

Modeling ultrafine particles and associated health metrics

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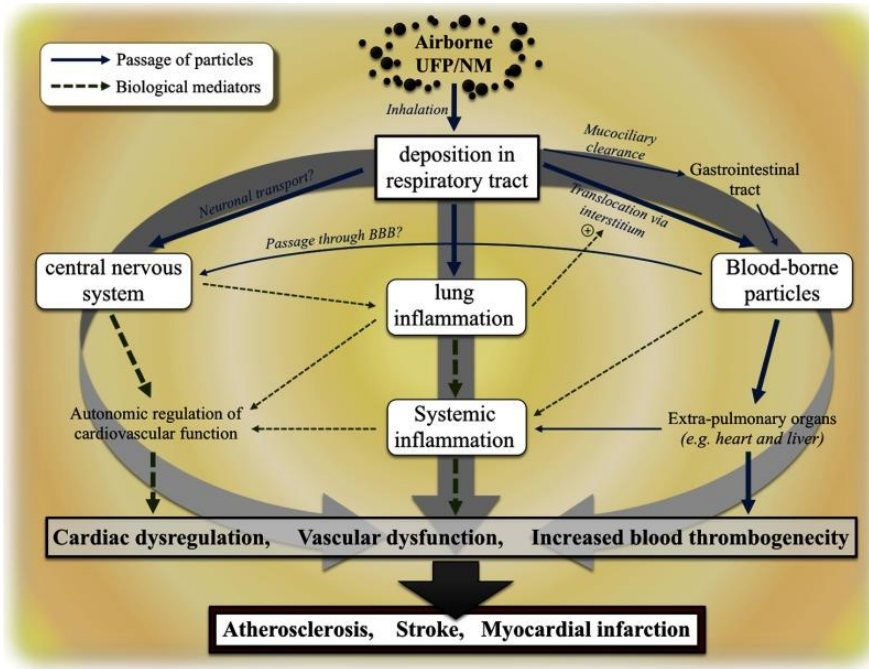
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Introduction



Schematic illustrating some of the key mechanisms through which inhaled ultrafine particles (UFPs) may influence secondary organs and systemic tissues (Stone et al. *Environ. Health Perspect.* 2017)

- **Air pollution and public health**

Major effects : respiratory, cardiovascular, neurological

- **Health effects** are dominated by fine particles ($PM_{2.5}$) whose mass is regulated
- **Ultrafine particles (UFP < 100 nm)** have a low mass but they can cross biological barriers, reach the bloodstream and the brain

⇒ **How to quantify exposure to particles and to UFP ?**

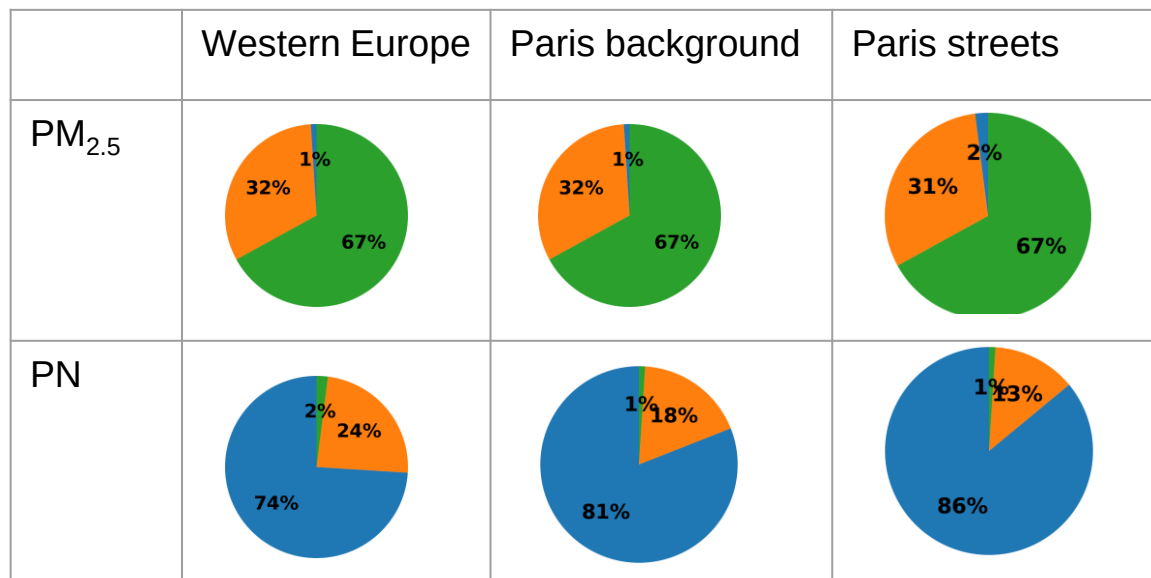
⇒ **What are the main sources?**

UFP characteristics

	10 μm (Coarse)	2.5 μm (Fine)	0.1 μm (Ultrafine)
			
Total mass	1	1	1
Particle number	1	64	1,000,000
Surface area per particle	1	0.0625	0.0001
Total surface area per mass	1	4	100
	- Filtered in proximal airway - May irritate skin, mucosa	- Reaches peripheral airway - Cannot enter systemic circulation	- Higher adsorbed toxic material on surface - May enter systemic circulation

Comparisons of number and surface of particles (Kwon et al. 2020)

➤ Low mass, high number concentrations



■ UFP (<100 nm)
 ■ 100-385 nm
 ■ >385 nm

Contribution to concentrations during winter 2020/2021
(Sartelet et al. Environ. Sci. Tech. 2026)

Estimation of UFP emissions using desagregation matrices

Table A1. Estimation of the size-distribution of emissions by estimating the ratio $PM_1/PM_{2.5}$ and $PM_{0.1}/PM_1$ for each activity sector.

	SNAP	$PM_1/PM_{2.5}$	$PM_{0.1}/PM_1$
Combustion in energy and transformation industries	01		
Public power and District heating plants	0101/0102	0.7945	0.4806
Petroleum refining plants	0103	0.8058	0.5428
Stationary engines	0105	1	0.5
Non-industrial combustion plants	02		
Commercial and institutional plants	0201	0.8577	0.4155
Residential plants	0202	0.6761	0.2006
Plants in agriculture, forestry and aquaculture	0203	0.7101	0.5565
Combustion in manufacturing industry	03	0.8072	0.5265
Production processes	04		
Processes in petroleum industries	0401	0.8072	0.5265
Processes in iron and steel industries and collieries	0402	0.5117	0.3684
Processes in inorganic and organic chemical industries, wood, food and other	0404/0405/0406	0.7711	0.5
Extraction and distribution of fossil fuels and geothermal energy	05	0.8072	0.5265
Solvent and other product use	06	0.7711	0.5
Road transport	07		
Passenger cars, light, heavy duty vehicles and buses	0701/0702/0703	0.8947	0.5882
Mopeds and Motorcycles < 50 cm ³ and > 50 cm ³	0704/0705	0.6842	0.3846
Gasoline evaporation from vehicles	0706	0.8947	0.5882
Other mobile sources and machinery	08		
Railways	0802	0.8947	0.1765
Inland waterways	0803	0.8975	0.3032
Air traffic	0805	0.67	0.2239
Agriculture and Forestry	0806/0807	0.8148	0.2575
Industry	0808	1	0.5
Household and gardening	0809	0.9043	0.5882
Waste treatment and disposal	09	1	0.15
Agriculture	10	1	0.5

- Emission inventory => Emissions of PM_{10} and $PM_{2.5}$ per activity sector
- Use $PM_1/PM_{2.5}$ and $PM_{0.1}/PM_1$ ratio to determine masses of $PM_{0.1}$ and PM_1 (<https://naei.beis.gov.uk>)
- Each size range is associated to a mean diameter => Estimation of the emission of the particle number
- Algorithm to discretize into sectional sections, while conserving mass and number

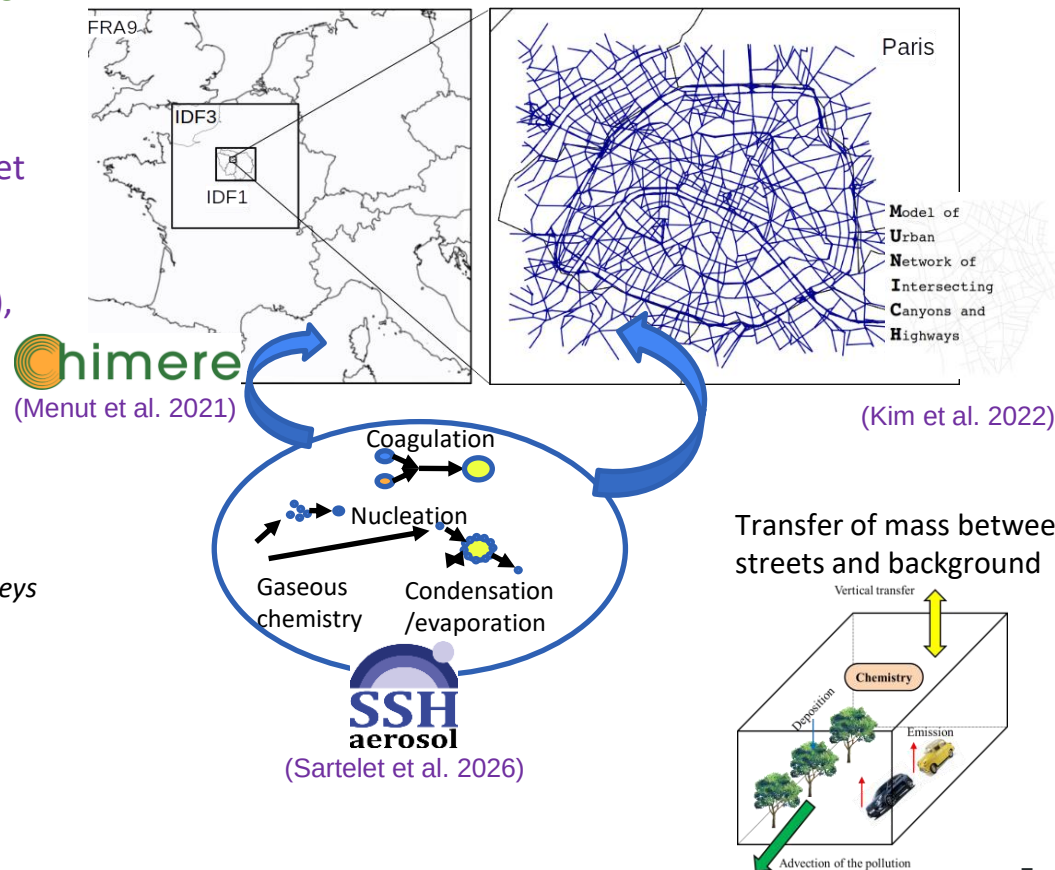
Multi-scale mapping of concentrations

- Use the modelling chain WRF-CHIMERE/MUNICH over Greater Paris
- Simulations performed over France/Greater Paris/ Paris streets during summer 2022 (Park et al. Atmos. Chem. Phys. 2025, Sartelet et al. Environ. Int. 2025, Lugon et al. 2025), , winter 2020/2021 (Lugon et al. J. Hazard. Mater. 2026), summer 2021 (Park et al. In preparation)

- **Anthropogenic emissions:** EMEP in France and Airparif in Greater Paris.

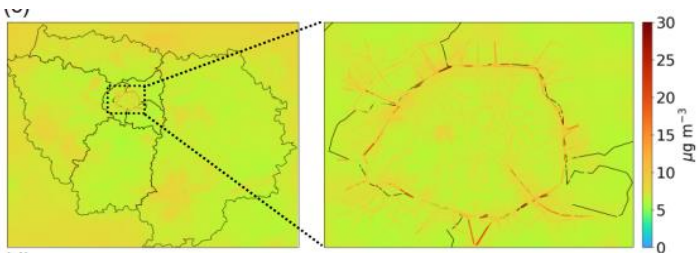
Observed traffic loop counts are used to correct modelled traffic emissions in Greater Paris.

Wood burning emissions improved using recent surveys and inclusion of condensables



Multi-scale mapping of concentrations

- Use the modelling chain WRF-CHIMERE/MUNICH over Greater Paris



PM_{2.5} concentrations in June/July 2022

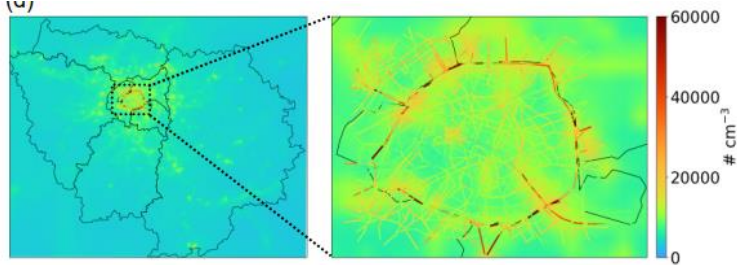
NO ₂	Station type	Nb of Stat.	Obs. (µg m ⁻³)	Sim. (µg m ⁻³)	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	21	15.0	14.7	33	0	90
	Traffic	10	40.0	38.3	31	0	92
Winter	Background	23	24.7	25.0	30	0	93
	Traffic	9	43.4	52.2	28	19	96

PM _{2.5}	Station type	Nb of Stat.	Obs. (µg m ⁻³)	Sim. (µg m ⁻³)	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	8	7.2	6.8	30	0	92
	Traffic	3	11.2	9.9	27	-10	95
Winter	Background	8	12.2	13.2	39	17	84
	Traffic	2	16.9	23.1	38	34	87

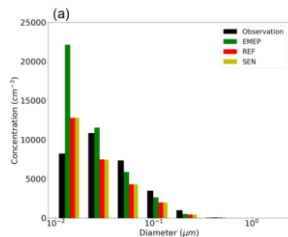
Strict criteria: MFE < 50%, MFB < 30%, FAC2 > 30%
Less strict criteria: MFE < 75%, MFB < 50%, FAC2 > 50%

Multi-scale mapping of concentrations

- Use the modelling chain **WRF-CHIMERE/MUNICH** over Greater Paris



PN concentrations in June/July 2022



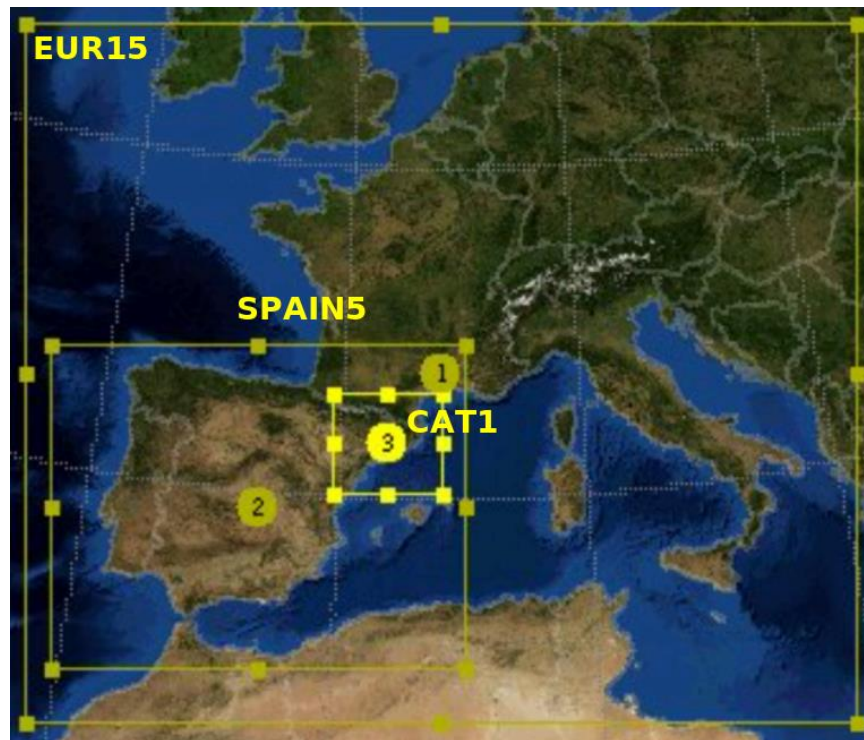
eBC	Station type	Nb of Stat.	Obs. ($\mu\text{g m}^{-3}$)	Sim. ($\mu\text{g m}^{-3}$)	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	4	0.78	0.64	39	-8	80
	Traffic	3	2.2	2.2	38	15	89
Winter	Background	5	1.2	1.3	43	22	79
	Traffic	2	3.2	3.7	46	28	79

PN	Station type	Nb of Stat.	Obs. ($\mu\text{g m}^{-3}$)	Sim. ($\mu\text{g m}^{-3}$)	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	4	8176	8173	25	4	98
Winter	Background	5	7091	8025	43	22	79

Strict criteria: MFE < 50%, MFB < 30%, FAC2 > 30%
 Less strict criteria: MFE < 75%, MFB < 50%, FAC2 > 50%

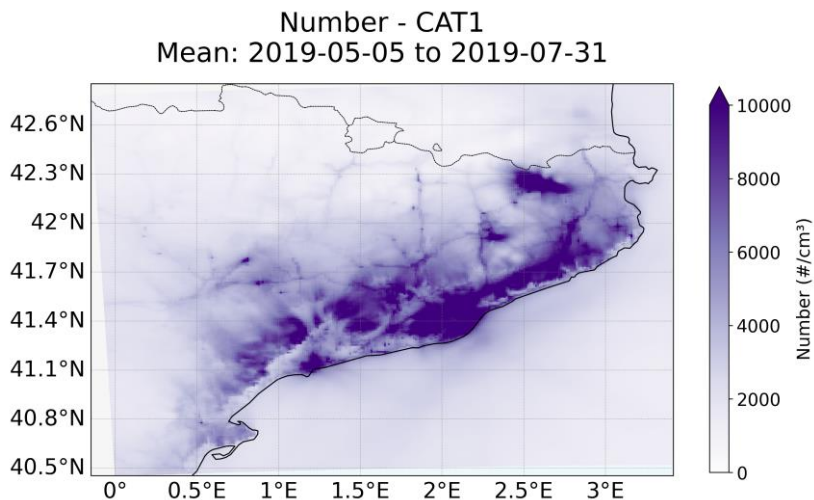
Multi-scale mapping of concentrations

- Use the modelling chain WRF-CHIMERE/MUNICH
- Simulations performed Europe and Barcelona (Olivares Lopez et al. Environ. Poll. 2026)
- Anthropogenic emissions: Top down EMEP ($0.1^\circ \times 0.1^\circ$) or bottom up HERMESv3 (1 km x 1 km)



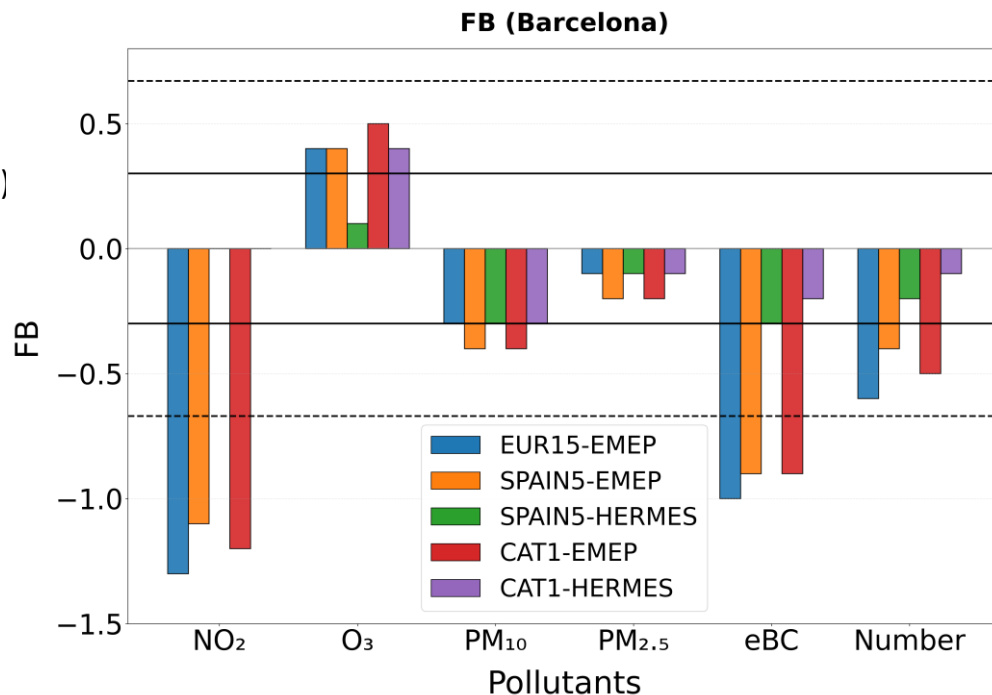
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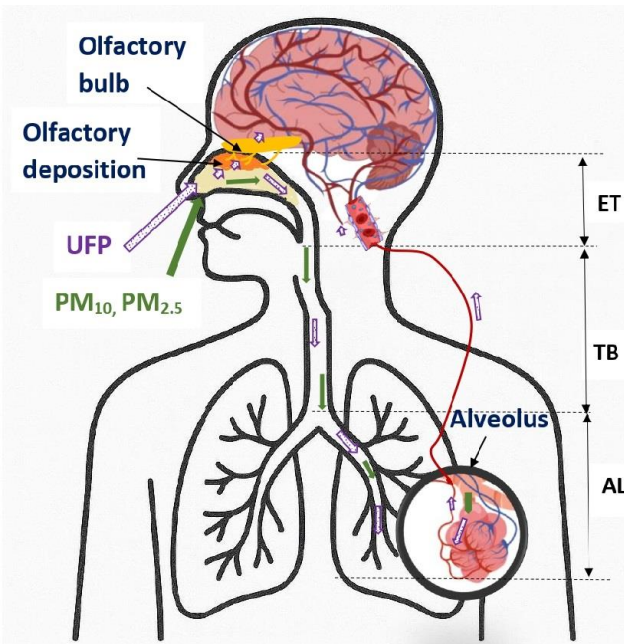
Multi-scale mapping of concentrations

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- **Anthropogenic emissions:** Top down EMEP ($0.1^\circ \times 0.1^\circ$) or bottom up HERMESv3 (1 km x 1 km)
- PN and BC simulations reach statistical skill comparable to regulated pollutants.
- Inventory choice dominates PN/BC/ NO_2 concentrations, outweighing grid refinement



Strict performance criterion: $-0.3 < \text{Fractional Bias} < 0.3$

Associated health metrics



- **Health-relevant exposure depends on**

- **where particles deposit** within the respiratory tract

- **Alveolar deposition:** potential translocation of UFP across the epithelial barrier → systemic circulation → secondary organs
- **Olfactory deposition:** neuronal transport of UFP along olfactory nerves → direct brain exposure

- **deposited particle surface area**, which controls interfacial reactivity and biological interaction

- **Lung Deposition Surface Area LDSA_r in region r**

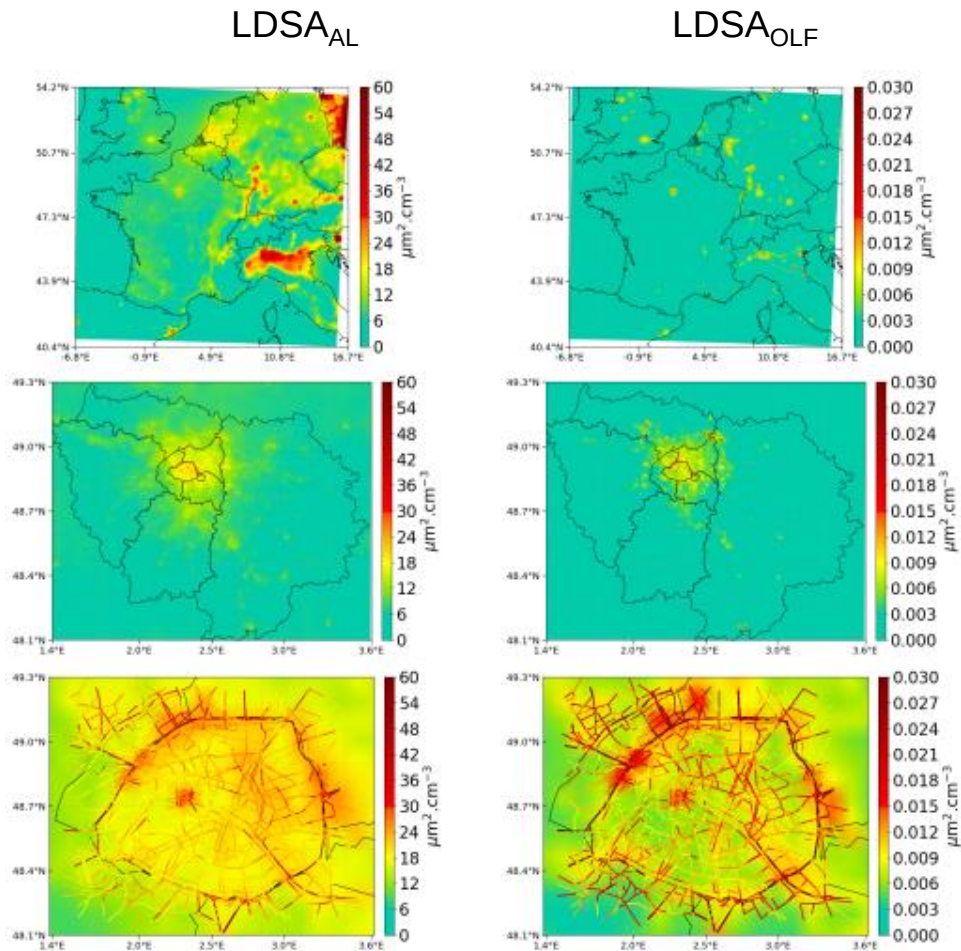
$$LDSA_r = \int N(d)S(d)F_r(d) dd$$

With $N(d)$ the number distribution, $S(d)$ the surface and F_r the deposition fraction

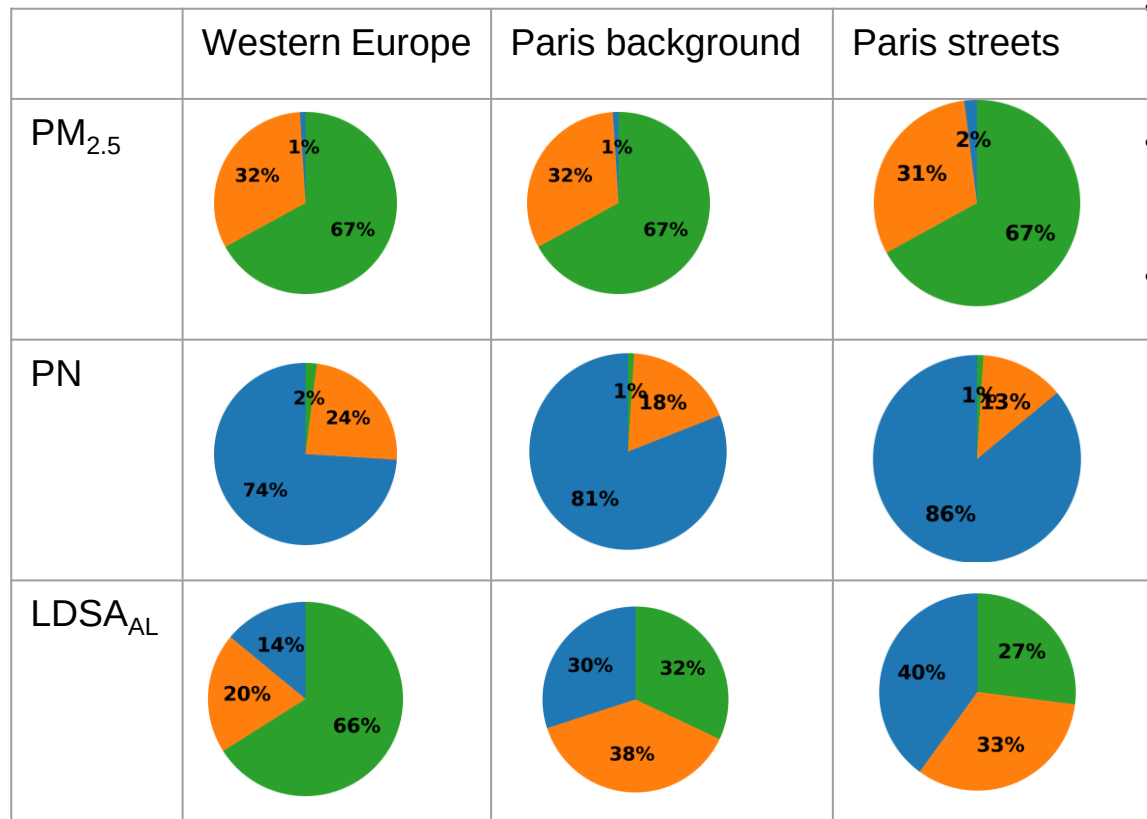
LDSA maps

- Account for the hygroscopic growth of particles in the respiratory tract
- At regional scale, LDSA_{AL} broadly follows $\text{PM}_{2.5}$ patterns → smooth gradients and clear urban/rural contrasts (e.g., Po Valley, Paris region)
- LDSA_{OLF} exhibits much stronger spatial heterogeneity → elevated concentrations confined to urban environments
- At city scale, LDSA_{OLF} closely follows the road network

(Sartelet et al. Environ. Sci. Tech. 2026)



Size contribution to alveolar deposition



■ UFP (<100 nm) ■ 100-385 nm ■ >385 nm

- **UFPs contribute little to PM_{2.5} mass**

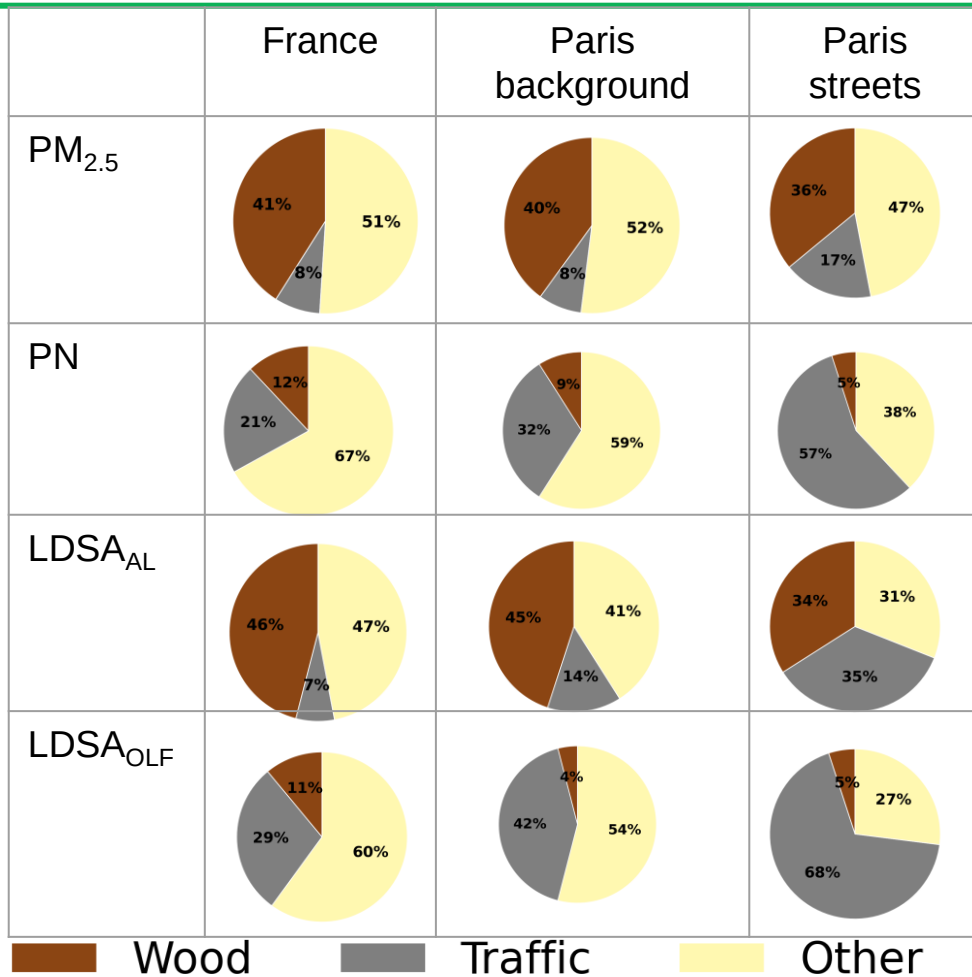
- **UFPs dominate particle number**

- **Substantial contribution to LDSA_{AL}**

- 13-14% at regional scale

- 30-40% in urban / street environments

Source contribution to alveolar and olfactory deposition



- Source contribution determined using **brut-force method**
- Wood heating** makes a very large contribution to **PM_{2.5}** and **LDSA_{AL}** over France and in cities
- Traffic** becomes an equally important contributor to **LDSA_{AL}** in **urban streets**.
- LDSA_{OLF}** and **PN** both exhibit a stronger **traffic influence**.

Conclusion

- **Simulations of UFP and BC concentrations with comparable scores as regulated pollutants**
- **Bottom-up detailed emission inventory better for accurate simulation of urban concentrations of UFP**
- **Ultrafine particles** contribute little to $PM_{2.5}$ mass but make **30-40% of alveolar-deposited surface area ($LDSA_{AL}$) in urban environments**
- **$LDSA_{OLF}$ exhibits stronger spatial heterogeneity** than $LDSA_{AL}$ with elevated concentrations confined to urban environments in winter
- **$PM_{2.5}$ concentrations** are strongly impacted by **wood heating in winter**, and little by traffic
- **Traffic** largely impacts number and hence **$LDSA_{OLF}$ and $LDSA_{AL}$ in urban environments**
- Preliminary calculations suggest that **UFP translocation to the brain via the olfactory route** may exceed alveolar translocation by a factor of several hundreds

Thank you for your attention

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Model validation for LDSA

- Size distribution measured using mobility particle size spectrometers
- LDSA is deduced from measurements and modelled concentrations
- Good model/measurement comparison in the different regions of the respiratory tract

