrid variability **CNRS M20** *sensitivity metrics defined*

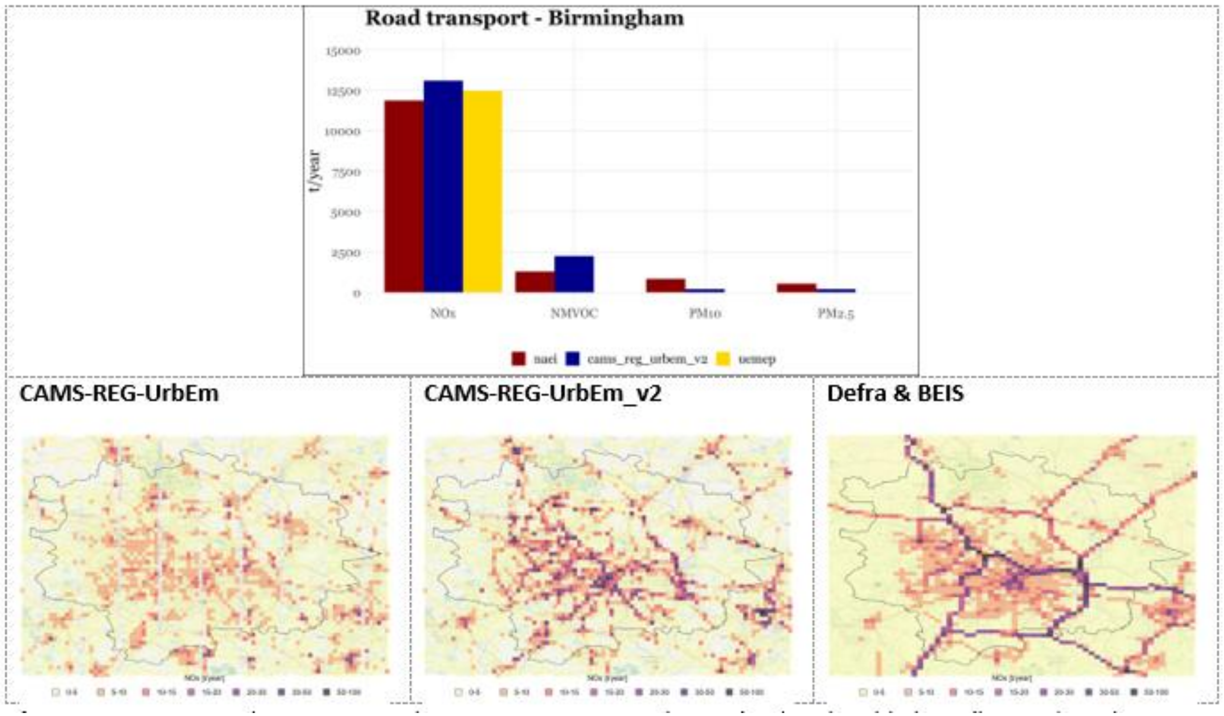
Publications

- P3.1. Strömberg, J. et al., 2023. Effect of radiation interaction and aerosol processes on ventilation and aerosol concentrations in a real urban neighbourhood in Helsinki, Atmos. Chem. Phys. 23, 9347-9364, https://doi.org/10.5194/acp-23-9347-2023
- P3.2. Siouti, E. et al., 2022. Development and Application of the SmartAQ High-Resolution Air Quality and Source Apportionment Forecasting System for European Urban Areas. Atmosphere, 13(10), 1693. https://doi.org/10.3390/atmos13101693
- P3.3. Aktypis, A., et al., 2023. Infrequent new particle formation in a coastal Mediterranean city during the summer. Atmos. Environ., 302, 119732. https://doi.org/10.1016/j.atmosenv.2023.119732
- In RP2
- P3.4. Navarro-Barboza, H., et al., 2024. Uncertainties in source allocation of carbonaceous aerosols in a Mediterranean region. Environment International, 183, 108252. https://doi.org/10.1016/j.envint.2023.108252
- P3.5 Fung P.L.,et al., 2023. Exploring the discrepancy between top-down and bottom-up approaches of fine spatio-temporal vehicular CO2 emission in an urban road network. Science of the Total Environment 901, 165827, https://doi.org/10.1016/j.scitotenv.2023.165827.
- P3.6. Vida et al, 2024. Modelling of atmospheric concentrations of fungal spores: a two-year simulation over France using CHIMERE. Atmos. Chem. Phys. 24, 18, 10601–10615, https://doi.org/10.5194/acp-24-10601-2024
- P3.7. Vida et al, 2025 Modelling oxidative potential of PM10: a 2-year study over France using CHIMERE, Science of The Total Environment, 967, 2025, 178813, https://doi.org/10.1016/j.scitotenv.2025.178813.
- P3.8. Siouti, E., et al., 2024. Simulation of the influence of residential biomass burning on air quality in an urban area., Atmospheric Environment, 309, 119897, 2023 https://doi.org/10.1016/j.atmosenv.2023.119897
- P3.9 Siouti, E., et al., 2024. Prediction of the Concentration and Source Contributions of PM2.5 and Gas-Phase Pollutants in an Urban Area with the SmartAQ Forecasting System. Atmosphere, 15, 1, 8. https://doi.org/10.3390/atmos15010008
- P3.10. Aktypis, A., et al., 2024. Significant spatial gradients in new particle formation frequency in Greece during summer, Atmos. Chem. Phys., 24, 65–84, https://doi.org/10.5194/acp-24-65-2024
- P3.11. Denby, B.R., et al., 2024. Sub-grid Variability and its Impact on Exposure in Regional Scale Air Quality and Integrated Assessment Models: Application of the uEMEP Downscaling Model. Atm. Env. 333. https://doi.org/10.1016/j.atmosenv.2024.120586
- P3.12. Savenets, M., et al., 2022. Enviro-HIRLAM model estimates of elevated black carbon pollution over Ukraine resulted from forest fires, Atmos. Chem. Phys., 22, 15777–15791, https://doi.org/10.5194/acp-22-15777-2022
- P3.13. Savenets, M., et al., 2024. Seamless Modeling of Direct and Indirect Aerosol Effects during April 2020 Wildfire Episode in Ukraine. Atmosphere, 15, 5, 550; https://doi.org/10.3390/atmos15050550
- P3.14. Myriokefalitakis S., et al., 2024. Analysis of secondary inorganic aerosols over the greater Athens area using the EPISODE–CityChem source dispersion and photochemistry model. Atmos. Chem. Phys., 24(13), 7815–7835. https://doi.org/10.5194/acp-24-7815-2024
- P3.15. Siouti, E. et al., 2025 High resolution source-resolved PM2.5 spatial distribution and human exposure in a large urban area, Atmos. Environ., 355 (2025) 121277, https://doi.org/10.1016/j.atmosenv.2025.121277
- P3.16. Patoulias, D., et al. 2025. Sensitivity of predicted ultrafine particle size distributions in Europe to different nucleation rate parameterizations using PMCAMx-UF v2.2, Geosci. Model Dev., 18, 1103–1118, https://doi.org/10.5194/gmd-18-1103-2025.
- P3.17. Kouznetsov, R., et al, 2025. Deposition velocity concept does not apply to fluxes of ambient aerosols, EGUsphere [preprint], https://doi.org/10.5194/egusphere-2025-2364, 2025.
- P3.18 Lugon L., et al. (2025) To what extent can we improve urban air quality and population exposure by changing mobility? A study case in Paris, Science of the Total Environment, in press.
- P3.19 Sartelet, K., Kerckhoffs, J., Athanasopoulou, E., Lugon, L., Vasilescu, J., Zhong, J., Hoek, G., Joly, C., Park, S.-J., Talianu, C., van den Elshout, S., Dugay, F., Gerasopoulos, E., Ilie, A., Kim, Y., Nicolae, D., Harrison, R. M., Petaja, (2025) Air pollution mapping and variability over five European cities. Environment International, 199, 109474. https://doi.org/10.1016/j.envint.2025.109474
- P3.20 Park, S.-J., Lugon, L., Jacquot, O., Kim, Y., Baudic, A., D'Anna, B., Di Antonio, L., Di Biagio, C., Dugay, F., Favez, O., Ghersi, V., Gratien, A., Kammer, J., Petit, J.-E., Sanchez, O., Valari, M., Vigneron, J., and Sartelet, K. (2025) Population exposure to outdoor NO2, black carbon, and ultrafine and fine particles over Paris with multi-scale modelling down to the street scale. Atmos. Chem. Phys., 25 (6), 3363-3387, https://doi.org/10.5194/acp-25-3363-2025.
- P3.21 Sartelet, K., Kim, Y., Couvidat, F., Merkel, M., Petäjä T., Sciare J. and Wiedensohler, A. (2022), Influence of emission size distribution and nucleation on number concentrations over Greater Paris. Atmos. Chem. Phys., 22, 8579-8596, doi:10.5194/acp-22-8579-2022.
- P3.22 Pekel, F., Uzu, G., Weber, S., Kranenburg, R., Tokaya, J., Schaap, M., ... & Timmermans, R. (2025). Comparison of modelled and experimental PM10 source contributions of mapping source-specific oxidative potential. Atmospheric Environment: X, 100339. https://doi.org/10.1016/j.aeaoa.2025.100339

TNO/BSC/NOA: Comparisons with new EU emissions

Examples Amsterdam & Birmingham show totals agree much better, also spatial patterns improved significantly





Modeling Health-Relevant Indicators

- Regional models were improved and downscaled to simulate health-relevant indicators over European cities, such as BC, OA, OP, $PM_{2.5}$, and UFPs.
- Challenges included aligning modelled and observed BC and OA components.
- Source apportionment modeling tools have been improved and intercompared to link pollutant sources to their concentrations in order to be used to evaluate potential health impacts and support clean area strategy (details in D3.4).

Model development in Task 3.3

WP3 tasks accomplished during RP3 (since the 3rd science conference in Helsinki, Sept 2024)

- **Deliverable D20 (D3.5)** Assessment of the modeling system supporting policy implementation (**M39**)

- **Deliverable D21 (D3.6)** Pan-European report on modeling health indicators, variabilities, sources, uncertainties, and roadmap in support of the pilots (**M40**)

- Liaising with WP5 to take stock of WP3 developments achieved M0 to M36 to design a Service Tool and prepare its upscaling in WP5 **(D5.4: STs for modelling novel urban air diagnostics and evaluation of regional AQ models over urban areas**, INERIS, R/PU, M48)

CNRS-LISA: OP Modeling Methodology

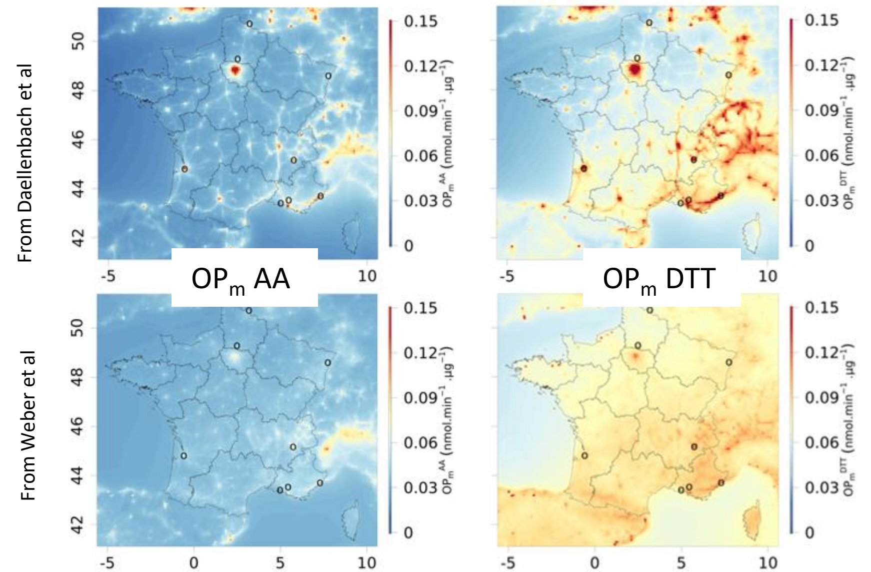
Implementation of a OP modeling module within the CHIMERE model

(Vida et al, subm. ACP)

- Based on PSAT tagging methods
- Modelling of PMF sources from Weber et al (2021) & Daellenbach et al (2020)

➡ OP modeling using OP attribution/sources by Weber & Daellenbach

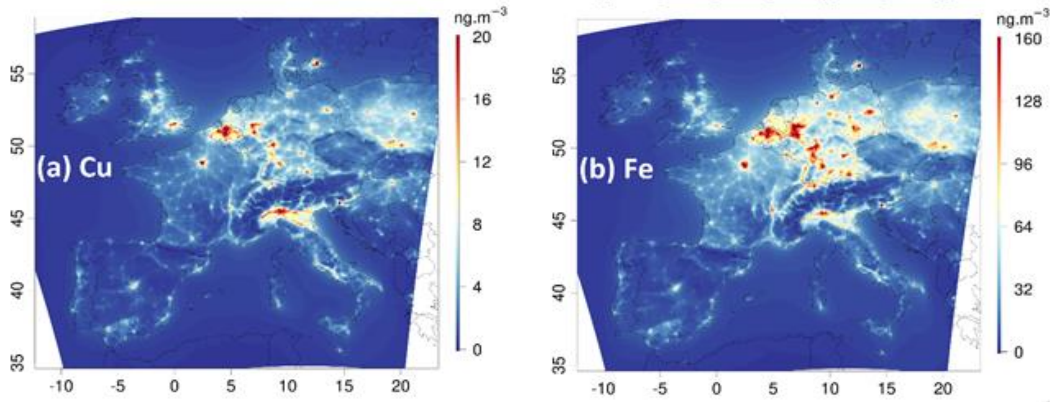
Vida et al, subm. ACP



Modeling of additional species contributing to OP

- Fungal spore modeling within CHIMERE (Vida et al, ACP, 2024)
- Development of Cu, Fe and Mn emission inventory for Europe (Dubois et al, in prep)

➡ Simulation of European atmospheric Cu, Fe & Mn concentrations



Dubois et al, in prep

Policy Support Applications

- Modeling tools were applied to assess sectoral contributions to pollutants like, PM_{10} and OP for past, present, and future scenarios (2005–2050).
- Residential heating and traffic emissions were found to be key contributors to OP.
- The in-city population weighted source contribution for OP (42% for OP DTTν and 60% for OP AAν) is found to be considerably higher than for $PM_{2.5}$ (16%), on average over the 10 studied cities, indicating that **OP exposure can be significantly reduced via emission reduction measures inside the cities themselves.**
- Surrogate models like ACT captured non-linear chemical regime changes in ozone concentrations, supporting mitigation strategy evaluations (details in D3.5).

Done in Task 3.4