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New tools for assessing personal exposure near urban air pollution hotspots

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Exposure Modelling: the basics

Emissions

COPERT
SYBIL
COPERT street level

**Dispersion
Modelling**

Exposure (“external”)

Concentrations (PN)
Sensitive receptors
Statistics/Indicators



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Exposure Modelling: the basics

Emissions

COPERT
SYBIL
COPERT street level

EZM Tools

Exposure (“external”)

Concentrations (PN)
Sensitive receptors
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Regional scale
Country scale
City scale
Block scale



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Exposure Modelling: the basics

Emissions

COPERT
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Regional scale
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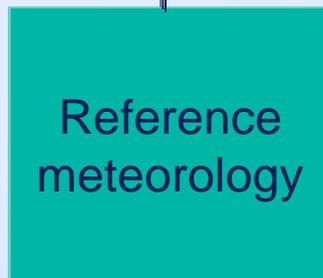
Reference
meteorology



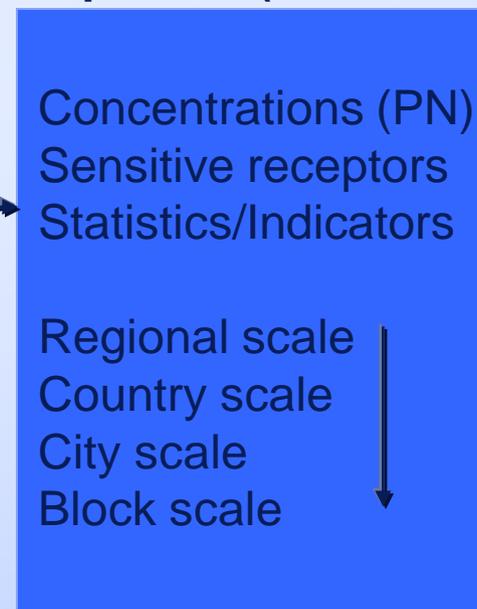
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Exposure Modelling: the basics

Emissions



Exposure (“external”)





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EZM: main modelling components

MEMO, v. 7.0

- Non-hydrostatic prognostic mesoscale meteorological model
- Flexible nesting configuration
- Code is ported to a variety of HPC platforms

MIMO, v. 91

- RANS CFD model
- Fully configurable nonequidistant meshsize in all three dimensions and near obstacles

MARS-aero, v. 6.0

- Multi-layer chemical transformation and dispersion model
- Modular support for multiple chemical mechanisms
- Secondary Organics Aerosol module



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MARS-aero: chemistry and PM physics

➤ Gas chemistry

- RACM (72 species, 234 reactions)
- EMEP (66 species, 136 reactions)
- KOREM (20 species, 39 reactions)
- CBM-IV (47 species, 92 reactions)

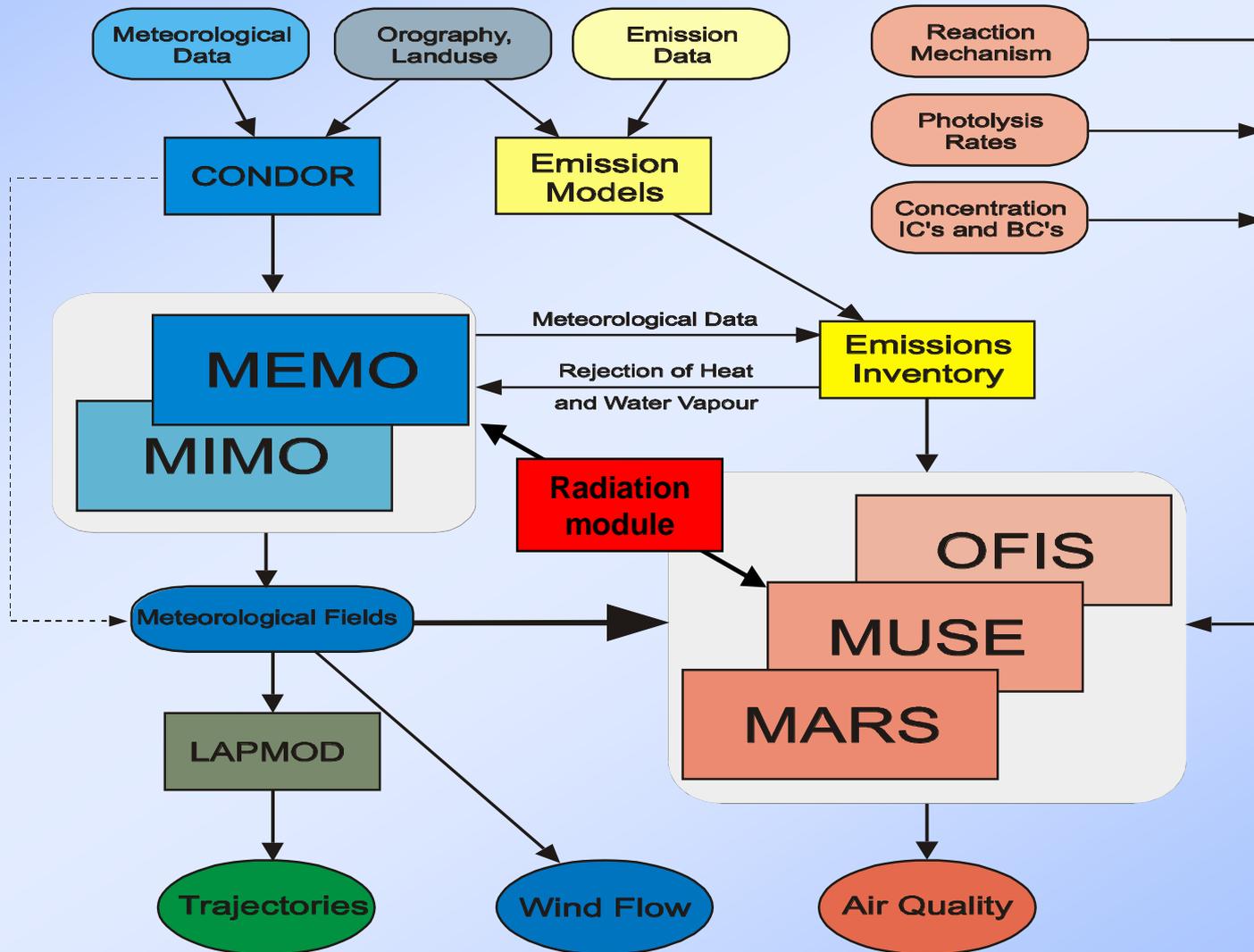
➤ Secondary PM

- Three-mode model
- Internally mixed assumption
- Na, H₂SO₄, NH₄, HNO₃, HCl, EC, OC, OTH (mainly mineral dust)
- Aerosol number concentrations
- Inorganics → ISOROPIA (sodium, sulfate, nitrate, ammonia, chloride, water)
- Organics → SORGAM (with improvements)
 - ARO1,2 (aromatic), ALK1 (oxidization), OLE1 (oleine), ALPI1,2 (α -pinene), LIM1,2 (limonene)



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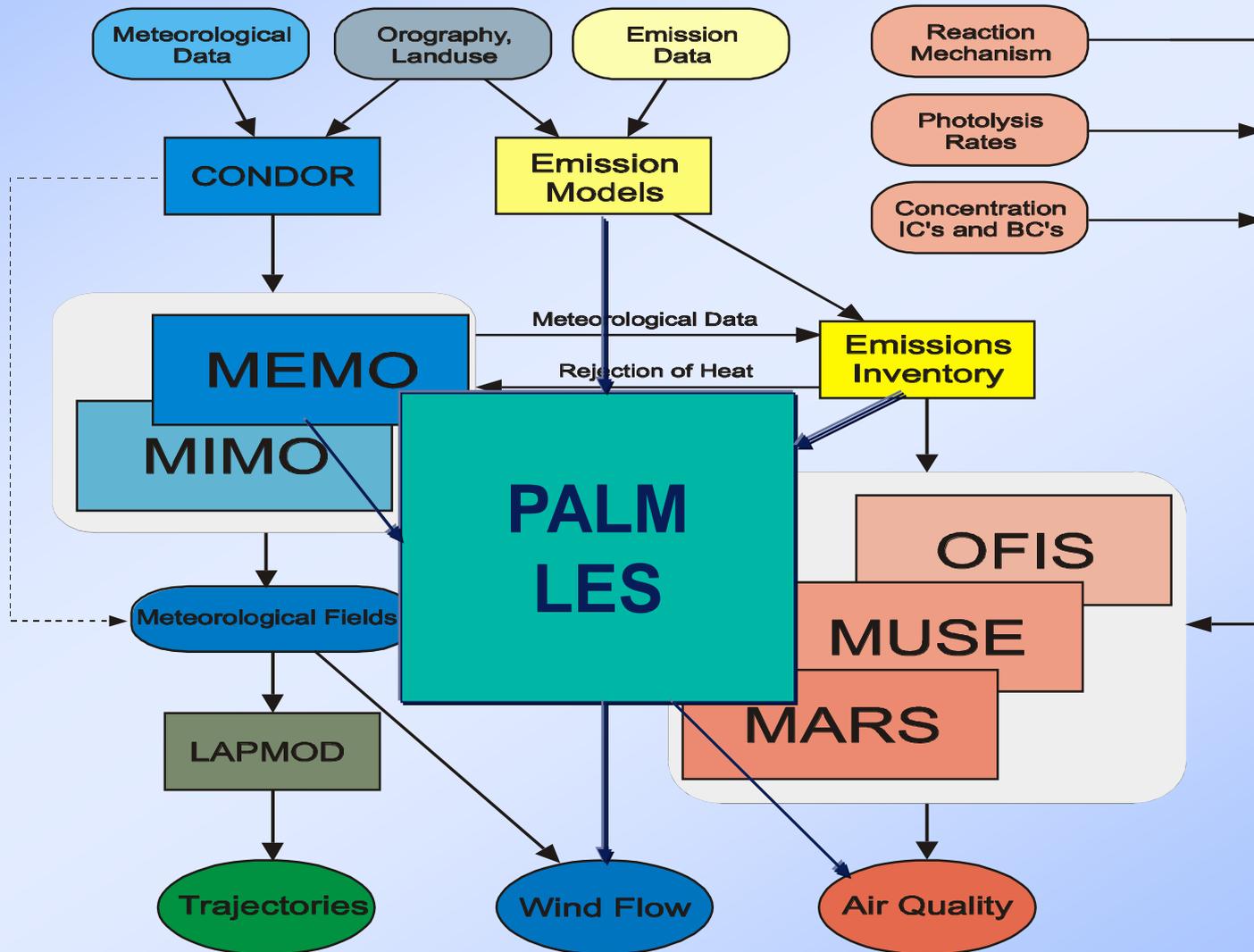
EZM: an arsenal of Modelling Tools





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EZM+PALM LES

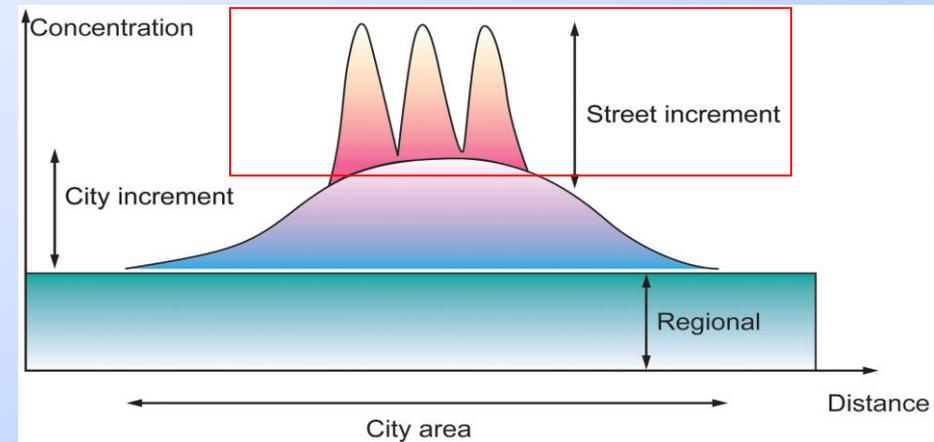
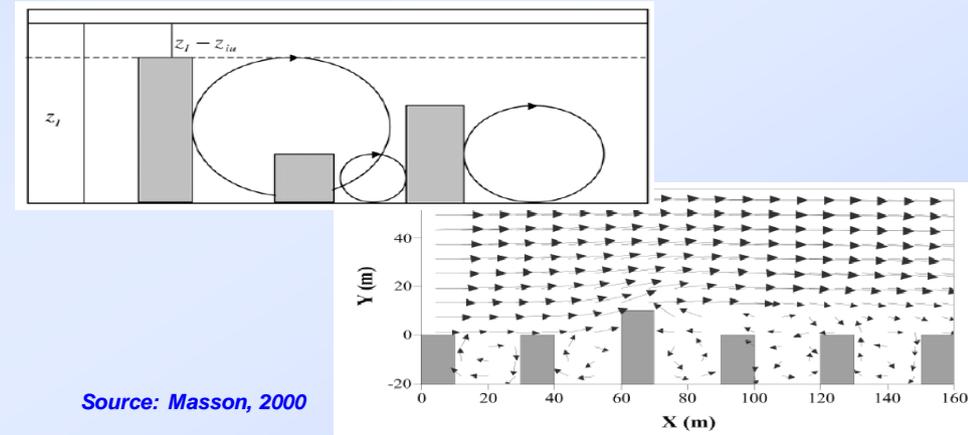




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Hotspot assessment : a multiscale problem

- Mesoscale models can typically simulate atmospheric flows in the 20 – 500 km scale, providing reliable 3D meteorological fields for simulating pollutant transport, diffusion and chemical transformation in and around urban areas.
- These models cannot resolve urban canopy effects or explicitly take into account obstacle geometries.
- Hotspot exposure encompasses contribution from at least three spatial scales: a regional, a higher city-scale background, and local-scale increments.

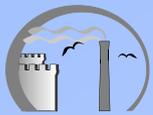




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Obstacles to multiscale modelling

1. Spatial scale gap → timestep gap → offline coupling
2. Chemistry combatibility → Aggregation (but online?)
3. Representativeness → How to treat point measurements

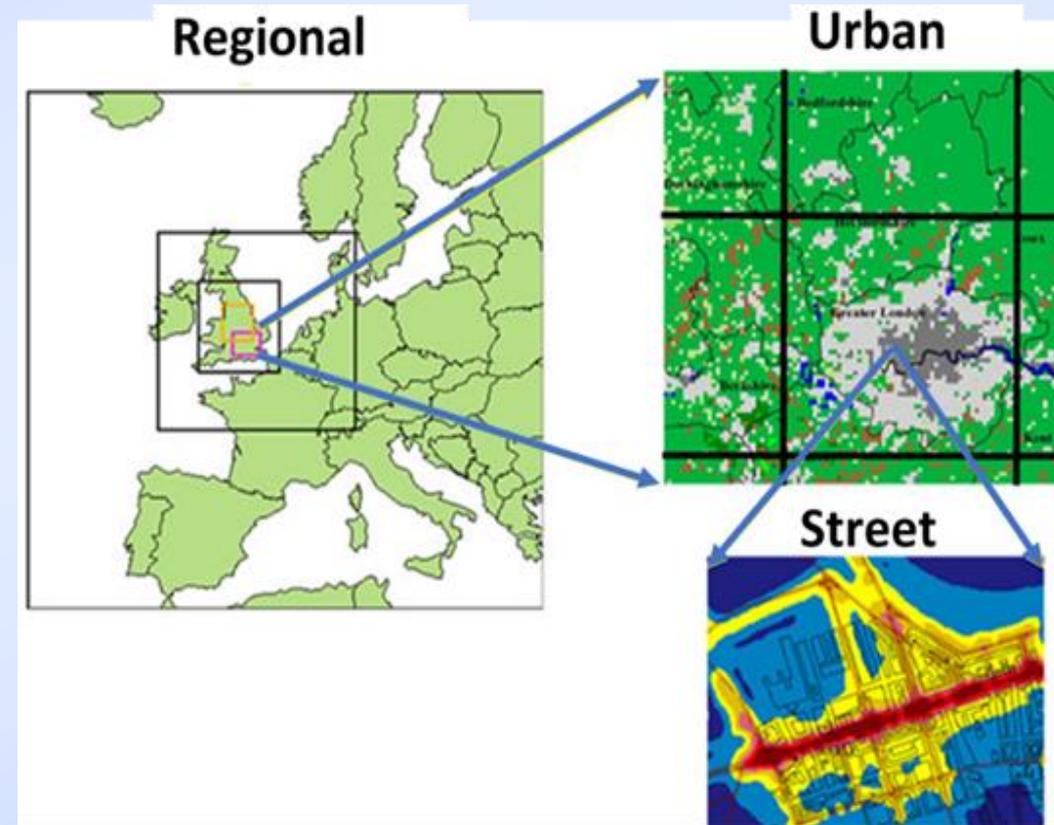


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Integration: Air Quality management system

What it does

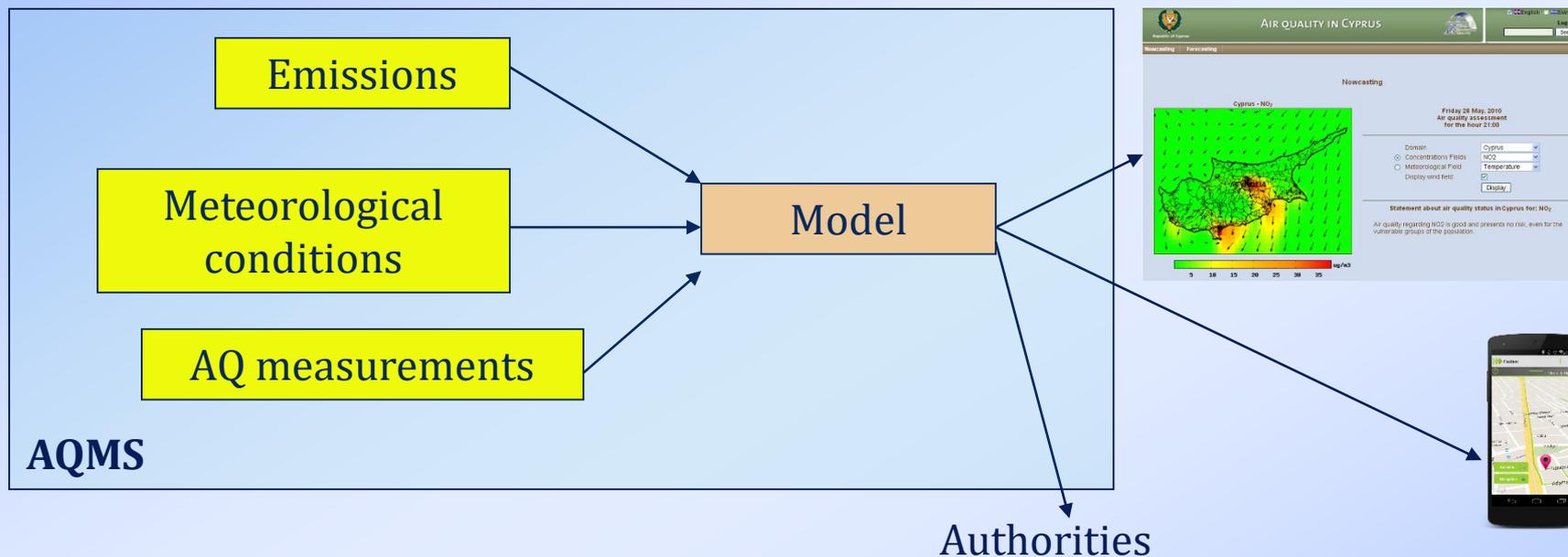
- ❑ Evaluate AQ in real-time and for the next day
- ❑ Regional down to street scale
- ❑ Emissions at different scale are taken into account
- ❑ Identify hotspots
- ❑ All major pollutants
- ❑ Impact assessment of (proposed) policy measures
- ❑ Customised coverage





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Operational Features



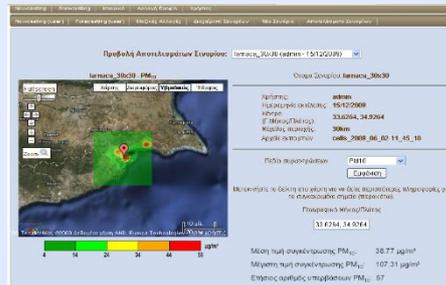
- Hourly AQ estimates (NO_x, SO₂, CO₂, CO, PM, PN, BC) for the whole region and zoomed over streets, hotspots
- Informational messages about the air quality situation are automatically displayed on the webpage, can also be sent to smart devices (phones).



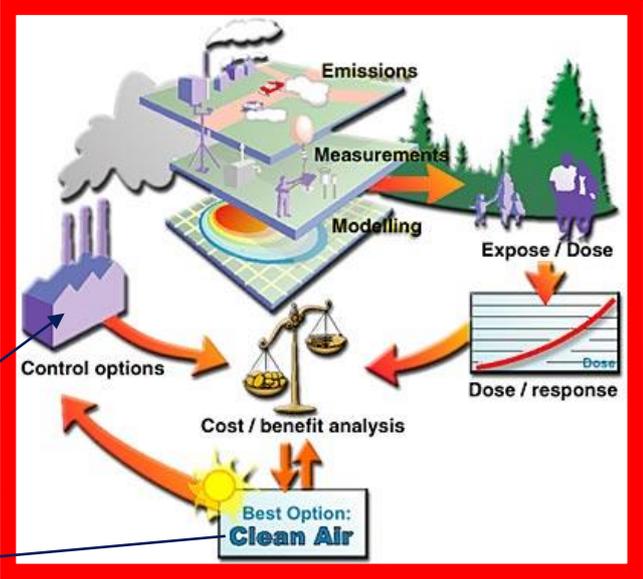
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Scenario Assessment

- ◆ Various control options can be tested as emission scenarios
- ◆ Calculations performed for user defined areas are chosen with the aid of a friendly interface
- ◆ Display of the results in the form of maps and statistical indices



Decision
Maker





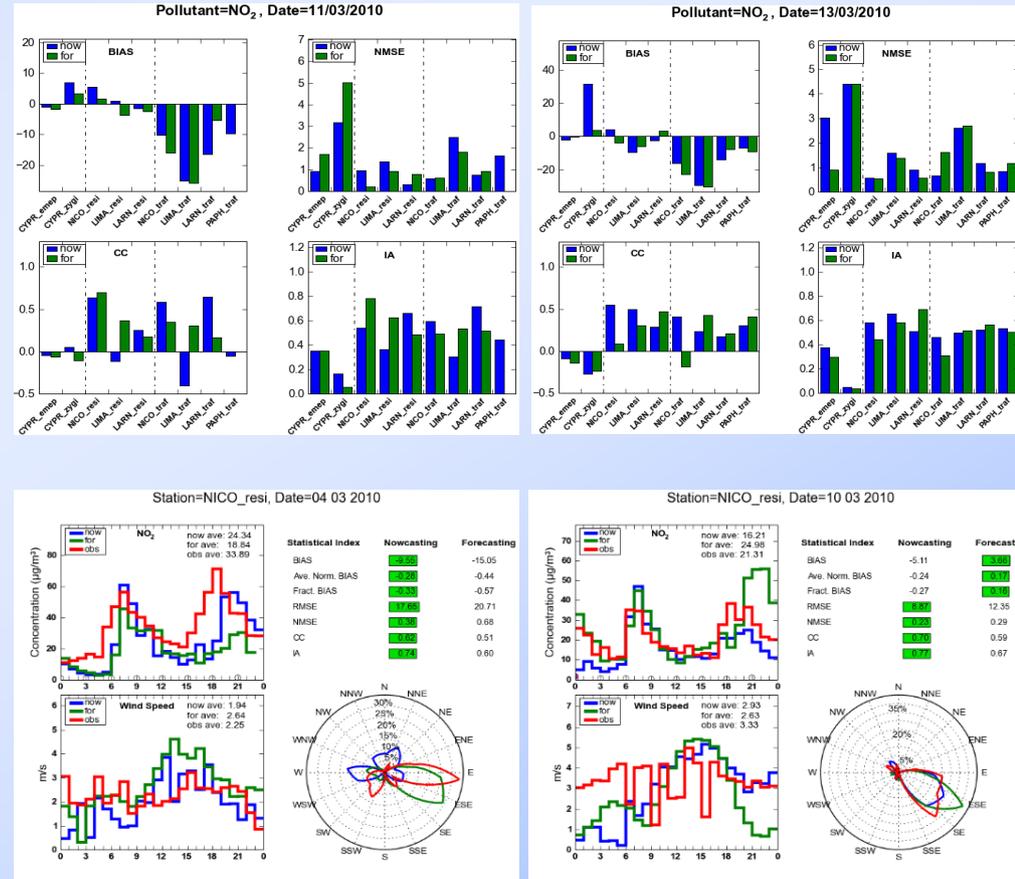
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Evaluation/Validation

A wide range of quality indicators are calculated according to the guidelines set by COST728, for the station locations and pollutants of interest

Numerous charts are automatically provided for visually assessing the accuracy of the simulations in both nowcasting and forecasting modes

Validation charts for the meteorological parameters are also provided

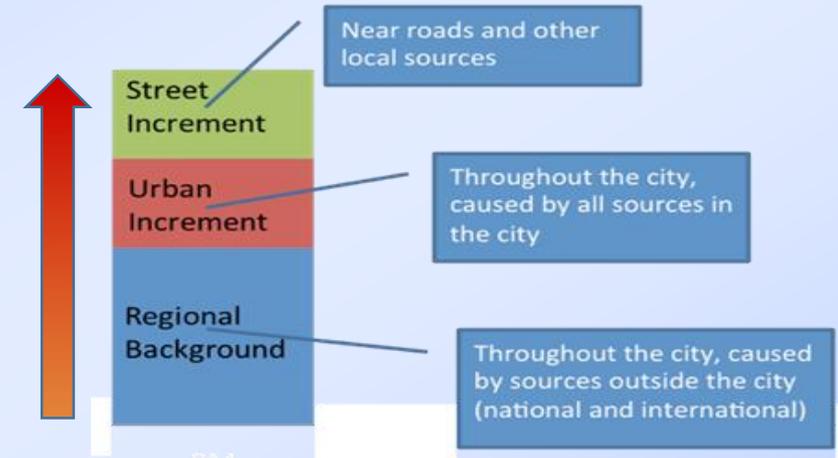




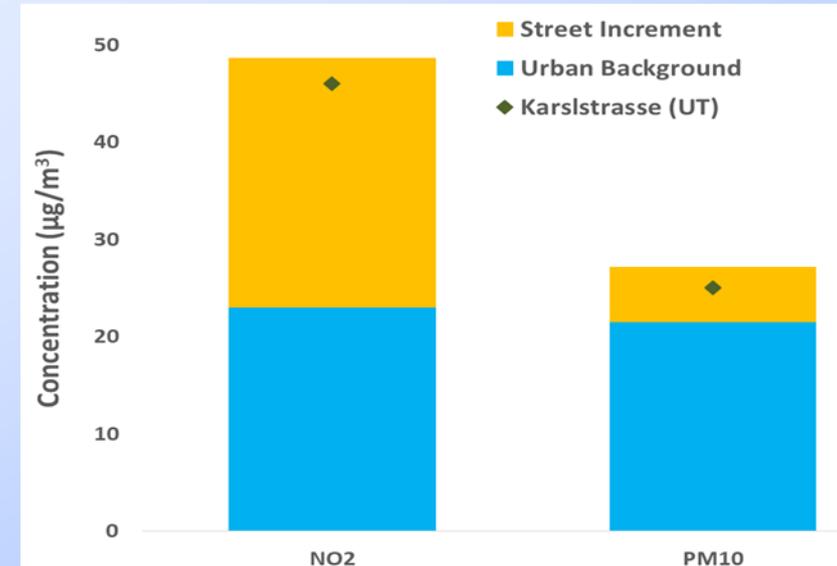
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Solution A: semiempirical increment models

- An approach allowing the operational assessment of urban and local scale air quality without the need of detailed input data.
- The method is based on the efficient calculation of concentration increments on top of the regional and urban background concentrations, respectively.
- Core elements: functional relationships between local meteorological parameters, urban and street geometrical characteristics and emissions, constructed on the basis of measured increments in representative locations.
- 3 steps:
 - ✓ Selection of urban background pairs
 - ✓ Multiple regression analysis
 - ✓ Calculation of time- and location-dependent increments



Application: Augsburg, Germany

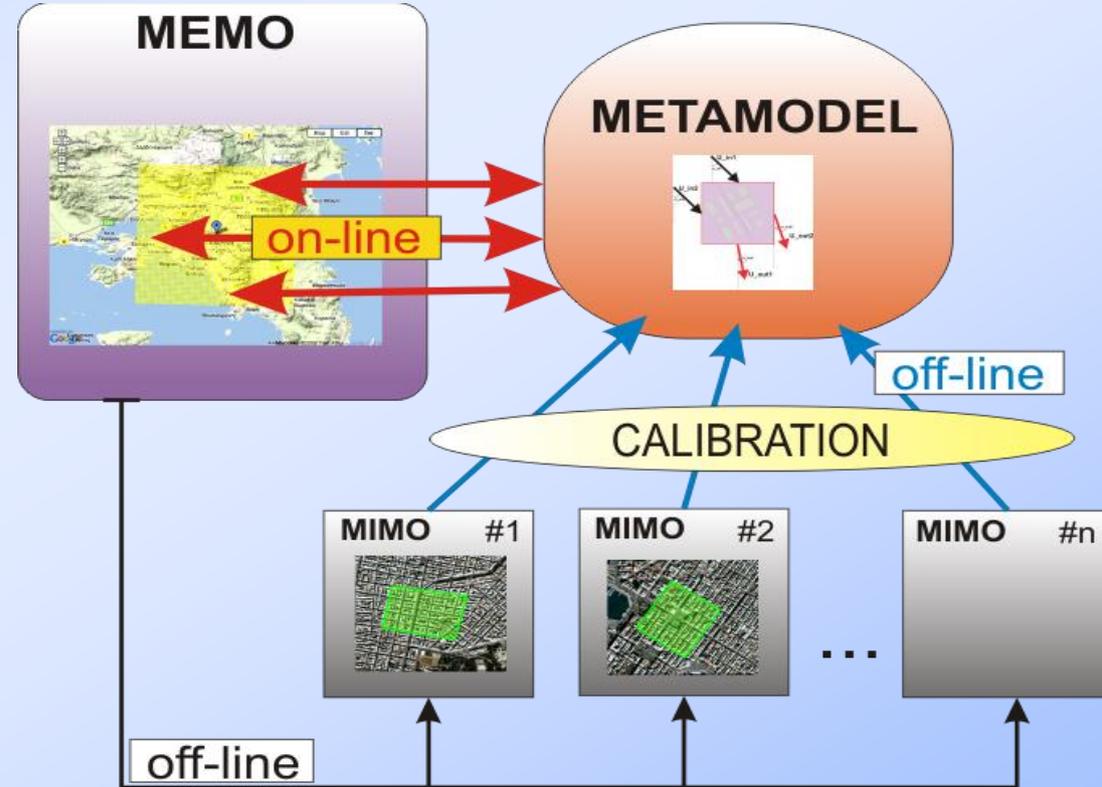




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Solution B: Explicit mesoscale-microscale coupling

- ❑ The calibration-application process can be applied iteratively, in order to increase accuracy of the mesoscale simulation
- ❑ Convergence is usually achieved in less than 3 iterations

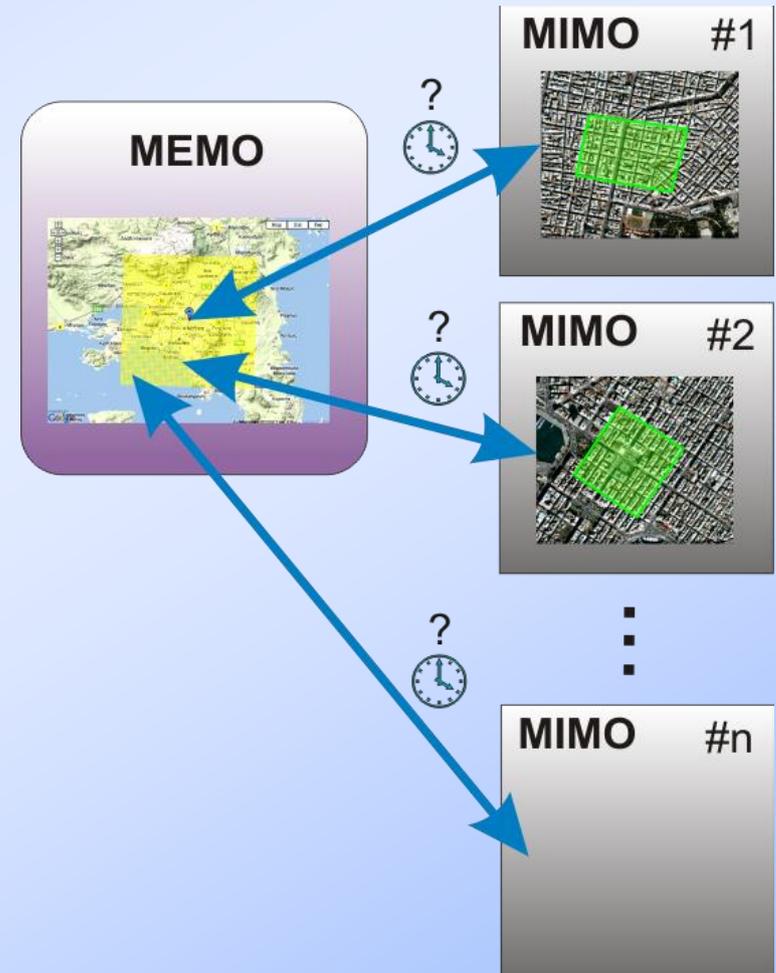




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Solution B: Explicit mesoscale-microscale coupling

- ❑ Big spatial **scale mismatches**:
 - mesoscale: $\sim 100 - 300$ km
 - microscale: < 4 km
- ❑ The selected microscale domain should be **representative** (geometry, orientation, etc.) of the larger urban area
- ❑ “One-way” \rightarrow **Cannot** estimate the effect of the microscale domain **on the mesoscale flow** (e.g. the combined effect from hundreds of urban cells)

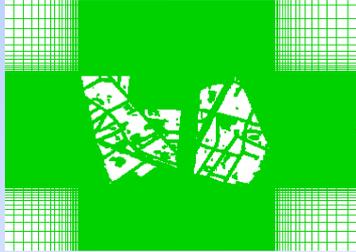




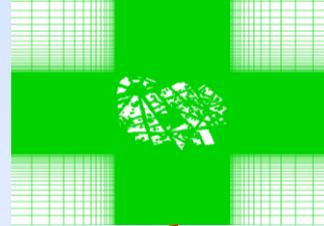
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Solution B: Explicit mesoscale-microscale coupling

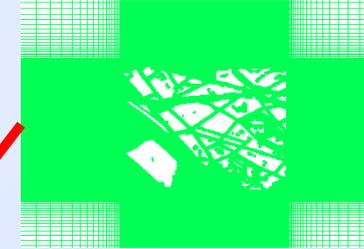
Northern sector



Middle sector

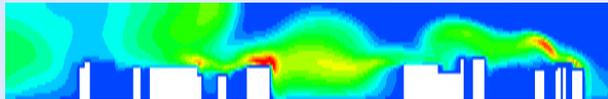


Eastern sector

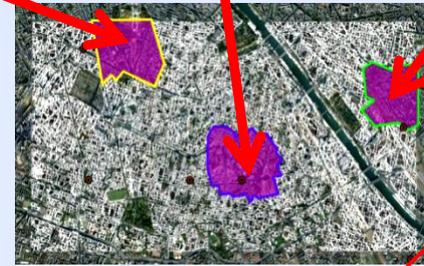
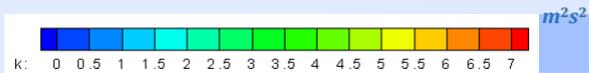
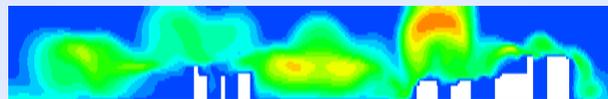


TKE

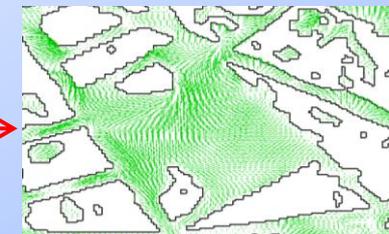
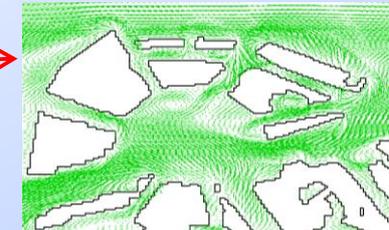
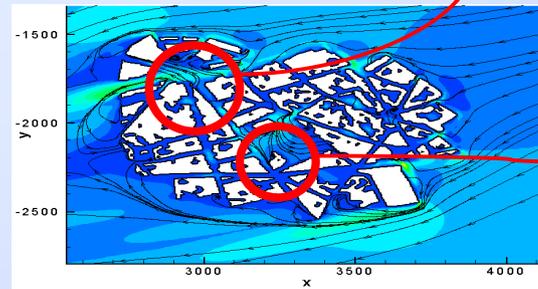
W to E plane at the domain centre



N to S plane at the domain centre



Middle sector

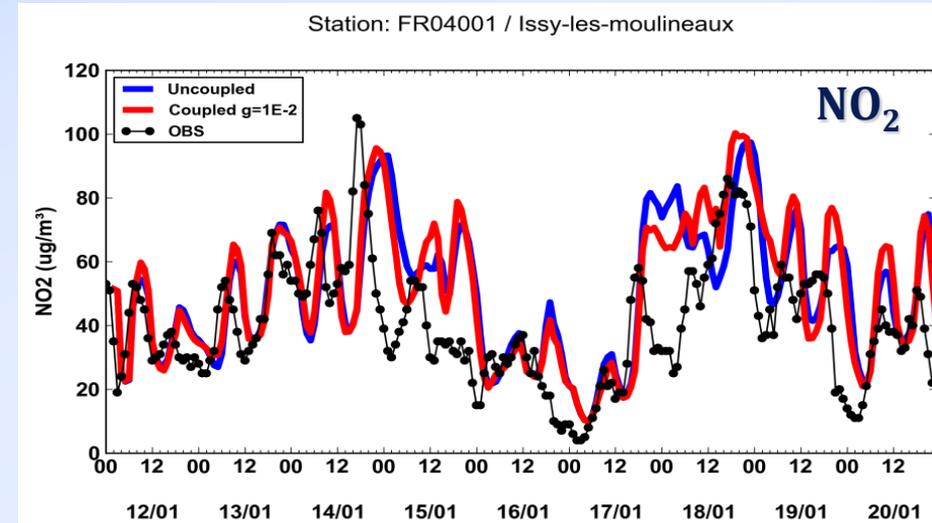
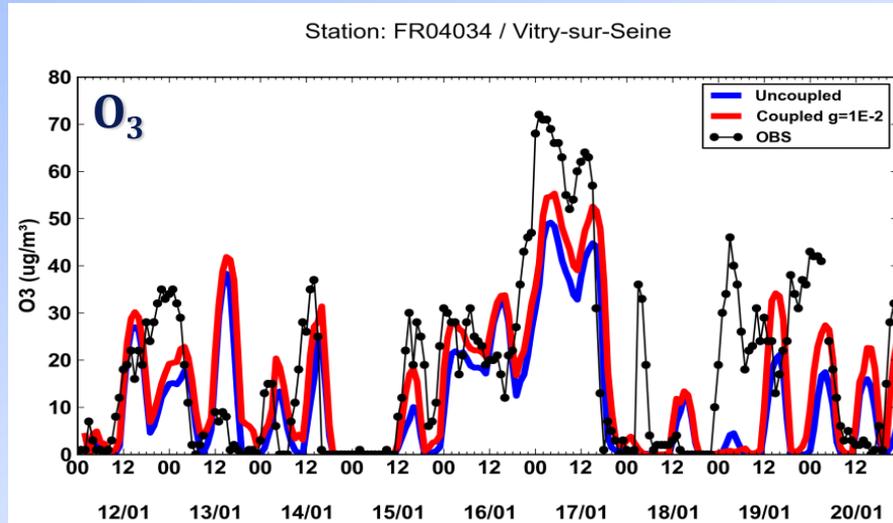


Test application in Paris, France

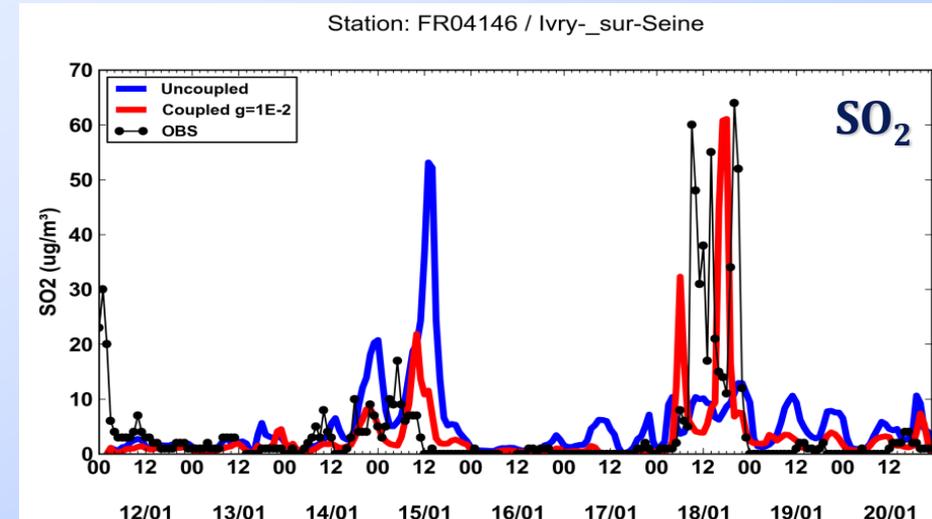


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Solution B: Explicit mesoscale-microscale coupling



- **O₃**: coupling improves bias
- **NO₂**: Coupling improves bias and correlation
- **SO₂**: significant improvement on background peaks



Test application in Paris, France



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Solution C: Assimilation of data from AQ sensors

Source: SmartAQNet project



Standard
(gravimetric)

Professional
(mostly optical)

Consumer
(mostly optical)

Low-Cost
(optical)

accurate ←
stable ←
expensive ←
low temporal
resolution ←
delayed ←
large ←
static ←



→ noisy
→ unstable
→ cheap
→ high temporal
resolution
→ low latency
→ small
→ mobile



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Solution C: Assimilation of data from sensors

Advantages

- Low installation and maintenance cost
- Large number, better spatial coverage
- Flexible in placement
- Can be incorporated in IoT networks!
- If portable: measure personal exposure!



Consumer (mostly optical) Low-Cost (optical)

AQMS models can mitigate these

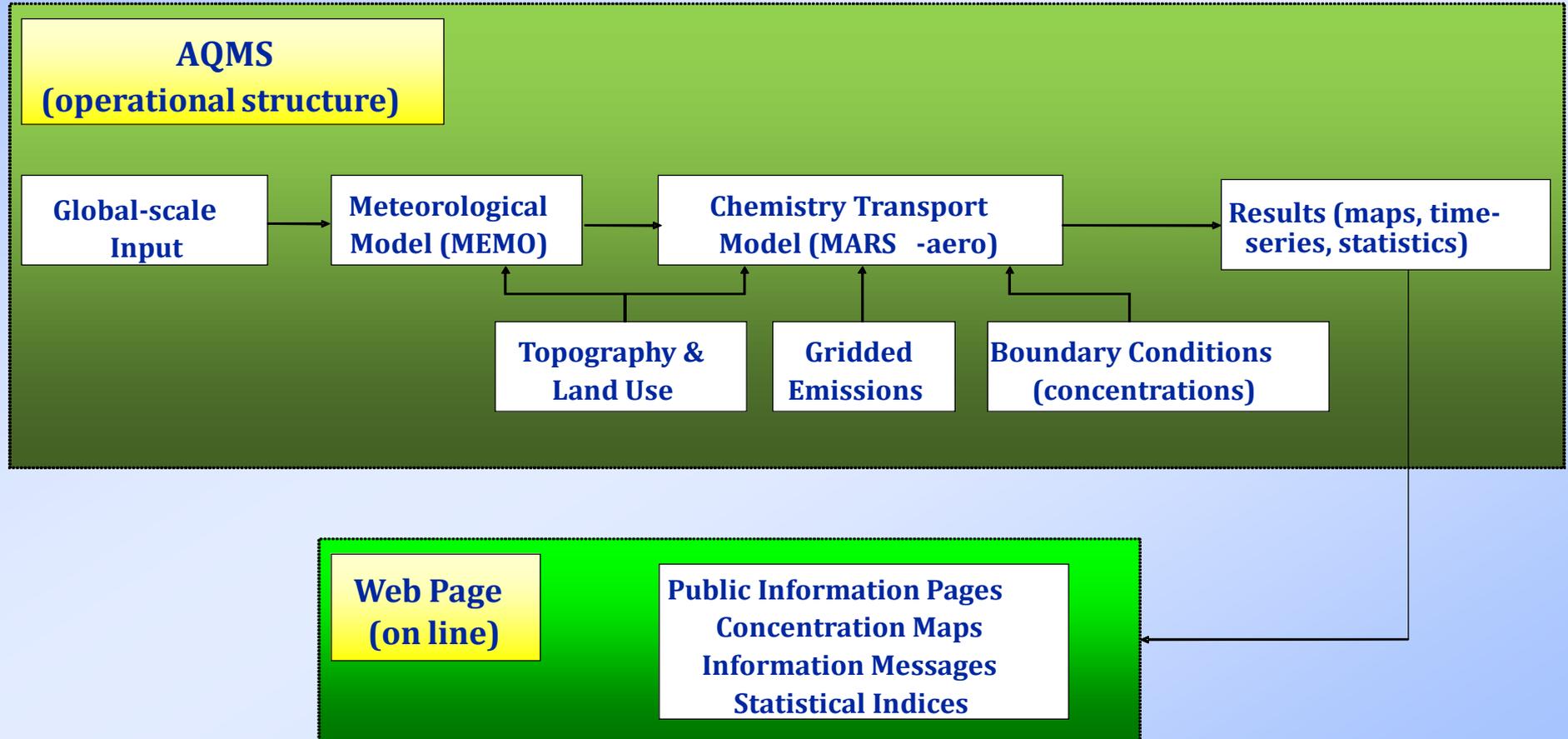
Shortcomings

- Systematic error (mainly “drift”)
- Sensitivity to environmental parameters
- Difficulty in spatial interpretation



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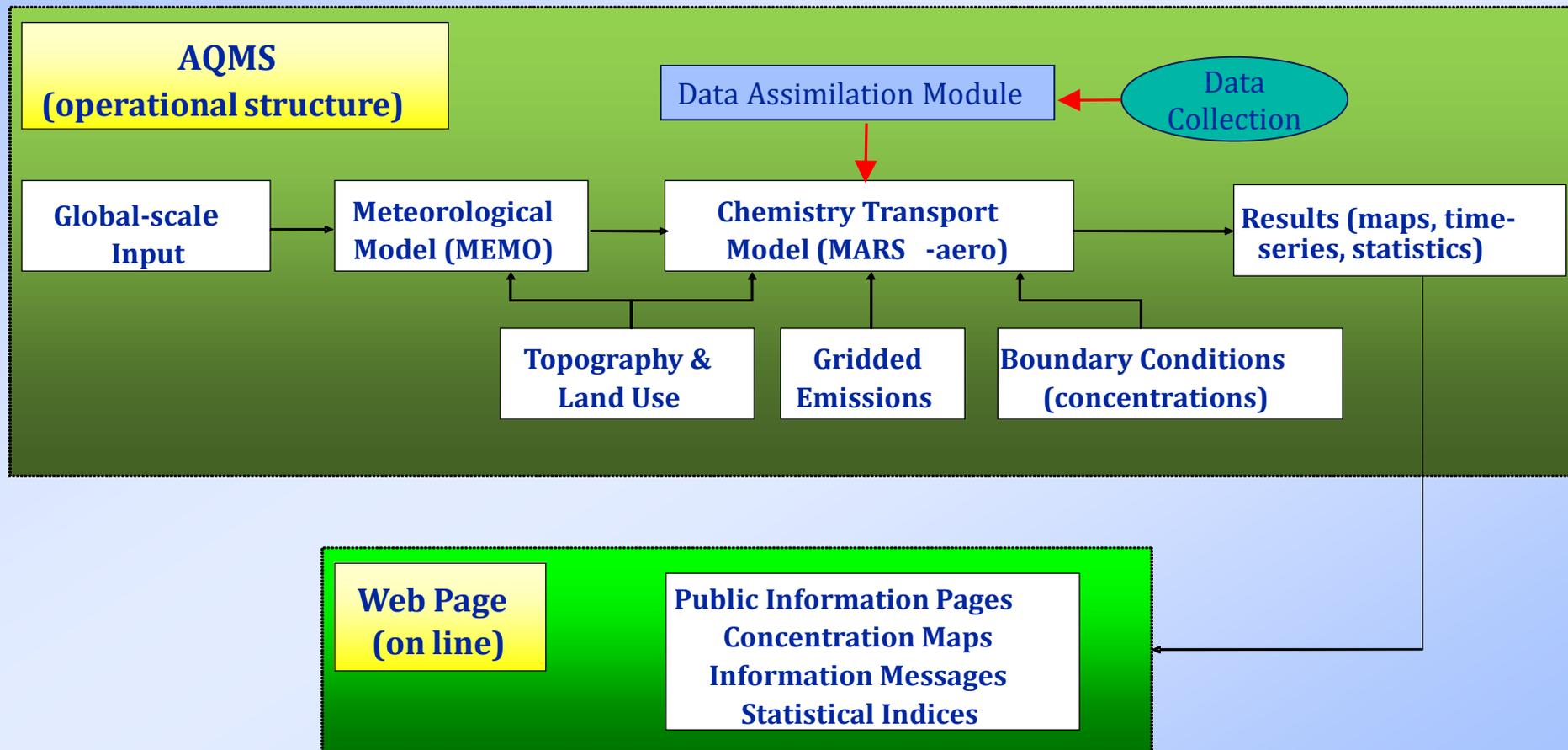
Solution C: Assimilation of data from sensors





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Solution C: Assimilation of data from sensors



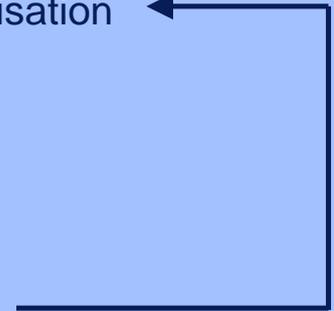


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Solution C: Assimilation of data from sensors

Data Assimilation Module

1. Transfer of concentration data
2. Timebase checking, rejection of out-of-sequence data
3. Sanity checking: ranges (species-dependent), derivatives, spatial correlation
4. Classification (regional background, urban background, street-scale) and normalisation
5. Calculation of numerical tendencies (forcing terms)
6. Spatial “smearing” of tendencies
7. Incorporation of tendencies in the dynamical terms and step integration
8. Extraction of corrective terms, to be used in next assimilation/integration steps





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PALM-LES: A flexible solution for smaller scales

- ❑ The Atmospheric Boundary Layer (ABL) is solved simultaneously with the small-scale street-canyon turbulent events
- ❑ Advantages:
 - Highly turbulent flows can be simulated - simulations which capture the turbulent motion within streets can be performed
 - Multi-scale interactions resolved via self nesting



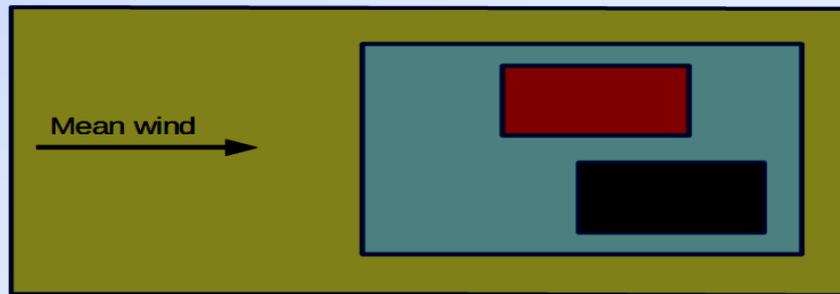


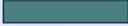
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PALM-LES: A flexible solution for smaller scales

Self nesting

- ❑ LES of wind flow in is a multi-scale problem
- ❑ High enough resolution for a sufficiently large domain is usually too expensive → resolution must be concentrated to the area of principal interest
- ❑ Model nesting is the only way to concentrate resolution to the principal area of interest as we gain from both fast solver and spatially varying resolution!



-  Root domain, the coarsest resolution
-  Nest domain, medium resolution
-  Nest domain, area of interest, the highest resolution
-  Nest domain, area of interest, the highest resolution

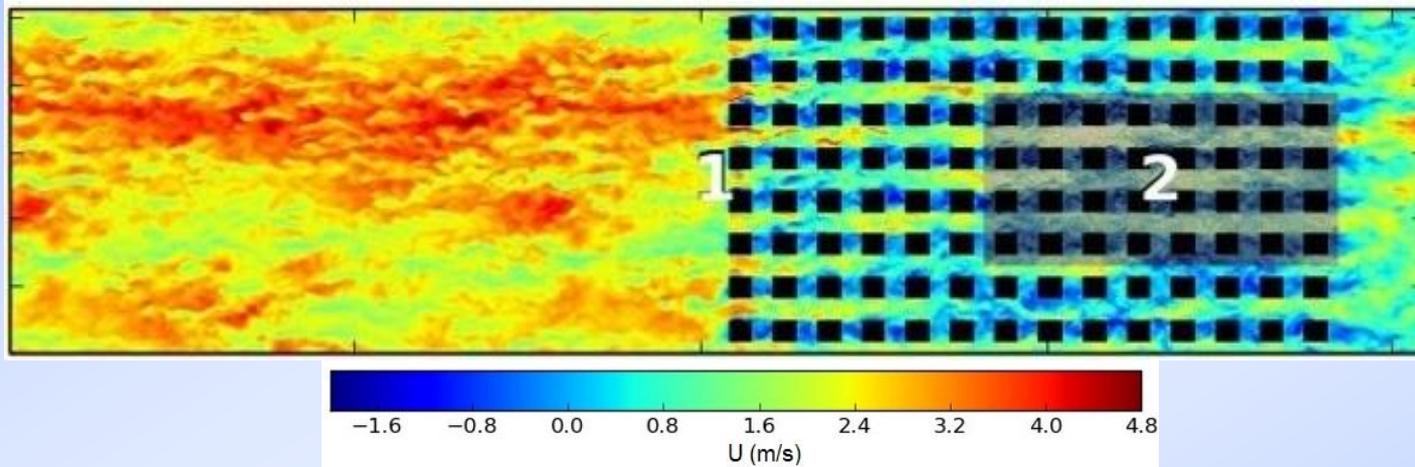
- ❑ The system of nested domains consists of the root and nest domains
- ❑ Nests can have their own nests and so on (cascading domain arrangement)
- ❑ Cascading and parallel nests can co-exist in the same run
- ❑ All nests must lay inside their parent model domain



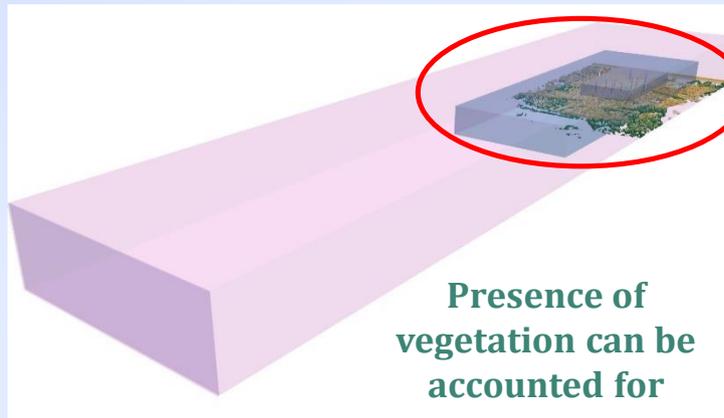
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PALM-LES: A flexible solution for smaller scales

Functional testing of an array of cubes approximating buildings: success!



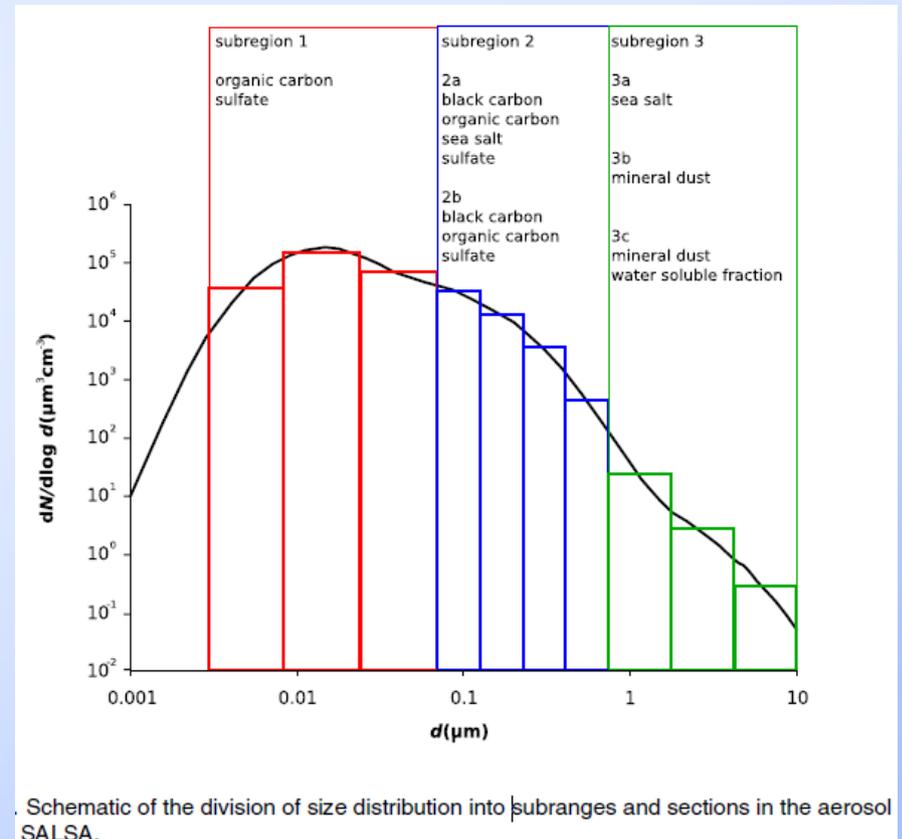
Example of PALM LES application in real city



Presence of
vegetation can be
accounted for



SALSA – a Sectional Aerosol module for Large Scale Applications



- A fully "online" coupled (Baklanov et al., 2014) chemistry module
- For the description of gas-phase chemistry the latest version of Kinetic Preprocessor (KPP 1) version 2.3 has been implemented into PALM-4U
- Fortran source code can be generated directly from a list of chemical rate equations, a special preprocessor automatically generates interface routines between the generated modules and PALM.
- A more complex chemistry module is available for the RANS mode
- A strongly simplified chemistry mechanism is available for the LES mode

Conclusions and final thoughts

- Hotspot exposure (external) modelling is a multiscale problem
- Significant technical obstacles in “naïve” coupling
- Recent developments in tools/methods show that the problems are not intrinsic
- Online coupling (including chemistry) has become feasible
- Integration of modelling tools provides benefits, also for validation
- Data from inexpensive sensors: added value under certain conditions
- Progress in tailpipe-to-roadside modelling (inc. work in DOWNT010 project, <http://www.downtoten.com>)



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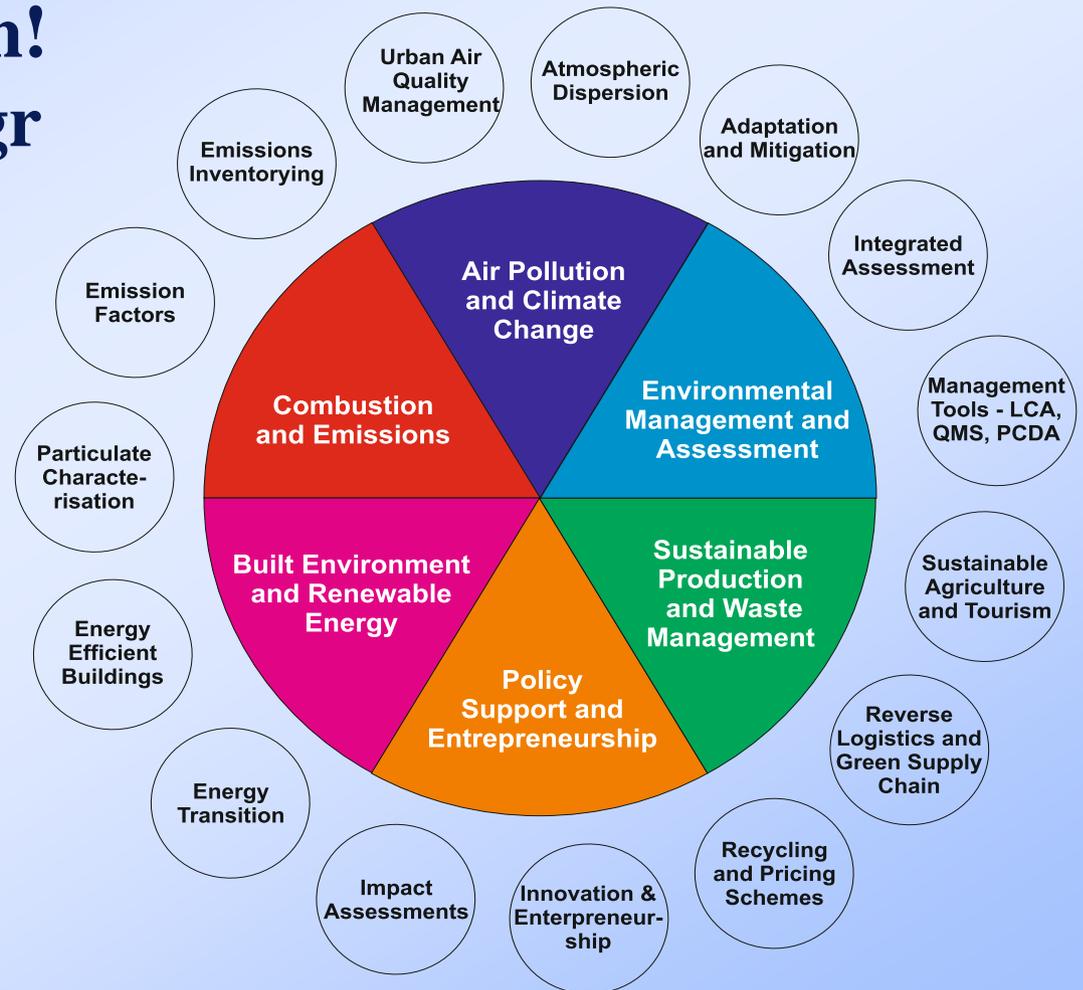
7th International Symposium on Ultrafine Particles – Brussels, May 15th 2019

Thank you for your attention!
URL: <http://aix.meng.auth.gr>

Laboratory of Heat Transfer
and Environmental
Engineering
Aristotle University
Thessaloniki, Greece

Main Research Topics:

- Air Pollution
- Waste Management
- Energy Systems and Technology

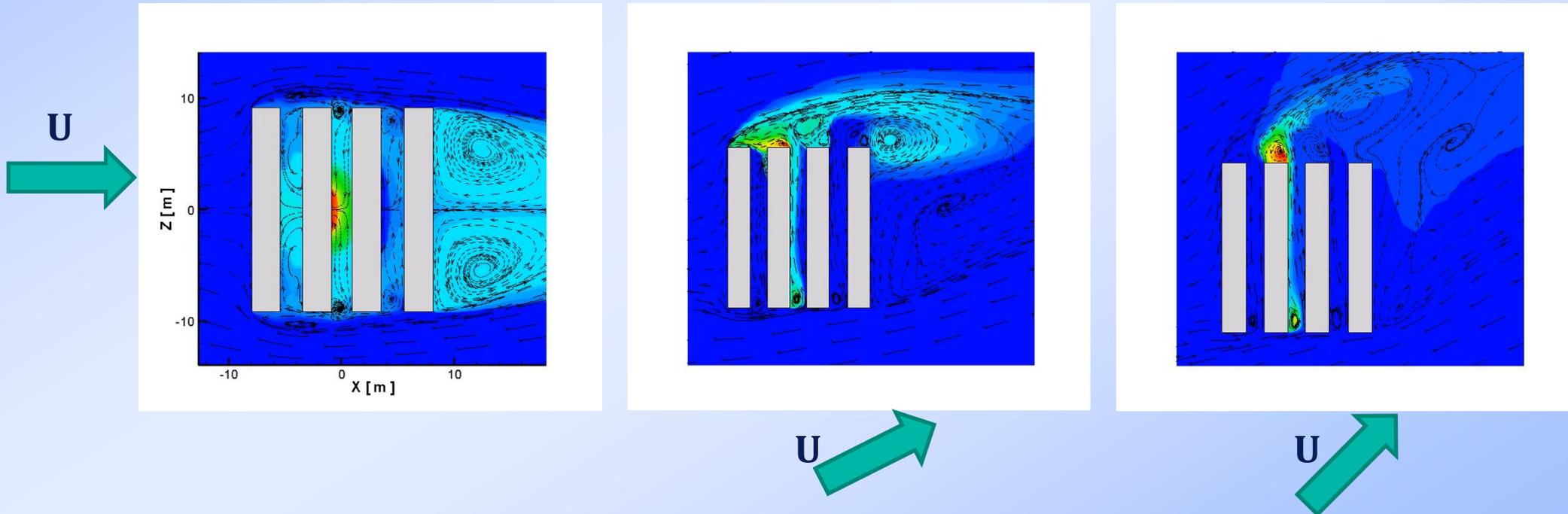




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Example of dispersion in streets

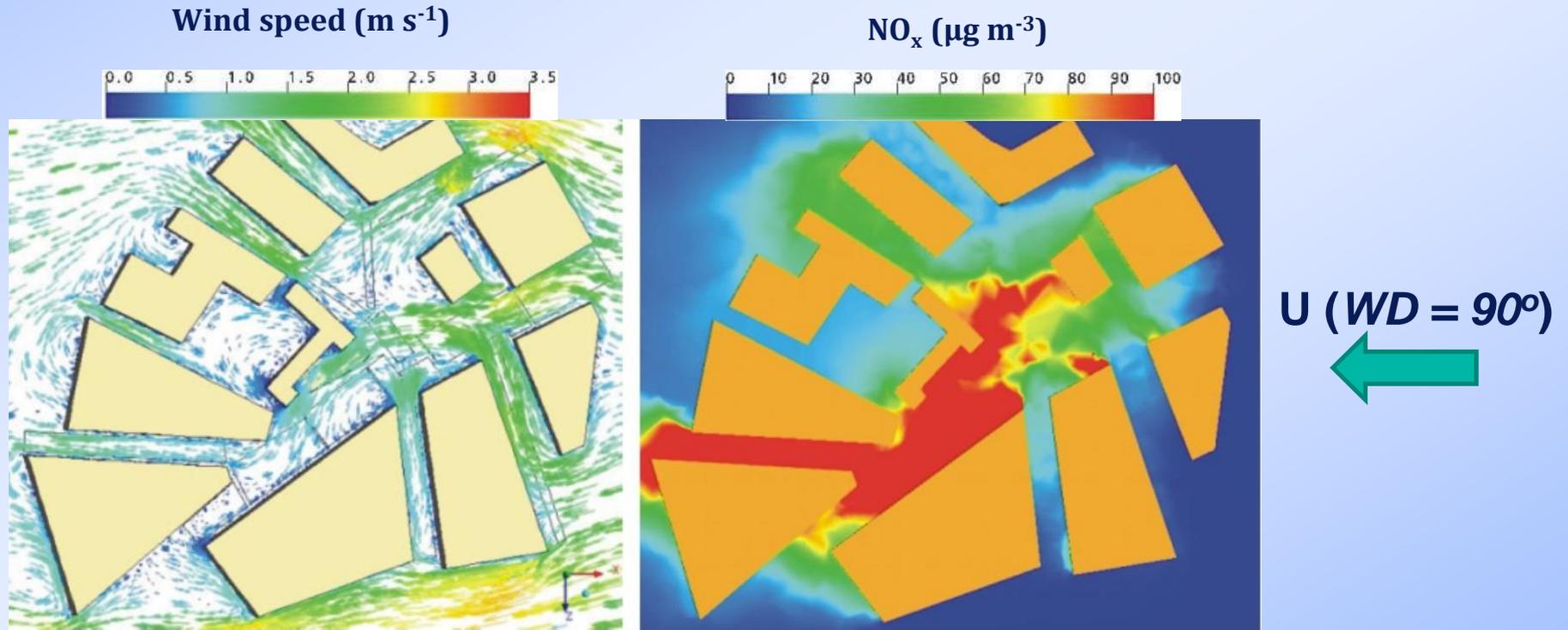
Flow and dispersion fields under the influence of 3D building geometry in an artificial series of streets (the PICADA project Guerville experiment) - Bird's eye view





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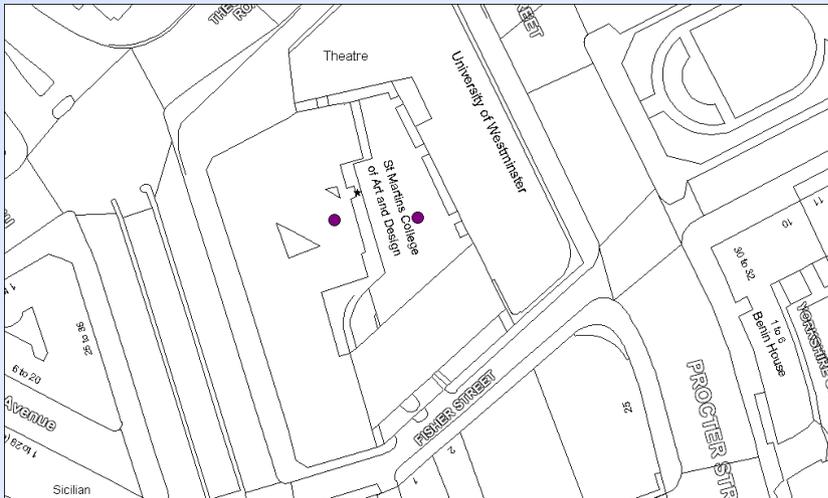
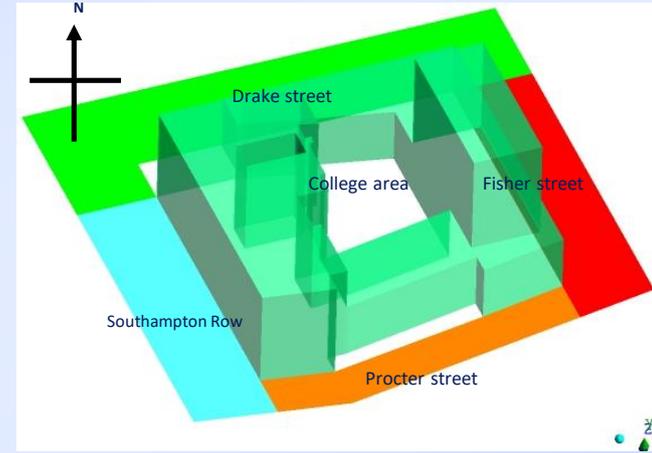
Example of numerically calculated flow and dispersion fields in Central London





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Example of numerically calculated flow and dispersion fields in Central London

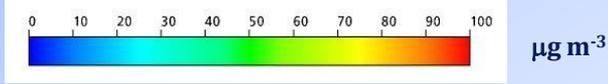




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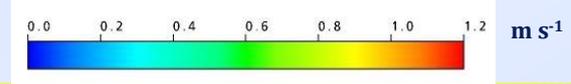
Example of numerically calculated flow and dispersion fields in Central London

NO_x

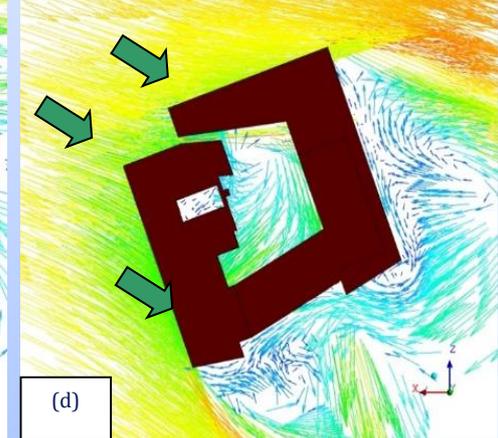
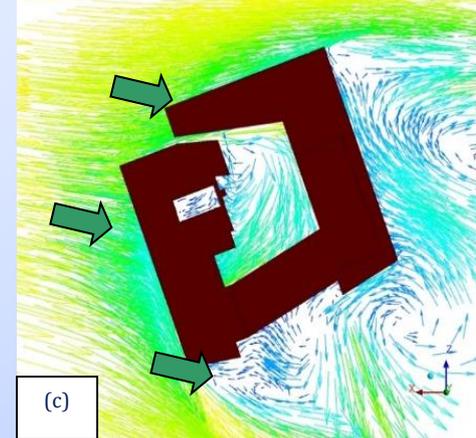
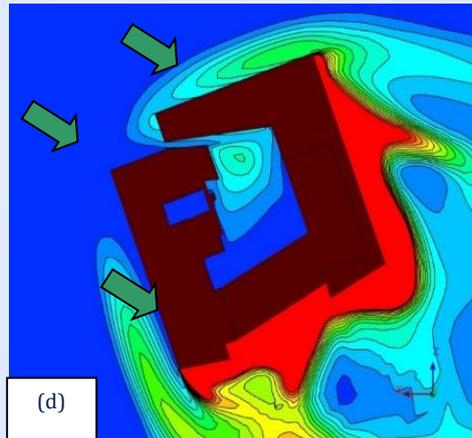
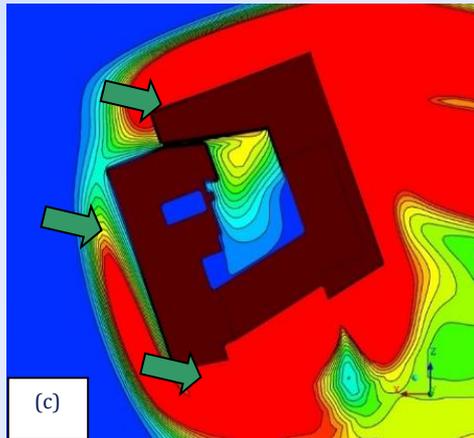
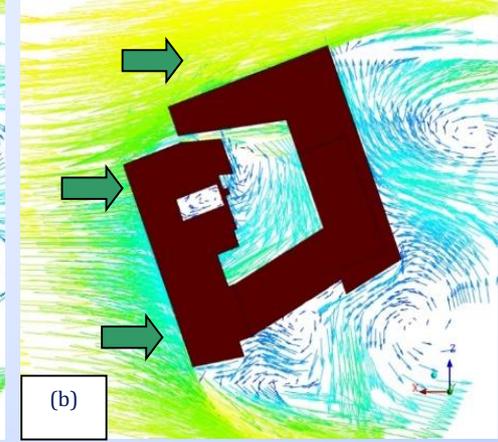
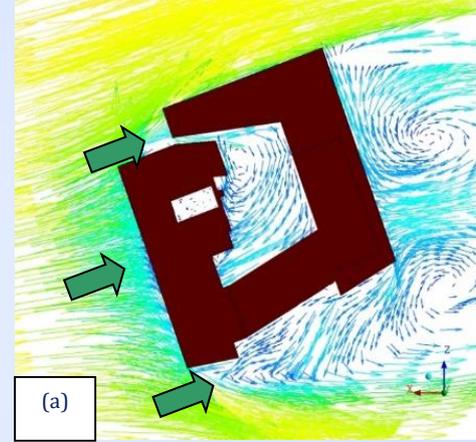
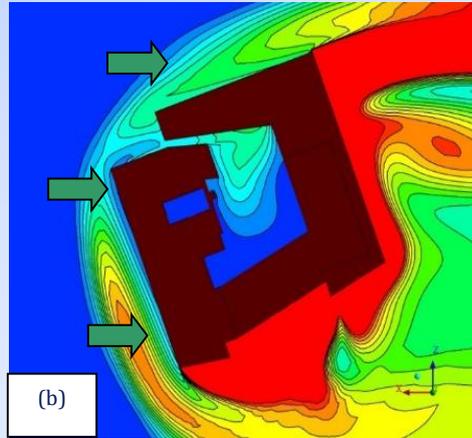
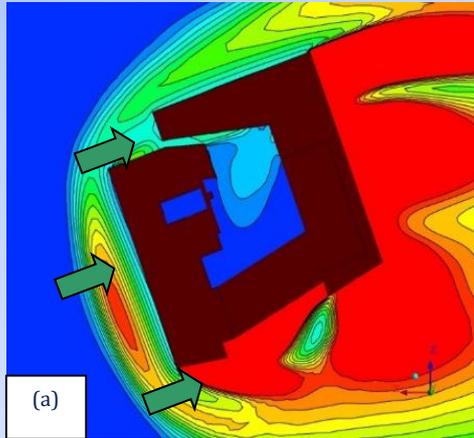


$\mu\text{g m}^{-3}$

Wind speed



m s^{-1}

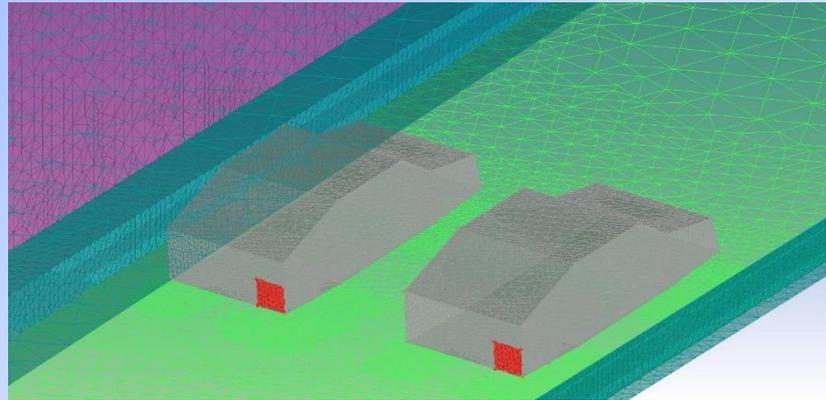




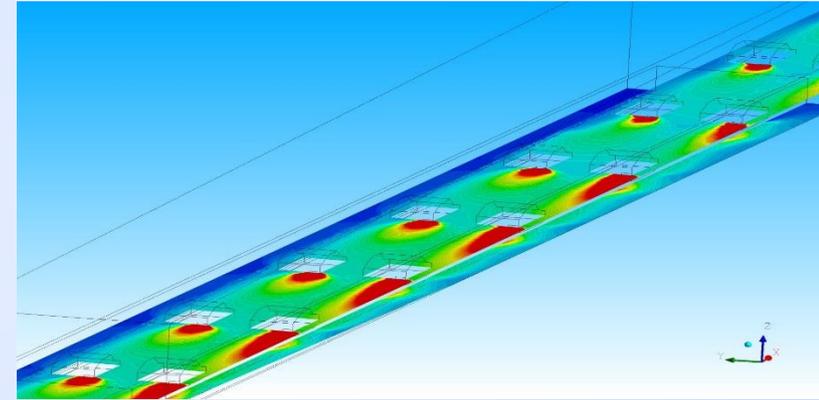
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Other examples of real life application of CFD

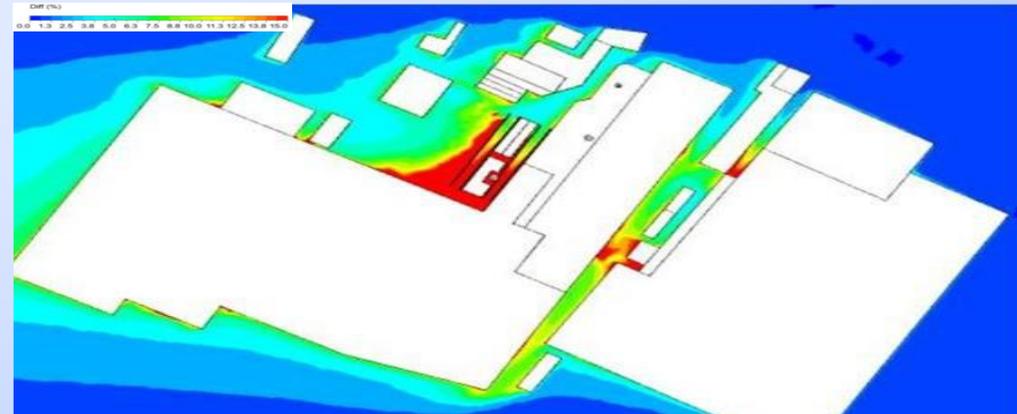
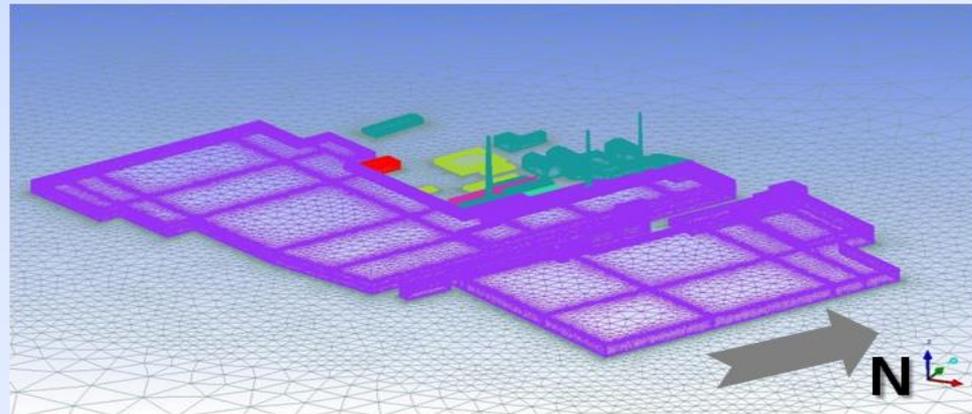
Leopold II road tunnel field trial, Brussels, Belgium



Moving mesh
technique applied –
impact of **vehicles**
motion quantified



Industrial site application (Italcementi), Bergamo, Italy





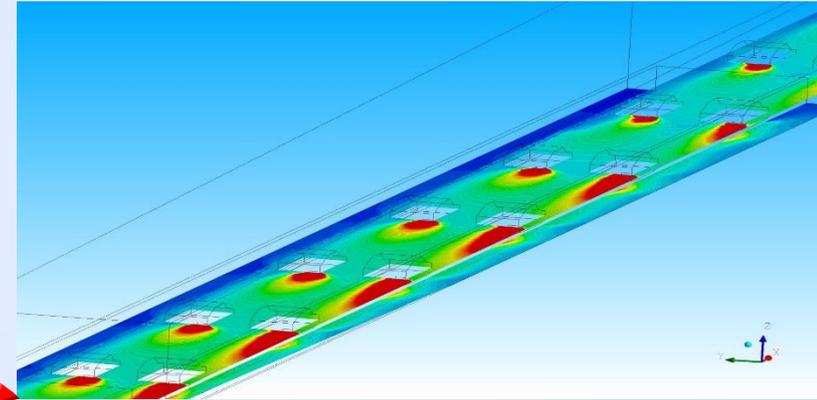
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Other examples of real life application of CFD

Leopold II road tunnel field trial, Brussels, Belgium

Simulation of dispersion-dilution of exhaust gases

Moving mesh
technique applied –
impact of **vehicles**
motion quantified



Industrial site application (Italcementi), Bergamo, Italy

