EXPERIENCES ABOUT THE USE OF CFD MODELS FOR AIR QUALITY STUDIES IN SPAIN

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FAIRMODE TECHNICAL MEETING
Tallinn, Estonia 26-28 June 2018

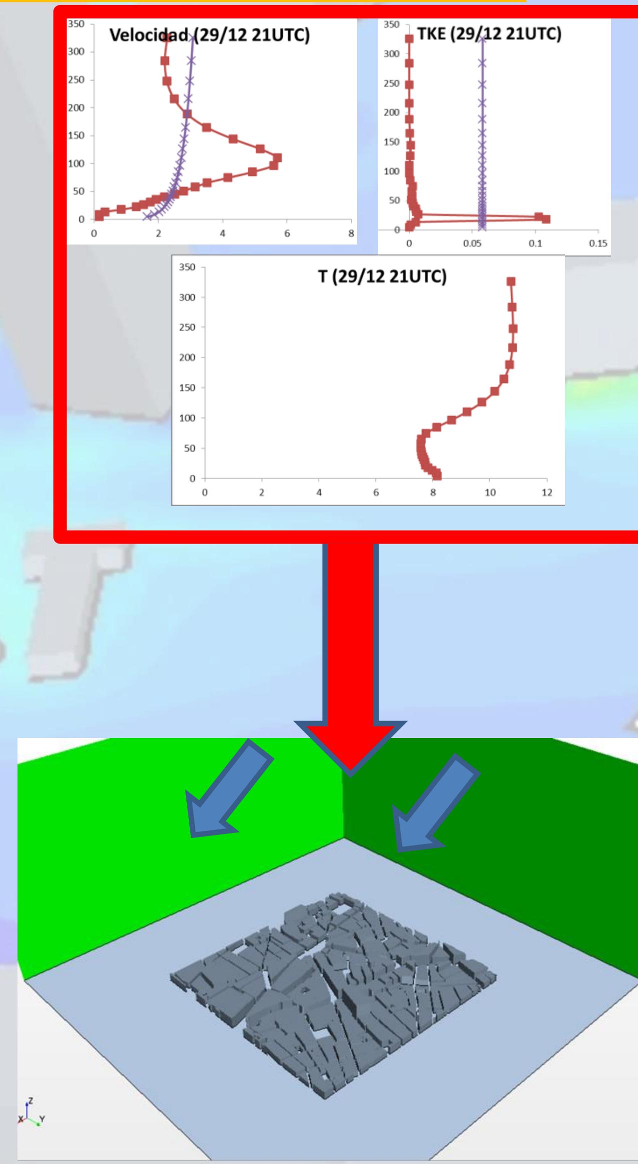
Outline

- **Q1**: How to couple local scale CFD output with (urban) background concentrations?
- **Q2**: How to derive AQD statistic (annual averages, percentiles) with CFD models?
- **Q3**: Quality of CFD calculations in formal AQ assessment?

Q1: How to couple local scale CFD output with (urban) background concentrations

Mesoscale meteorology for CFD boundary conditions

- **Variables**:
  - **Wind speed and direction (V)**: Vertical profile at inlet, time evolution
  - **Turbulent kinetic energy (TKE)**: Vertical profile at inlet, time evolution
  - **Turbulent dissipation rate (ε)**: Vertical profile at inlet, time evolution
  - **Temperature (T)**:Vertical profile at inlet, time evolution. Usually neutral stability profiles assumed.
  - **Heat fluxes**: Urban surfaces (ground, building walls), time evolution
- **Data from**:
  - **Meteorological stations**:
    - **Compute profiles from point measurements at one height (10 m)** of meteorological station.
    - Meteo station should not be influence by nearby buildings.
    - Usually **neutral profiles assumed** from these measurements
  - **Mesoscale models (same grid cell where the microscale domain is located)**:
    - **Mesoscale model vertical profiles** imposed at inlet.



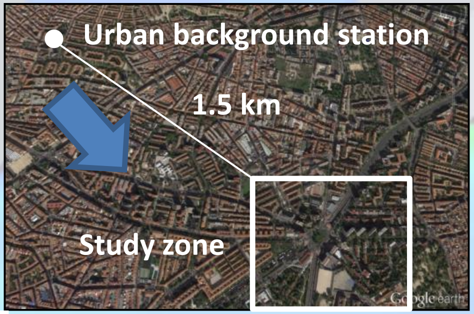
Q1: How to couple local scale CFD output with (urban) background concentrations

Urban background concentration for CFD boundary conditions

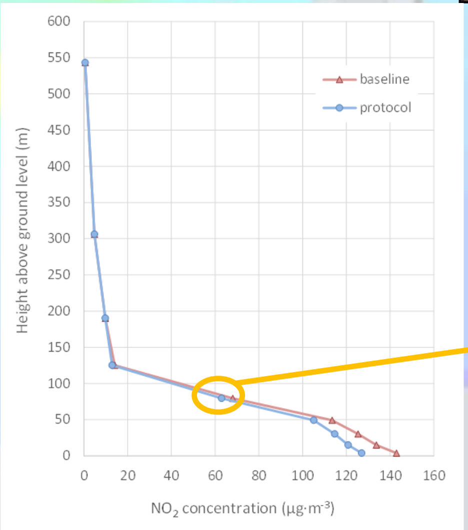
- Pollutant concentration at inlet. Time evolution.
- Data from:
  - **Air Quality monitoring stations**:
    - Concentration **urban background station** (added to concentration computed by CFD)

Close to simulated area

Located upwind the simulated area



  - **AQ Mesoscale models (same grid cell where the microscale domain is located)**:
    - **Mesoscale concentration profiles** imposed at inlet. (Problems: Double counting of emissions, not accurate concentration profiles)
    - Background concentration (added to concentration computed by CFD) from a **vertical level just above the mixing layer**. *Similar values to urban background stations??*



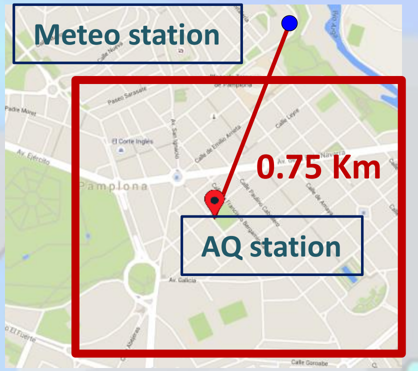
Vertical Profile mesoscale

Background concentration for CFD computations

Q1: How to couple local scale CFD output with (urban) background concentrations

Experiences in Spain

- **Plaza de la Cruz (Pamplona)**: Meteorological station, no background. Evaluation with Time evolution only with one AQ station.



Objective: Effect of urban vegetation on NOx

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Reference: Santiago JL, Rivas E, Sanchez B, Buccolieri R, Martin F, 2017. The Impact of Planting Trees on NOx Concentrations: The Case of the Plaza de la Cruz Neighborhood in Pamplona (Spain). *Atmosphere* 8, 131.

- **Escuelas Aguirre (Madrid)**: Meteorological station, urban background monitoring station. Evaluation with time evolution with AQ station and time average concentration with passive samplers (see Q2 section)

Objective: Evaluation methodology (WA CFD_RANS) to compute annual statistics of NO_2 by CFD modelling.

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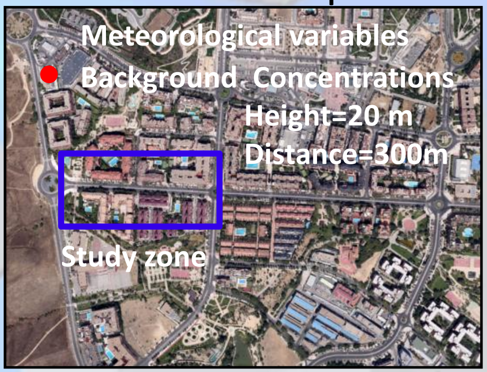
Reference: Santiago JL, Borge R, Martin F, de la Paz D, Martilli A, Lumbreras J, Sanchez B, 2017. Evaluation of a CFD-based approach to estimate pollutant distribution within a real urban canopy by means of passive samplers. *Sci. Total Environ.* 576, 46-58.

Q1: How to couple local scale CFD output with (urban) background concentrations

Experiences in Spain

- **Alcobendas (Madrid):** Meteorological station, concentration measured at a building roof in an experimental campaign. Evaluation with measurements at road.

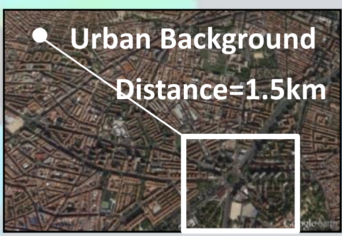


Objective: Evaluation of chemical scheme implemented and impact of photochemical materials on air quality

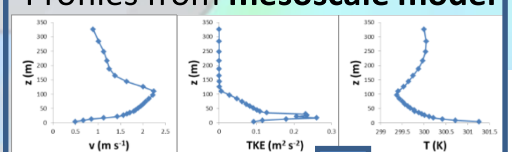
MiNOx street Life

Reference: Sanchez B, Santiago JL, Martilli A, Palacios M, Pujadas M, Nuñez L, German M, Fernandez-Pampillon J, Iglesias JD, 2016. CFD Modeling of Reactive Pollutants Dispersion and Effect of Photocatalytic Pavements in a Real Urban Area. *HARMO17 Conference*. Budapest, Hungary.

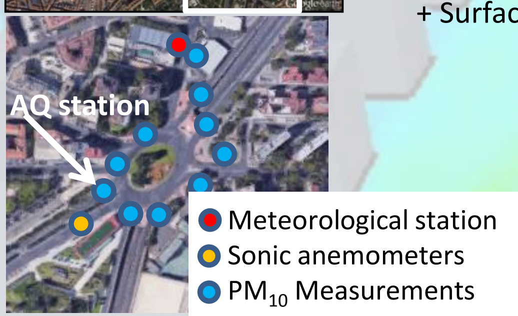
- **Plaza Elíptica (Madrid):** Meteorological mesoscale model, Meteo station, urban background monitoring stations (Chemistry implemented for NO_2). Evaluation with AQ station and passive samplers (NO_X, NO_2), particle matters monitors (PM_{10}).



Profiles from **mesoscale model**



+ Surface Heat Flux



Objective: Evaluation of chemical scheme implemented and coupling mesoscale-microscale model.

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References:

Sanchez B, Santiago JL, Martilli A, Martin F, Borge R, Quaassdorff C, de la Paz D, 2017. Modelling NOx concentration through CFD-RANS model in an urban hot-spot using high resolution traffic emissions and meteorology from a mesoscale model. *Atmospheric Environment* 163, 155-165.

Santiago JL, Sanchez B, Martin F, Martilli A, Quaassdorff C, de la Paz D, Borge R, Gómez-Moreno FJ, Artiñano B, Yagüe C, Blanco C, Vardoulakis S, 2017. CFD modelling of particle matter dispersion in a real hot-spot. HARMO18. Bologna, Italy.

Sanchez B, Santiago JL, Martin F, Martilli A, Quaassdorff C, de la Paz D, Borge R, 2017. Modelling reactive pollutants dispersion in an urban hot-spot in summer conditions using a CFD model coupled with meteorological mesoscale and chemistry-transport models. HARMO18. Bologna, Italy.

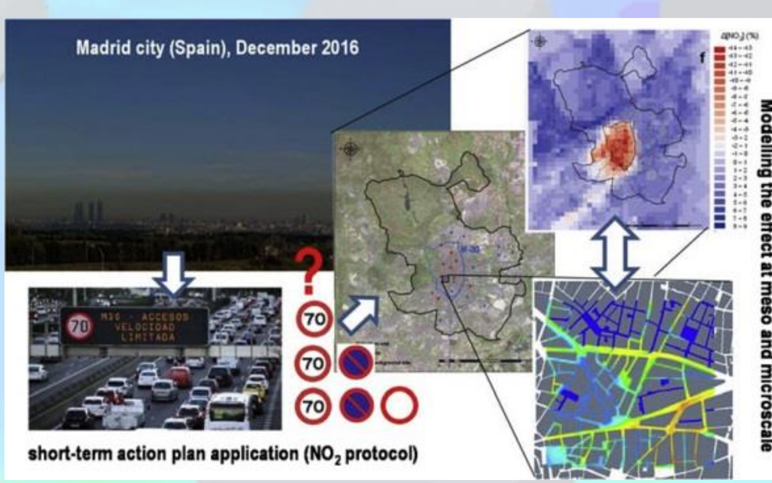
Q1: How to couple local scale CFD output with (urban) background concentrations

Experiences in Spain

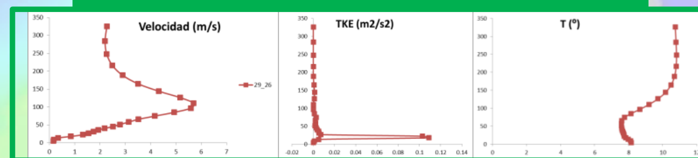
- **Plaza del Carmen (Madrid)**: Meteorological mesoscale model and AQ mesoscale model. Assessment from multi-scale modelling to high pollution episode of NO_2 in Madrid

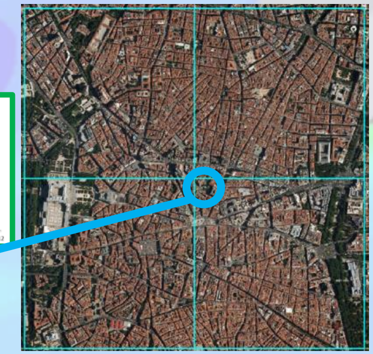
Objective with CFD model: Evaluation at microscale of traffic restriction (one hour simulated)

Mesoscale grid cells

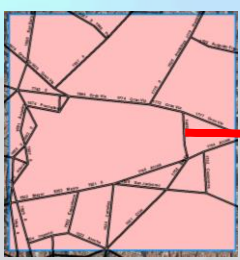


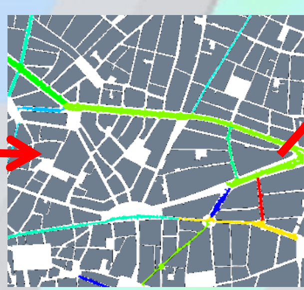
Meteorology from **WRF model**

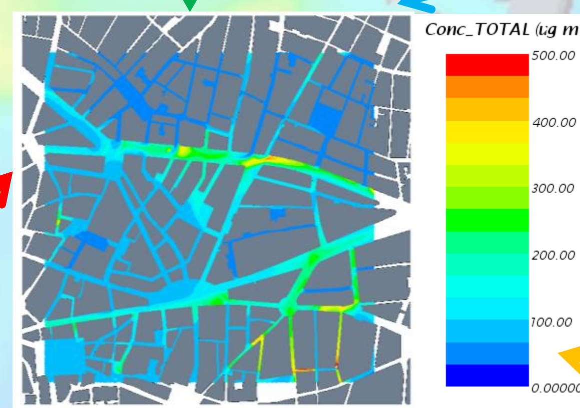




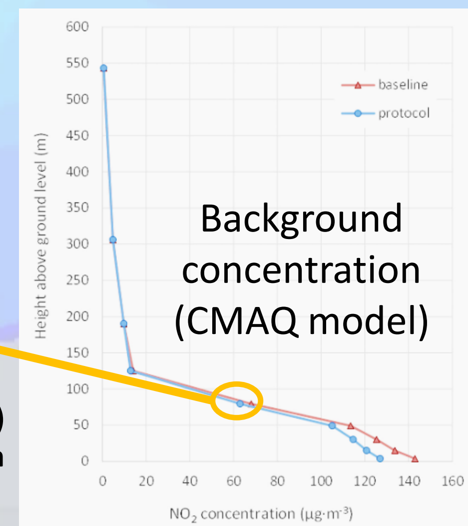
Emissions used in CMAQ







NO_2 predicted on December 29th 2016 (20-21 LT) in the Gran Vía area assuming traffic restrictions in Madrid (stage 3)



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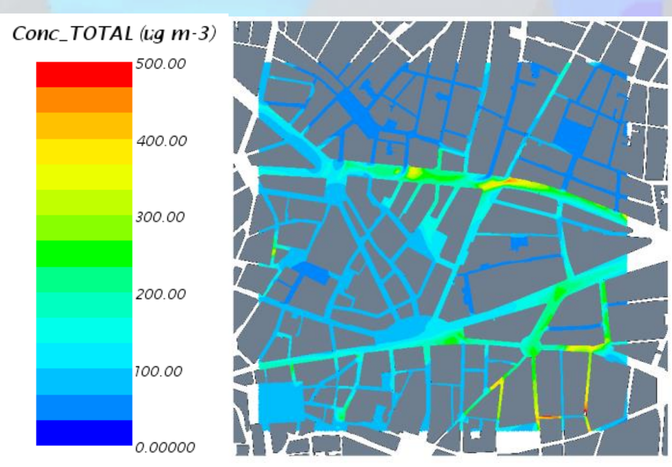
Reference: Borge R, Santiago JL, de la Paz D, Martín F, Domingo J, Valdés C, Sanchez B, Rivas E, Rozas MT, Lazaro S, Pérez J, Fernandez A, 2018. Application of a short term air quality action plan in Madrid (Spain) under a high-pollution episode-Part II: Assessment from multi-scale modelling. *Science of The Total Environment*, *635*, 1574-1584.

Q1: How to couple local scale CFD output with (urban) background concentrations

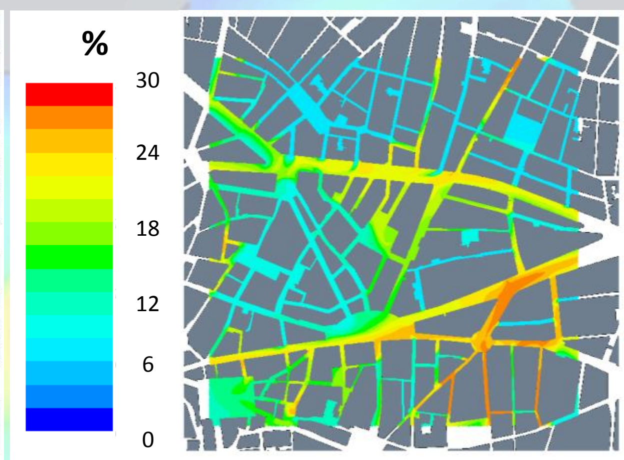
Experiences in Spain

- **Plaza del Carmen (Madrid)**: Meteorological mesoscale model and AQ mesoscale model. Assessment from multi-scale modelling to high pollution episode of NO_2 in Madrid

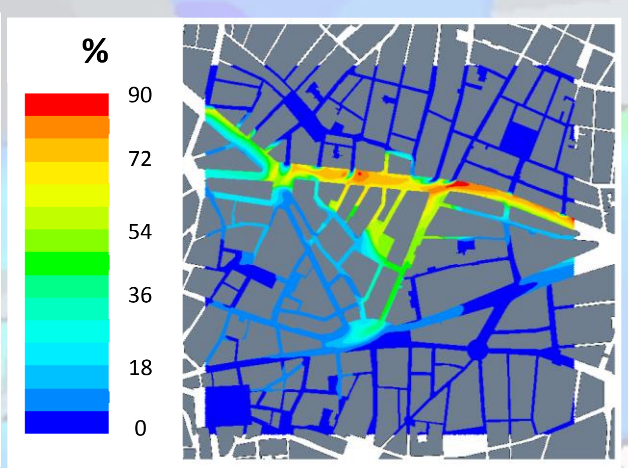
Objective with CFD model: Evaluation at microscale of traffic restriction (one hour simulated)



NO_2 predicted on December 29th 2016 (20-21 hours) in the Gran Vía area considering traffic restrictions (stage 3)



Avoided NO_2 concentration increase in Gran Via due to the NO_2 Protocol on December 29th 2016 (20-21 hours) according to CFD simulations (% relative to the baseline –no action- scenario)



NO_2 concentration reduction under the **hypothetical scenario of closing Gran Vía Street to road traffic**

TECNAIRE PROJECT

Comunidad de Madrid

Reference: Borge R, Santiago JL, de la Paz D, Martín F, Domingo J, Valdés C, Sanchez B, Rivas E, Rozas MT, Lazaro S, Pérez J, Fernandez A, 2018. Application of a short term air quality action plan in Madrid (Spain) under a high-pollution episode-Part II: Assessment from multi-scale modelling. *Science of The Total Environment*, *635*, 1574-1584.

Q2: How to derive AQD statistic (annual averages, percentiles) with CFD models

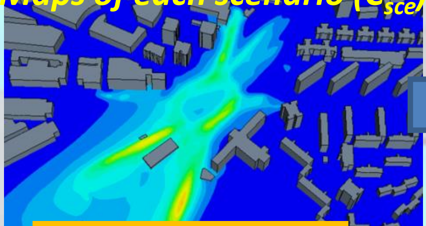
- Nowadays, **impossible to run unsteady simulations for one year with CFD** (huge computational cost).
- Solution? Computing averages and percentiles from a set simulated representative scenarios.
- How many scenarios? Depends on the available data.
- **Simplest option when**:
  - No traffic (main source) emission data but at least annual street traffic intensity
  - Meteorological data (wind) of a meteorological station or a mesoscale model for a year
  - Pollutant concentration data from air quality station in the modelling domain and from background stations (or a mesoscale CTM model) close to the domain for a year.

Database of CFD simulations:
- 16 wind directions
- Same wind speed
- Emission proportional to traffic intensity

Annual meteorological statistics
Hourly wind direction and wind speed frequencies from meteo station or mesoscale model

Adding urban background concentration AQ station or model
$C_{tot} = C_{loc} + C_{back}$

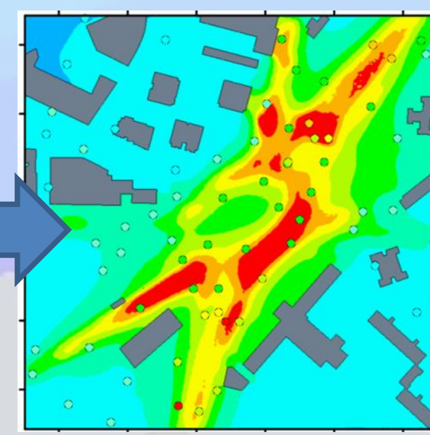
Maps of each scenario (C_{sce})



16 concentrations maps (scenarios)

Weighted average

WA CFD-RANS methodology



Correction of scenario maps for hourly wind speed:
$C_{loc} \sim (1/v)\, C_{sce}$

Calibration of concentration maps using concentration measured in a urban AQ station

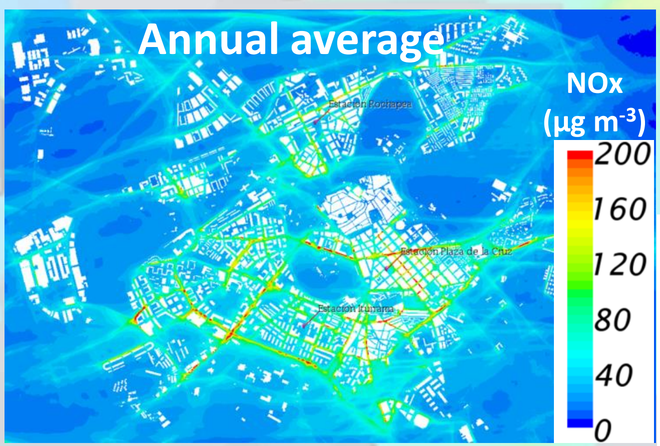
Q2: How to derive AQD statistic (annual averages, percentiles) with CFD models

Experiences in Spain

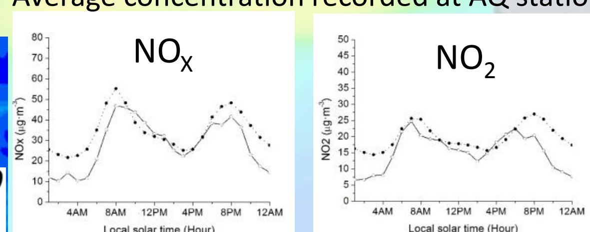
- **Pamplona**: Meteorological station (reference velocity: wind speed), no background. 7 x 5 km^2 approx. (a complete medium city)

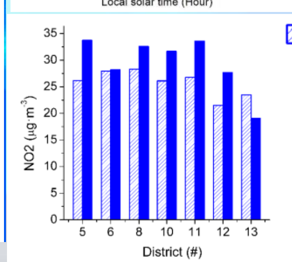
Objective: High resolution maps of annual average of NO_X and NO_2 throughout the entire city. Application to spatial representativeness and health impacts.

- 16 simulations for different wind directions.
- Meteorology from a station. Wind speed is used as reference velocity to composed the annual average maps and hourly maps of annual average day.
- Calibration with data from one AQ station
- NO_X maps neglecting chemistry. To compute NO_2 maps without simulating chemistry the ratio **NO_2/NO_X recorded at a traffic AQ station is applied to NO_X maps**.
- Evaluation with data from the two remaining AQ stations and sensors carried by cyclists (Relative errors < 30%).

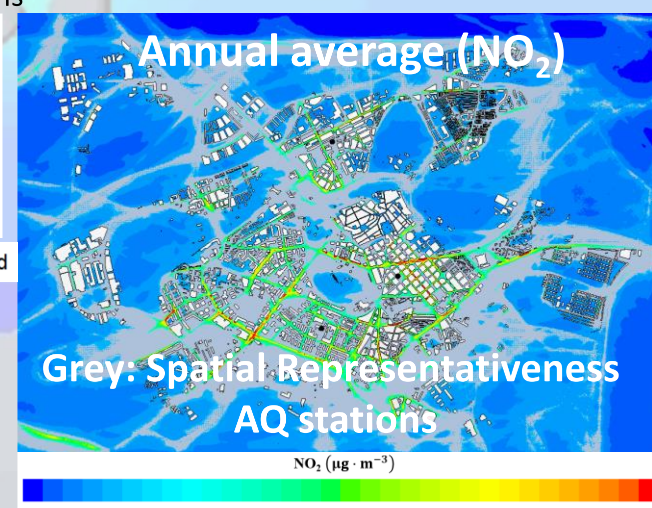


Average concentration recorded at AQ stations





NO_2 Average concentration measured by cyclist during 2016 in different neighbourhoods.



Reference: Rivas E, Santiago JL, Lechón Y, Martin F, Ariño A, Pons JJ, Santamaría JM. Progress in urban air quality assessment: CFD modelling of a whole city in Spain. *Science of the Total Environment* (under review).

Q2: How to derive AQD statistic (annual averages, percentiles) with CFD models

- Nowadays, **impossible to run unsteady simulations for one year with CFD** (huge computational cost).
- Solution? Computing averages and percentiles from a set simulated representative scenarios.
- How many scenarios? Depends on the available data.
- **More complex option** when:
  - Good emission data, for example, from traffic emission models which provides emission data depending on time of the day/ labour day, weekend day/ season, etc. This data can be grouped in *N* emission scenarios.
  - Meteorological data (wind) of a meteorological station or a mesoscale model for a year
  - Pollutant concentration data from air quality station in the modelling domain and from background stations (or a mesoscale CTM model) close to the domain for a year.

Database of CFD simulations:
- 16 wind directions
- Same wind speed
- *N* hourly emission scenarios

Maps of each scenario (C_{sce})

16 x *N* concentrations maps (scenarios)

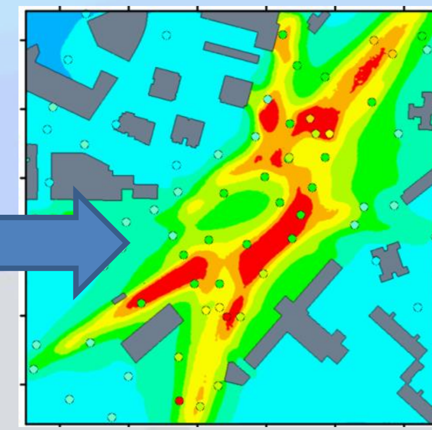
Meteorological data
Hourly wind direction and wind speed **data** from meteo station or mesoscale model

Adding urban background concentration AQ station or model
$C_{tot} = C_{loc} + C_{back}$

Estimated hourly concentration maps

Correction of scenario maps for hourly wind speed: $C_{loc} \sim (1/v)\, C_{sce}$

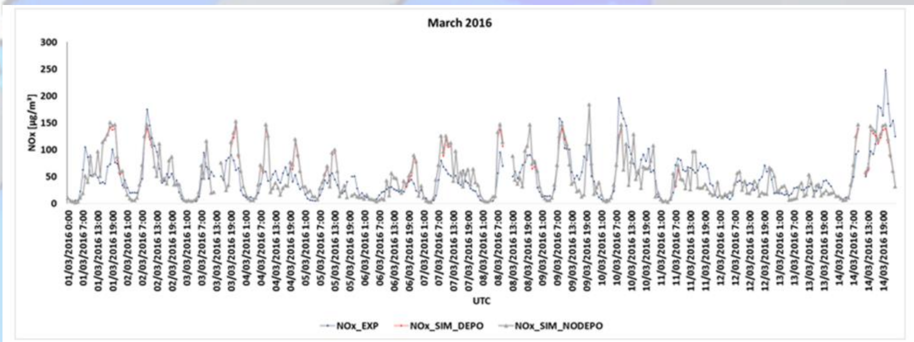
Annual average of hourly maps



Q2: How to derive AQD statistic (annual averages, percentiles) with CFD models

Experiences in Spain

- **Plaza de la Cruz (Pamplona)**: Meteorological station (reference velocity: wind speed), no



Objective: Effect of urban vegetation on NOx. Average NOx during two weeks considering vegetation deposition.

Reference: Santiago JL, Rivas E, Sanchez B, Buccolieri R, Martin F, 2017. The Impact of Planting Trees on NOx Concentrations: The Case of the Plaza de la Cruz Neighborhood in Pamplona (Spain). Atmosphere 8, 131.

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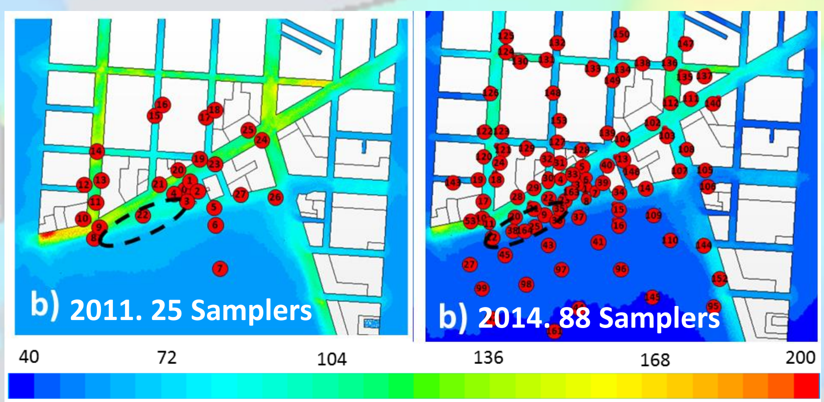
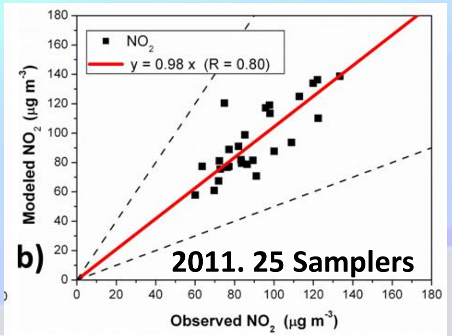
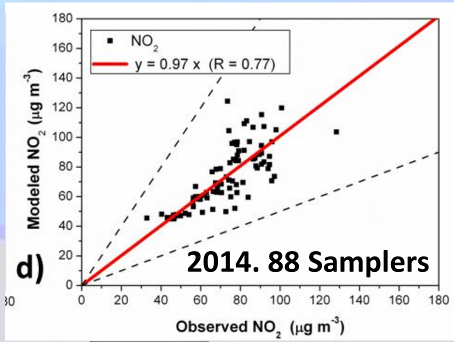
- **Escuelas Aguirre (Madrid):** Meteorological station (reference velocity: wind speed), urban background monitoring station.

Objective: Evaluation methodology to compute NO_2 long time average by CFD modelling. Two experimental campaigns of passive samplers. Winter → Chemistry neglected







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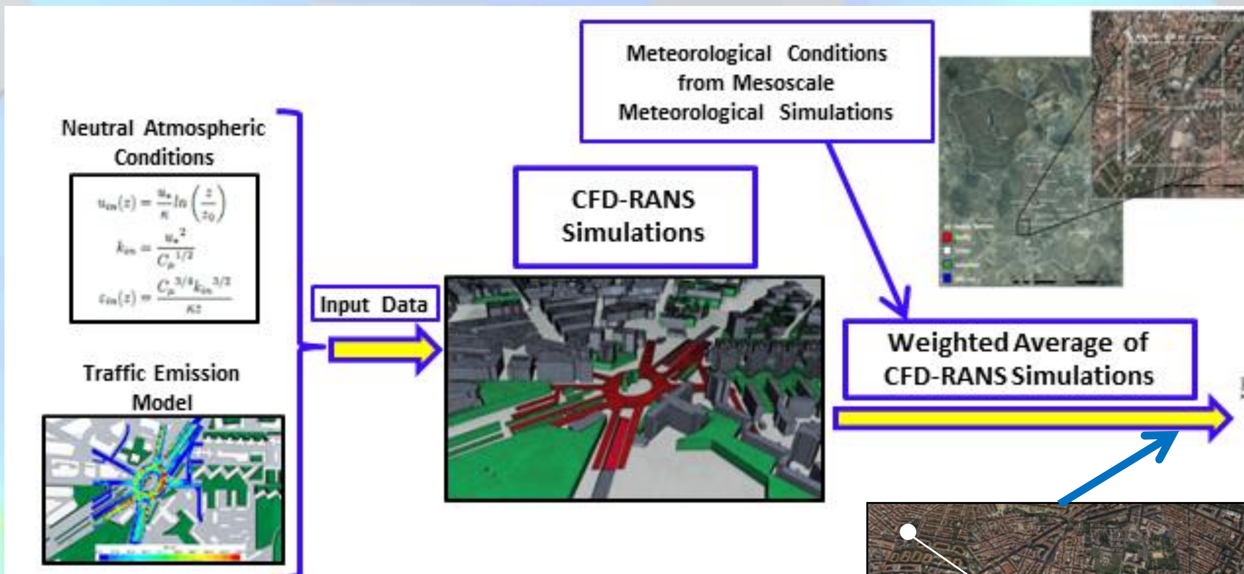
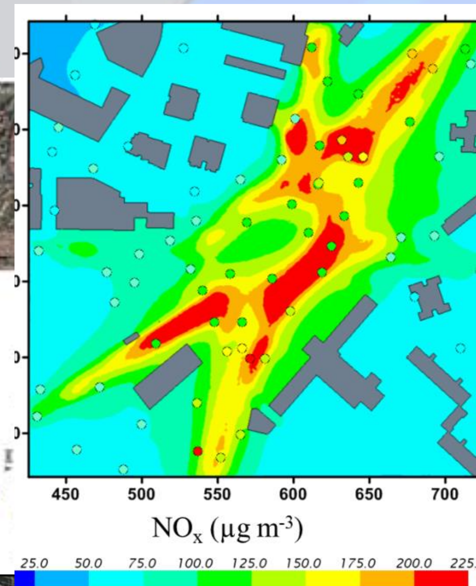
Q2: How to derive AQD statistic (annual averages, percentiles) with CFD models

Experiences in Spain

- **Plaza Elíptica (Madrid):** Meteorological mesoscale model, Meteo station, urban background monitoring stations.

Objective: Methodology using mesoscale model information.

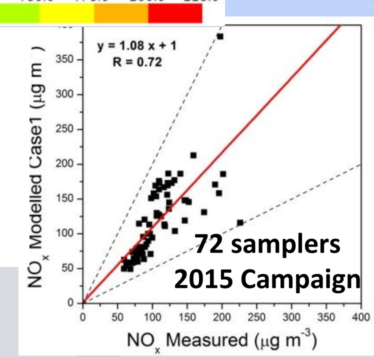




NOX Average Map

Better results Reference Velocity → Friction Velocity from mesoscale model

Background concentration from Urban Background Station



Reference: Sanchez B, Santiago JL, Martilli A, Martin F, Borge R, Quaassdorff C, de la Paz D, 2017. Modelling NOx concentration through CFD-RANS model in an urban hot-spot using high resolution traffic emissions and meteorology from a mesoscale model. Atmospheric Environment 163, 155-165.

Q3: Quality of CFD calculations in formal AQ assessment

- Problems of microscale validation
  - Strong spatial concentration gradients and usually few experimental data available.
- Experimental data:
  - Air quality monitoring stations:
    - Usually only one point in the numerical domain.
    - Provide time evolution of concentration at this location
  - Experimental campaigns:
    - Passive samplers:
      - Usually study area is covered by a high number of samplers
      - NO_2 averaged during several weeks. No time evolution.
    - Monitors and DustTrack (Particle Matter)
      - Point and paths concentration measurements
      - Time evolution of concentration
    - Sensors (NO_2)
      - More uncertainty in comparison with other experimental techniques.
      - Time evolution.

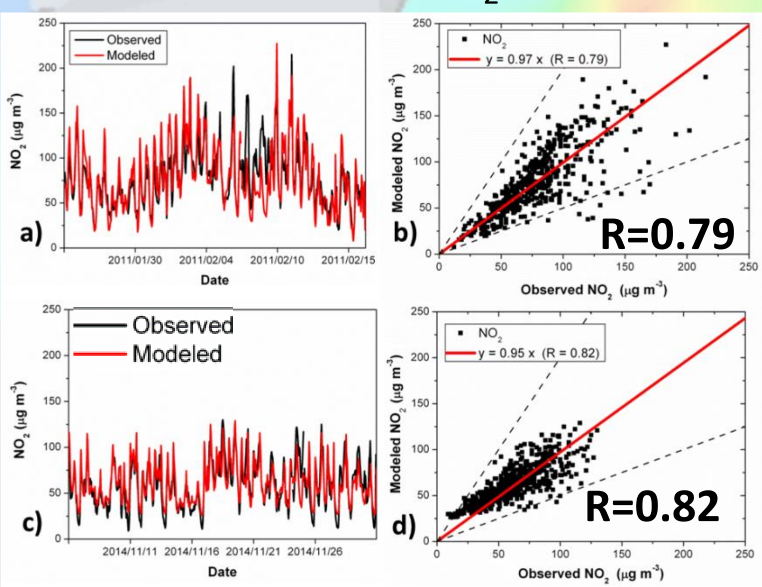
Q3: Quality of CFD calculations in formal AQ assessment

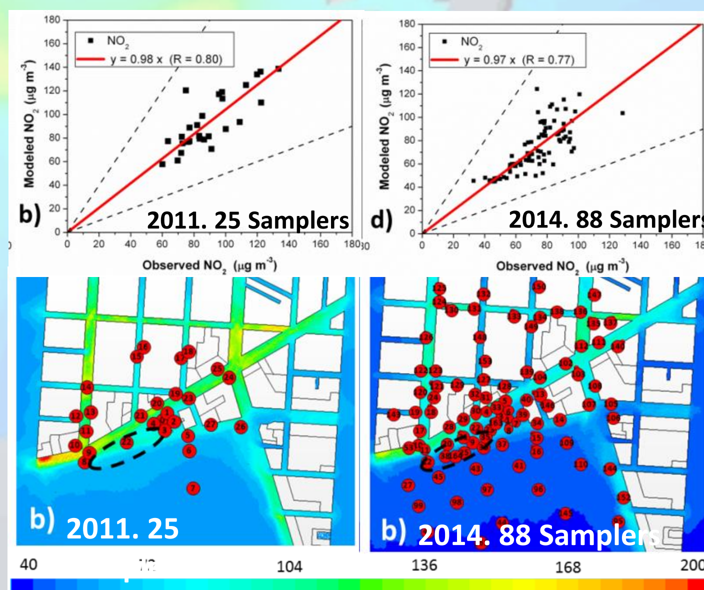
- Validations:
  - Statistics used: NMSE, FB, FAC2, R
  - Difficult to define standard values for a “good” model performance. We usually used Chang et al. (2005) criteria (NMSE<1.5 ; -0.3<FB<0.3)
  - Graphical representations: scatter plots, time series.

Experiences in Spain

- Escuelas Aguirre (Madrid): Passive samplers and AQ monitoring station (NO_2)

Time evolution NO_2 AQ station





Time average NO_2 concentration at location of Passive samplers AQ station

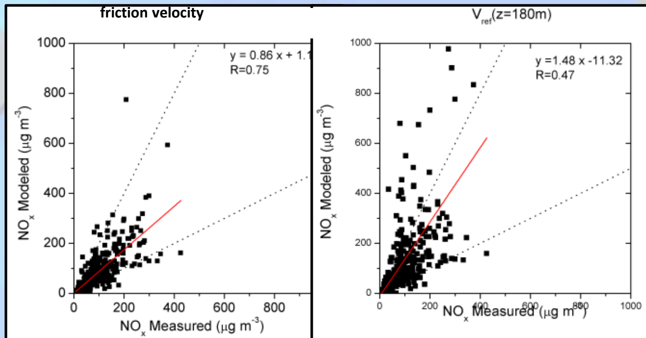
Reference: Santiago JL, Borge R, Martin F, de la Paz D, Martilli A, Lumbreras J, Sanchez B, 2017. Evaluation of a CFD-based approach to estimate pollutant distribution within a real urban canopy by means of passive samplers. *Sci. Total Environ.* 576, 46-58.

Q3: Quality of CFD calculations in formal AQ assessment

Experiences in Spain

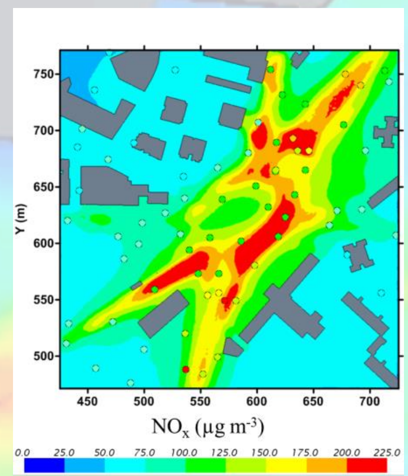
❑ Plaza Elíptica (Madrid): Passive samplers, monitors and AQ monitoring station. (NO_X, PM_{10})

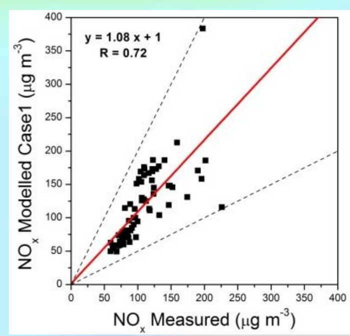
Time evolution NO_X AQ station



	$C_{mod}[u_*]$	$C_{mod}[V]$	Acceptance Criteria (Goricsan et al., 2011 and Chang et al., 2005)	
NMSE	0.28	2.40	<1.5	Good
FB	-0.13	0.29	-0.3 <0 <0.3	Good
R	0.75	0.47	0.5<R<0.8	Fair

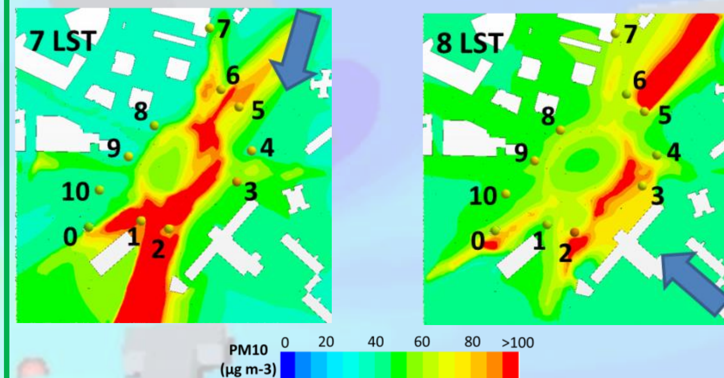
Time average NO_X samplers

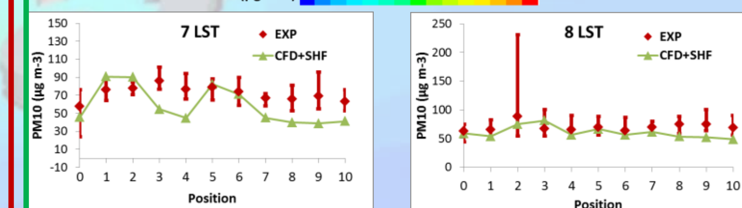




	Samplers	Acceptance Criteria	
NMSE	0.11	<1.5	Good
FB	-0.09	-0.3 <0 <0.3	Good
R	0.72	0.5<R<0.8	Fair

PM_{10} recorded by DustTrack (different time)





WINTER+ SUMMER	PM10 (CFD)	PM10 (CFD+SHF)
NMSE	0.48	0.085
FB	0.17	-0.15
FAC2	0.84	0.89

Reference:

Sanchez B, Santiago JL, Martilli A, Martin F, Borge R, Quaassdorff C, de la Paz D, 2017. Modelling NOx concentration through CFD-RANS model in an urban hot-spot using high resolution traffic emissions and meteorology from a mesoscale model. Atmospheric Environment 163, 155-165.

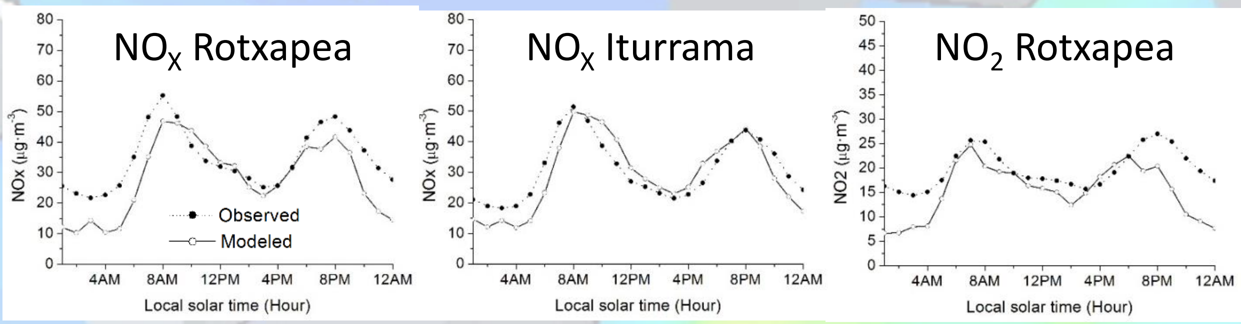
Santiago JL, Sanchez B, Martin F, Martilli A, Quaassdorff C, de la Paz D, Borge R, Gómez-Moreno FJ, Artiñano B, Yagüe C, Blanco C, Vardoulakis S, 2017. CFD modelling of particle matter dispersion in a real hot-spot. HARMO18. Bologna, Italy.

Sanchez B, Santiago JL, Martin F, Martilli A, Quaassdorff C, de la Paz D, Borge R, 2017. Modelling reactive pollutants dispersion in an urban hot-spot in summer conditions using a CFD model coupled with meteorological mesoscale and chemistry-transport models. HARMO18. Bologna, Italy.

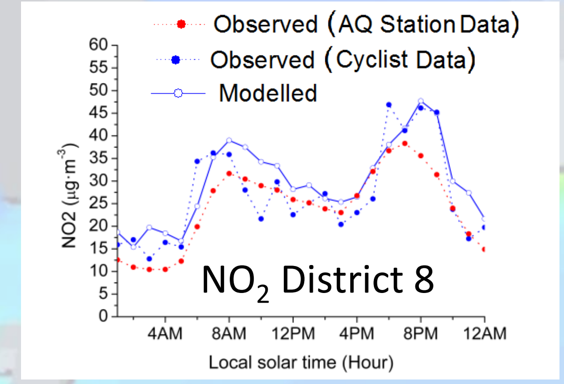
Experiences in Spain

- Pamplona (entire city modelled): Sensors and air quality monitoring stations (NO_X, NO_2)

Time evolution NO_X and NO_2 AQ stations of 2016 average day

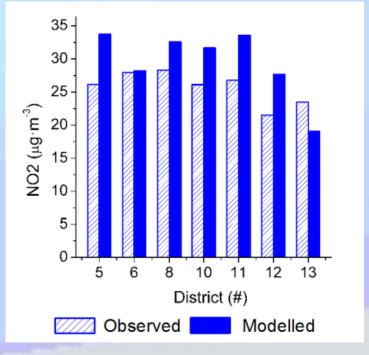


NO_2 cyclists with microsensorshours



AbsoluteError[µg·m^{-3}] / RelativeError [%]	Rotxapea		Iturrama
	NO_X	*NO_2*	*NO_X*
2016-average annual map	-6.6 / 19.1	-4.4 / 22.5	-1.5 / 4.9
2016-average spring map	-4.4 / 19.3	-3.7 / 23.1	-2.4 / 11.1
2016-average summer map	-1.1 / 8.1	-2.7 / 25.4	-3.0 / 17.9
2016-average autumn map	-11.4 / 22.2	-7.7 / 28.6	-2.0 / 4.7
2016-average winter map	-14.9 / 29.7	-6.6 / 26.1	-4.8 / 11.0

	R	*NMSE*	*FB*	*FAC2*
NO_X (Rotxapea): 2016-average annual day	0.843	0.087	0.211	0.833
NO_X (Iturrama): 2016-average annual day	0.890	0.035	0.050	1
NO_2 (Rotxapea): 2016-average annual day	0.683	0.118	0.254	1



NO_2	*R*	*NMSE*	*FB*	*FAC2*
2016-average annual map	0.565	0.040	-0.136	1

Reference:

Rivas E, Santiago JL, Lechón Y, Martin F, Ariño A, Pons JJ, Santamaría JM. Progress in urban air quality assessment: CFD modelling of a whole city in Spain. *Science of the Total Environment* (under review).

Rivas E, Santiago JL, Lechón Y, Martin F, Ariño A, Pons JJ, Santamaría JM. Progress in urban air quality assessment: CFD modelling of a whole town in Spain. HARMO18. Bologna, Italy.

Open questions

- How to validate CFD model: Need of data of field experiments:
  - Madrid. TECNAIRE project. Passive sampler, AQ monitoring stations, Dust-track,
  - Pamplona. LIFE RESPIRA project. Sensors, AQ monitoring stations, black carbon monitoring
  - Alcobendas. LIFE MINOx project. AQ monitoring.
- Uncertainties depending on atmospheric conditions, hour of day, season of year,…. Data from one met station or a model are well representative of atmospheric conditions?
- Uncertainties in local emissions. Main source of uncertainty?
  - Micro-emission model?
  - Traffic intensity + daily profiles + emission factors , then CFD
  - Traffic intensity , CFD and output calibration with traffic AQ station data?
- How these uncertainties affect to compute annual average for AQ assessment?
- How these uncertainties affect to reproduce high pollution episodes?
- Other ideas to couple local scale with mesoscale?
- Other processes: vegetation, thermal fluxes,…
- Need of chemistry schemes? Simple schemes as photostationary?
- Applications of CFD modelling,
  - High resolution maps → e.g. AQ assessment and spatial representativeness of AQ stations
  - Testing air pollution abatement strategies
  - Population exposure?

Thank you for your attention

- Borge R, Santiago JL, de la Paz D, Martín F, Domingo J, Valdés C, Sanchez B, Rivas E, Rozas MT, Lazaro S, Pérez J, Fernandez A, 2018. Application of a short term air quality action plan in Madrid (Spain) under a high-pollution episode-Part II: Assessment from multi-scale modelling. *Science of The Total Environment*, *635*, 1574-1584.
- Rivas E, Santiago JL, Lechón Y, Martin F, Ariño A, Pons JJ, Santamaría JM. Progress in urban air quality assessment: CFD modelling of a whole city in Spain. *Science of the Total Environment* (under review).
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- Sanchez B, Santiago JL, Martilli A, Palacios M, Pujadas M, Nuñez L, German M, Fernandez-Pampillon J, Iglesias JD, 2016. CFD Modeling of Reactive Pollutants Dispersion and Effect of Photocatalytic Pavements in a Real Urban Area. *HARMO17 Conference*. Budapest, Hungary.
- Sanchez B, Santiago JL, Martin F, Martilli A, Quaassdorff C, de la Paz D, Borge R, 2017. Modelling reactive pollutants dispersion in an urban hot-spot in summer conditions using a CFD model coupled with meteorological mesoscale and chemistry-transport models. *HARMO18*. Bologna, Italy.
- Santiago JL, Borge R, Martin F, de la Paz D, Martilli A, Lumbreras J, Sanchez B, 2017. Evaluation of a CFD-based approach to estimate pollutant distribution within a real urban canopy by means of passive samplers. *Sci. Total Environ.* 576, 46-58.
- Santiago JL, Sanchez B, Martin F, Martilli A, Quaassdorff C, de la Paz D, Borge R, Gómez-Moreno FJ, Artiñano B, Yagüe C, Blanco C, Vardoulakis S, 2017. CFD modelling of particle matter dispersion in a real hot-spot. HARMO18. Bologna, Italy.
- Santiago JL, Rivas E, Sanchez B, Buccolieri R, Martin F, 2017. The Impact of Planting Trees on NOx Concentrations: The Case of the Plaza de la Cruz Neighborhood in Pamplona (Spain). *Atmosphere* 8, 131.

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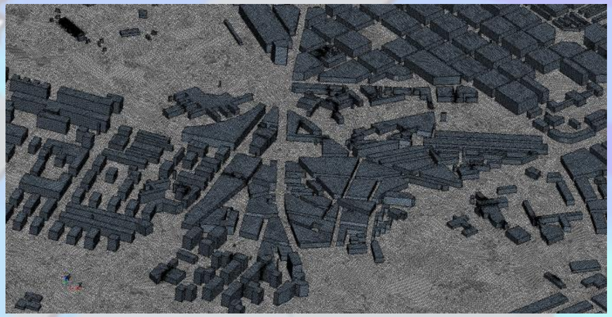
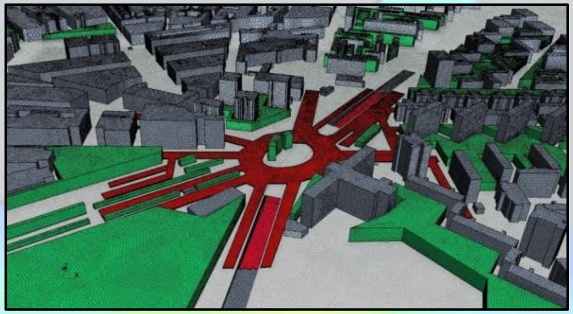
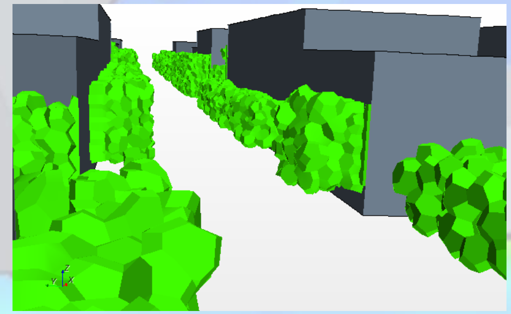
Q2: How to derive AQD statistic (annual averages, percentiles) with CFD models

- Nowadays, **impossible to run unsteady** simulations for **one year** with CFD (several millions of computational cells). **Solution?**





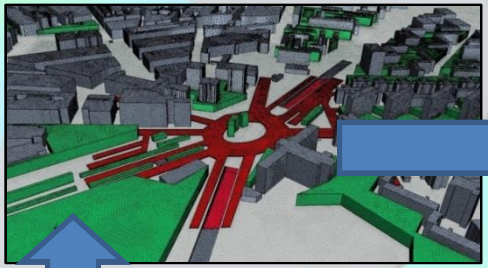


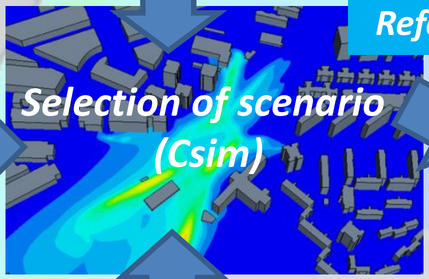
Proposal: **WA CFD-RANS methodology**

Database CFD simulations:
- 16 wind directions
- Emissions scenarios
- One wind speed

Meteorological conditions at each hour from:
- meteo station or
- mesoscale model

Urban background at each hour from:
- AQ station or
- mesoscale model



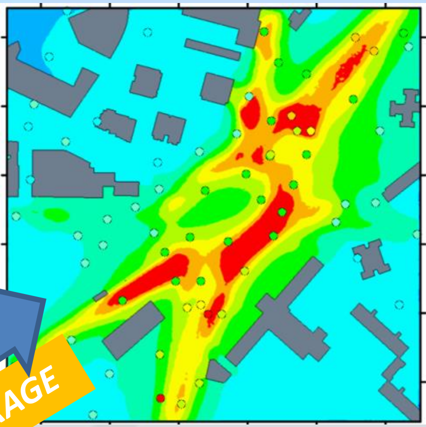


Reference velocity

Cmod_Local + Cbackg

Cmod (t=h)

AVERAGE



Hourly Emissions scenarios

Hour and Day