





Ciemol MINISTERIO DE CIENCIA INNOVACIÓ

Centro de Investinci

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FAIRMODE TECHNICAL MEETING 2021 CT4 – Microscale modelling session

F. Martin (CIEMAT), S. Janssen (VITO)

October 7th, 2021

Agenda

- 10:45 –11:00 Status of the intercomparison exercise
- 11:00 –11:30 Modelling group's presentations
- 11:30 –12:00 First look at the results
- 12:00 12:45 Discussion
- 15:00 –15:30 Wrap-up & next steps.

Status of the intercomparison exercise

- The aim is to compare methodologies for deriving annual statistics (using microscale modelling) to identify best practices.
- Participant groups:

ENEA, VITO, NILU, IVL, RIVM, RICARDO, CERC, Aveiro University, University of West Macedonia (UOWM), Széchenyi István University (SZE), Aarhus University, UPM and CIEMAT.

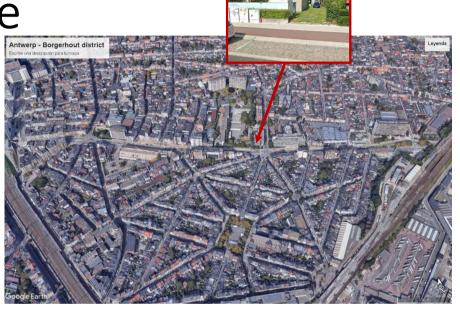
- Design of the exercise during second half of 2020
- Started in March 2021
- Delivery of modelling results along September 2021

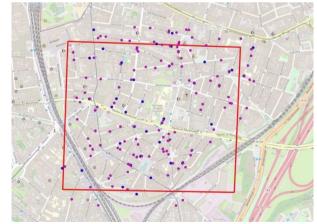
Models and methodologies:

- Many are using CFD models (RANS mostly) but there are also other type of models (parametric, lagrangian, etc).
- Different methods for computing annual indicators of pollutant concentrations.
 - Methods based on simulating a set of selected scenarios (wind scenarios and/or emission scenarios) and then a postprocessing (PDF of scenarios, rebuilding a entire year, etc) of model results for retrieving annual indicators.
 - Methods based on simulating the complete year, which is mostly for the case of no CFD models but some of them run CFD models a complete year.

Exercise details:

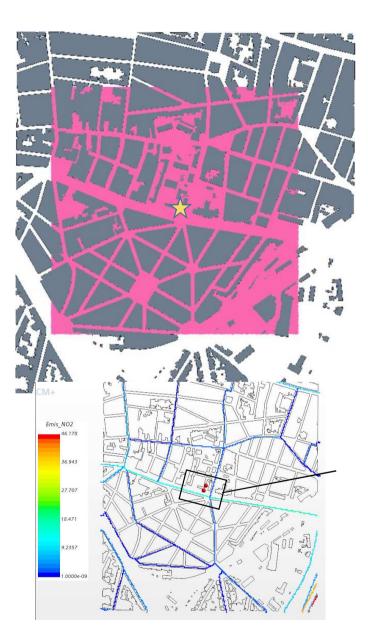
- Firstly focused on the Antwerp (Belgium). NO₂
 - Area around two air quality stations.
 - Used in a FAIRMODE spatial representativeness intercomparison exercise in 2016.
 - Urban morphology, emission data from traffic, meteorological data and air quality data (two stations and passive NO₂ samplers (VITO).
 - Campaign of 2016 (April 30 May 28) selected.
 - Precomputed NO₂ and PM10 CFD simulations for 16 scenarios corresponding to 16 wind sectors (CIEMAT).
- Extension to other city as Gyor (Hungary) should be foreseen for 2022.
- Possible future extension to PM10 or PM2.5 as well.





Exercise details:

- A similar domain would be used for all the groups.
- Each group could decide the model domain and resolution of their simulations and computations.
- It should be good to finally give results in a common mesh for all, but not mandatory.
- The precomputed CIEMAT CFD simulations are for a domain of 800 m x 800 m (pink area) centered at the traffic AQ station (yellow star) with a resolution of 1m x 1m close to obstacles approx.
- Pollutant emission from traffic.



Exercise details:

3 steps:

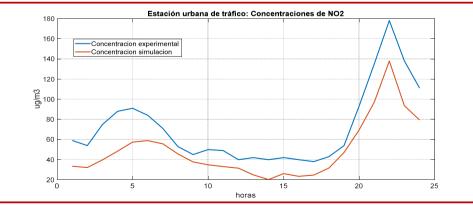
- 1. To simulate a selected day/episode from one of the one-month passive sampler campaigns.
 - Good for <u>comparing only modelling results</u> before applying the annual indicators methodologies.
- 2. To compute averages (concentration maps) for the complete campaign period applying the methodologies of each group.
 - Aim to *intercompare results from every methodology*.
- **3.** To compute averages (concentration maps) for one complete year applying the methodologies of each group.
 - Aim to *intercompare results from every methodology*.

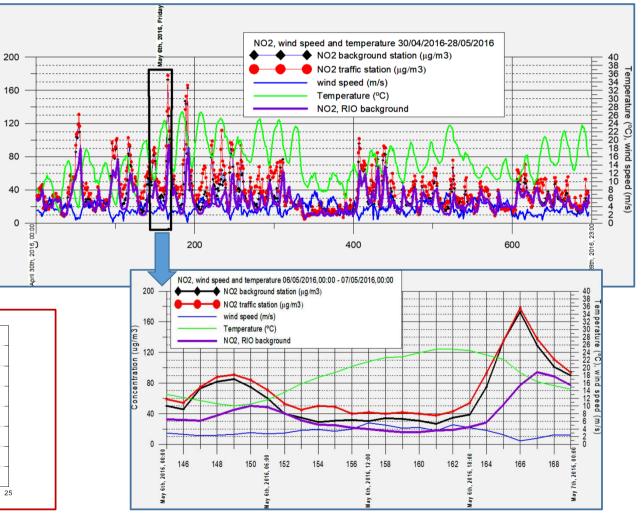
tion (ug/m3)

Exercise details:

3 steps:

- 1. To simulate a few selected hours from the one-month passive sampler campaigns.
 - May 6th, 2016 selected to simulate.
 - The model results would be compared with AQ stations data
 - Models results would be intercompared.

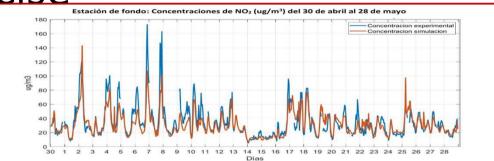




Exercise details:

3 steps:

- 2. To compute averages (concentration maps) for the complete campaign period (April 30 – May 28) applying the methodologies of each group.
 - 1. Comparison with passive samplers' data and AQ station data
 - 2. Intercomparison among models results.



Mapa promedio de NO₂ del 30 de abril al 28 de mayo-Promedio considerando intervalos de velocidad de viento



Exercise details:

3 steps:

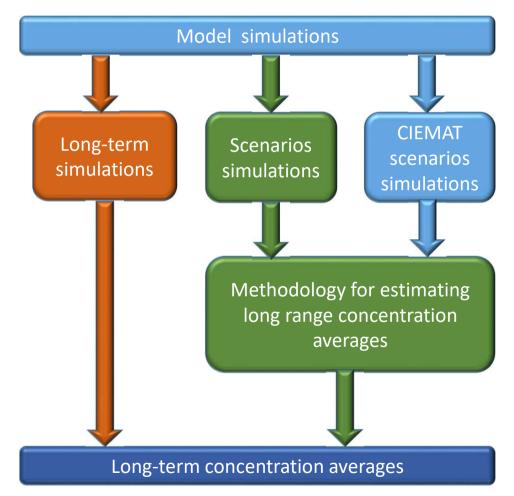
3. To compute averages (concentration maps) for 2016 year applying the methodologies of each group.

> Intercompare results from every methodology.



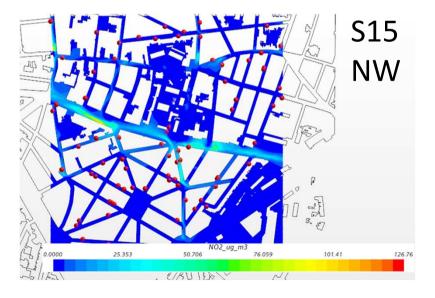
Ways of participating in the exercise:

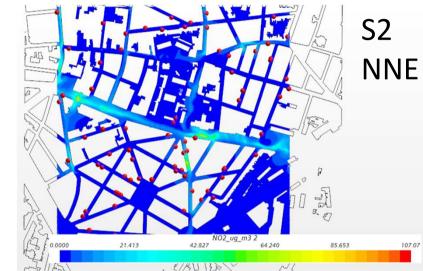
- Running your own model for the complete period.
- Running your own model for representative scenarios and then applying your own methodology for computing long term concentration indicators.
- Using the precomputed simulations of CIEMAT as starting point for applying a methodology for estimating long-term averages of pollutant concentration.

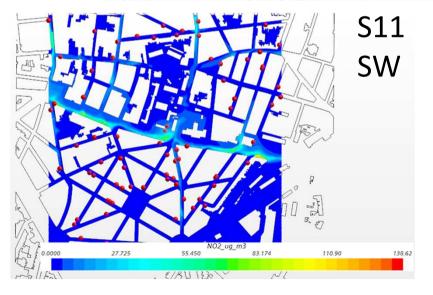


Precomputed CIEMAT CFD simulations:

- Simulations sent to participants, who required this information.
- 16 concentrations maps (one per direction sector) for anual averaged emissions of NO₂ and NOx







Timing

- Input data collection → February 2021
- Modeling simulations and methodology computations
 March June 2021
- Sending results

 September 2021
- Statistical intercomparison
 End 2021-Early 2022 (Hackathon)??
- Presentation of results
 → February/March 2022 (Plenary meeting)??

Status of results' reception

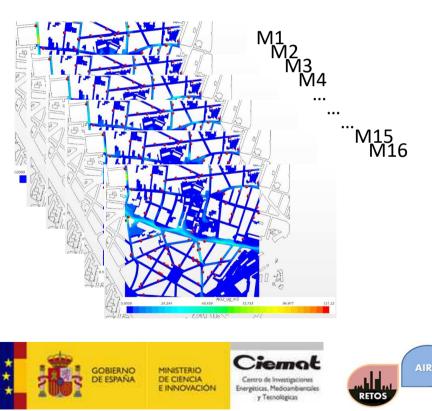
GROUP	STEP1	STEP2.1	STEP2.2	STEP3	Model	Methods for averaging
CIEMAT	Х	Х	Х	х	CFD/STAR CCM+	3 techniques (wind scenarios)
CERC	х	Х	Х	Х	ADMS-URBAN	Running model Processing CIEMAT CFD data
UOWM	Х	х	х	х	CFD/ADREA HF	Running model
ENEA	Х	Х	Х	х	Micro-SWIFT-SPRAY (PMSS)	Running model
NILU	Х	Х	Х	х	EPISODE	Running model + interpolation
SZE	х	х	Х	х	CFD/OPENFOAM CFD/ANSYS	Running models (2 results OPEN FOAM/ 1 ANSYS)
UPM	х	Х	х	х	CFD-LES PALM-4U	Representative day
VITO	Х	х	х		CFD-RANS	Averaging hourly maps Wind statistics
	х	Х	Х	х	ATMO-Street model	Running models
RICARDO				х	RapidAir	Running model (all Antwerp)
Aveiro Univ	0	0	0	0	CFD/VADIS CFD/OPENFOAM	Typical days Meteo and emission scenarios

IVL, Aarhus University, RIVM he resigned to participate

Modelling groups' presentations about used methodolgies

Methodology for Retrieving Annual Average Concentrations

Database of CFD simulations: 16 wind directions for a fixed inlet wind speed and annual average traffic emissions



<u>Methodology 1</u>: Using frequency (f_i) and mean wind speed (Vmean,i) for each wind direction (i).

$$M_{av} = \sum_{i=1,16} M_i \frac{Vref, CFD}{Vmean, i} f_i + C_{backg, av}$$

Methodology 2: Similar to methodology 1 but also considering 6 intervals of wind speed (v<1m/s; 1<v<2....;v>5m/s) for each wind direction.

$$M_{av} = \sum_{i=1,16} \sum_{j=1,6} M_i \frac{Vref, CFD}{Vmean, i, j} f_{i, j} + C_{backg, av}$$

<u>Methodology 3 (WA CFD-RANS)</u>: At each hour a concentration map is computed considering wind direction for selecting one map for the database and wind speed, traffic emission factors (TF) and background concentration at this hour for computing modelled concentration at this hour. For estimating annual average map, hourly maps are averaged.

$$M_{hour} = M_{i=WindDir(hour)} \frac{Vref, CFD}{Vhour} TF_{hour} + C_{backg,hour}$$

$$M_{av} = \frac{\sum_{hours} M_{hour}}{Nhours}$$

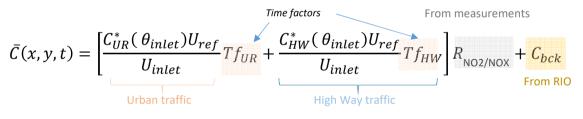


General:

- 72 RANS simulations at different angles [0:5:355] and same velocity U_{ref}
- Passive scalar equations:
 - o 1 passive scalar equation for urban traffic sources
 - o 1 passive scalar equation for high-way traffic source

Methodology for hourly averages

- Select closest wind direction 3 wind directions and do weighed average (account for hourly variability)
- Apply time factors for the 2 types of sources, NO2/NOx ratio and background



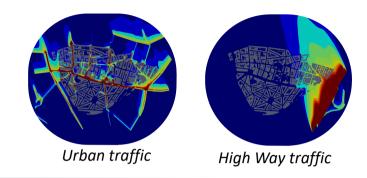
Methodology for Long term averages

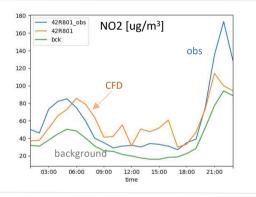
1) Averaging hourly maps

$$\bar{C}(x,y) = \sum_{h}^{N_{hours}} C(x,y,t) / N_{hours}$$

2) Using wind statistics

$$\bar{C}(x,y) = \sum_{\theta_{inlet}} \frac{C_{UR}^*(\theta_{inlet})U_{ref}}{U_{mean}} (P(\theta_{inlet})) + \sum_{\theta_{inlet}} \frac{C_{HW}^*(\theta_{inlet})U_{ref}}{U_{mean}} (P(\theta_{inlet}))$$







11/10/2021 ©VITO – Not for distribution

UOWM Methodology for the Antwerp data

- Neutral stability approximation
- <u>Fixed 32 directions</u> reference steady state CFD Simulations with UREF=5.0m/s and annual mean traffic emission rate : *MREF array*
- Hourly concentrations M_{hour} at a specific 'sensor' using :
- the wind speed and traffic emission factor given at the specific hour
- > the reference concentrations at the specific i-direction $MREF_i$ derived by interpolation from the CFD MREF array.

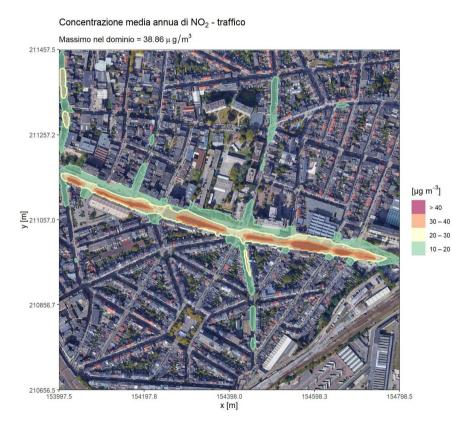
 $M_{hour} = MREF_i \frac{UREF}{Vhour} TF_{hour} + C_{backg,hour}$

$$M_{av} = \frac{\sum_{hours} M_{hour}}{Nhours}$$

ENEA

Methodology for Retrieving Annual Average Concentrations with the Model PMSS

Example of PMSS simulations:



Methodology: In order to calculate the annual average of the NO2 concentrations we simulated NO2 concentrations hourly over the entire year.

For this intercomparison exercise we performed the simulations on a regular grid with X from 153995 to 154797 and with Y from 210654 to 211456, at the resolution of 3m x 3m. Vertical levels are (in m): 0, 1, 4, 5, 7, 10, 15, 21, 50, 120, 220, 300, 500.

Since we did not implement the chemistry module, we calculated the NO2 concentrations from the simulated NOx concentrations using a simplified version of the relationship that is used by the RIO model for the background NO2, that we verified against the station's measurements.

One day simulation took on average 12 min for the meteo simulation and 15 min for the dispersion part, totaling 73 hrs for the meteo preprocessing + 90 hrs for the dispersion.

The post processing phase for transforming NOX to NO2 requires few seconds for each day, totaling 1 hour for the yearly simulation.

We are now studying a statistical tool to calculate the annual average from simulations of representative days.

- 'Advanced canyon' module within quasi-Gaussian plume dispersion model ADMS-Urban, allows for:
 - Recirculating (cross-wind) and channelling (along-wind) flow
 - Total building 'porosity' (not explicit representation of each building)
 - Canyon asymmetry height, width and/or porosity
 - Pavements and multiple lanes of traffic
 - Wide range of canyon height to width aspect ratios
 - Smooth transition between differing geometries
- Other relevant ADMS-Urban model features include:

Upstream wind U

Hourly temporal resolution

ADMS-Urban

CER

• Explicit photolytic NO_x chemistry scheme

- Meteorological pre-processor converts measured met. parameters into boundary layer profiles
- Hourly background concentrations: NO₂, NO_x, PM₁₀, PM_{2.5} and O₃
- GIS pre-processor derives street canyon parameters from 3D buildings dataset
- Some modifications to data provided:
 - Road nearest monitor modelled as 2 segments with different canyon properties & corrected centreline
 - Canyon widths were modified to ensure samplers were located within canyons, where appropriate
- Model output points at all monitor locations and on an irregularly spaced output grid for contour plots

	Source	Туре
1	Along canyon	Road with reflections
2	Across canyon	Simplified road
3	Recirculation	Well-mixed cells
4	Non-canyon	Road
5	Canyon-top	Volume
6	Canyon-end	Volume

Source data

- 1. CIEMAT CFD simulations:
 - 16 wind directions
 - Fixed inlet wind speed (measured annual average)
 - Annual average traffic emissions
- 2. Measured concentration time series: background, urban background, roadside

Motivation for bias correction methodology

- Meteorological conditions have a strong influence on pollutant dispersion: magnitude of wind speed has a near-inverse relationship with pollutant concentrations
- Pollutant concentrations in urban areas are strongly influenced by the temporal variations of traffic emissions
- Use pollutant measurements to quantify influence of meteorology / diurnal emissions variations on dispersion

Inconsistency between background & measurements impacts on methodologies that rely on quantification of 'urban increments'

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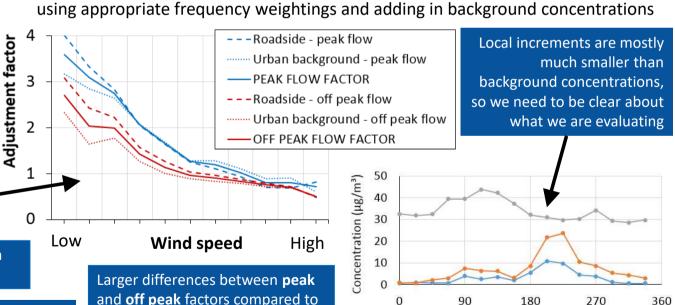
Methodology

- Define 11 wind speed bins with approx. same no. of hours in each bin
- Categorise each hour of the day as 'peak' or 'off-peak', resulting in 22 bins
- Calculate NO_x and NO₂ urban background and roadside increments by subtracting background concentrations from measurements (*note*: some negatives, set to zero)
- Calculate adjustment factors **per bin per measurement site for NO2** (and NOx) =

Land use regression?

Average measured incremental concentration within the bin

Average CFD concentration within the bin Derive spatially independent set of factors and use to scale CIEMAT CFD data,



and **off peak** factors compared to between **roadside** and **urban background** – supports method

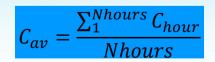
Wind direction (degrees) ---- Urban background ---- Background

EPISODE: 3D Eulerian grid model + Integrated gaussian dispersion model (no buildings)

- Meteorology: WRF meteo model with a 1km horizontal resolution and ~20m vertical resolution
 - **Traffic emissions**

$$C_{hour} = C_{grid,hour} + \sum_{1}^{Nroads} L_{hour}$$

$$L = \frac{Emission}{Wind} \times \int_0^l gfdl$$



FAIRMODE CT4 MICROSCALE MODELLING NTERCOMPARISON EXERCISE

Roberto San José and Juan L. Pérez Environmental Software and Modelling Group Computer Science School - Technical University of Madrid (UPM) Campus de Montegancedo - 28660 Madrid (Spain) <u>http://artico.ma.fi.upm.es</u>



Environmental Software and Modelling Group http://artico.lma.fi.upm.es



Model: CFD LES PALM-4U (BMBF,DE) <u>https://palm.muk.uni-hannover.de/trac/wiki/palm4u</u> Photo-stationary Chemistry mechanism (NO2, NO, O3 and 2 reactions plus PM10 tracer)

Computational 3D domain: 200 x 200 x 70 (z) Vertical and horizontal spatial resolution 5 m. LL corner (Belge Lambert 72): X=153896, Y=210555 CPU Time: 10-12 hours (400 cores) by one day of simulation

Input datasets

Buildings and traffic emissions (CT4) Topography (20 m.) and type of trees (Antwerpn open data GIS)

https://portaal-stadantwerpen.opendata.arcgis.com/ Monthly and daily time profiles: (CT4) Hourly emission time profile: EMIMO-UPM

Meteorological and chemical initial and boundary conditions

WRF/Chem 25-5-1 km

Off-line nesting, BCs frequency 10 min. Wind components (u, v, w) Potential temperature and humidity Soil temperature and moisture Pollutants concentrations



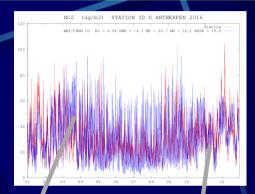


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METHODOLOGY FOR RETRIEVING MONTHLY AND ANNUAL AVERAGE CONCENTRATIONS MAPS (UPM-ESMG)

WRF/Chem 1 km & monitoring station data (one year, hourly temporal resolution)



Monthly representative day 01/05/2016

Daily avg station 30.0 Daily avg WRF/Chem 34.0 Monthly avg station 37.0 WRF/Chem daily R2 0.87

Annual representative day 11/11/2016

Daily avg station 41.5 Daily avg WRF/Chem 36.0 Annual avg station 42.0 WRF/Chem R2 0.76

The search of the representative day for the requested month/year average

1° BIAS of the station data daily average vs monthly/annual average value (min. < 30%)

2º BIAS of the WRF/Chem daily average vs station data monthly/annual average value . (min. < 30%)

 3° Correlation coefficient of hourly data of the WRF/Chem and station data for the representative day (min. > 0.6)

Run the CFD-LES PALM-4U during 24 hours of the representative day

The 24 hourly maps are hourly averaged to obtain one annual/monthly average map



Environmental Software and Modelling Group http://artico.lma.fi.upm.es



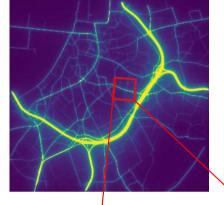
Ricardo RapidAir: Methodology to estimate annual concentrations

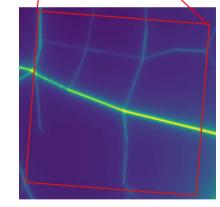
- RapidAir was used to predict 1 m gridded concentrations for Antwerp see ¹ for model details:
 - All hours of meteorology were used to run AERMET to produce hourly SFC and PFL files for the year
 - An idealised annual dispersion kernel was produced using AERMOD
 - Using convolution, the dispersion kernel was passed over gridded road emissions to directly generate <u>1 m gridded annual average concentrations</u>
 - Street canyons were accounted for using the AEOLIUS canyon model
- RapidAir models were produced for urban, rural and highway roads separately, then the concentrations grids were added together to get the total road NOx
- Modelled annual average road concentrations were combined with annual average background concentrations to produce total NOx concentrations
- The gridded concentrations for the FAIRMODE domain were clipped from the full city model
- Conversion of NOx to NO2 used the method published in the SHERPA model, assuming the Romberg coefficients²

$$NO2 = NOx * \left(\left(\frac{103}{NOx + 130} + 0.005 \right) * 1.2 \right)$$

The RapidAir dispersion model has been designed to address the operational needs of clients to produce highly spatially resolved gridded estimates of concentrations in short run times without the need for large, expensive computing requirements.







¹ https://www.sciencedirect.com/science/article/pii/S1364815217307806?via%3Dihub

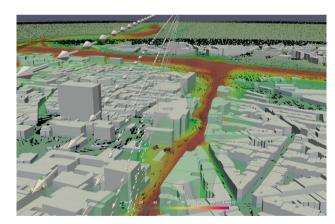
² <u>https://www.sciencedirect.com/science/article/pii/S1364815220309610</u>



Methodology used by the Széchenyi István University (SZE) HiDALGO-project team

- Software: **OpenFOAM**
- Mesh: Octree mesh with 3.3M cells, resolution: 2 meter at street level
- Air flow: Unsteady incompressible RANS with k-e turbulence model
 - Wind ABL boundary conditions (log-profile based on IE provided wind data)
 - Plant canopies are modelled by **porous zones**
 - Surface roughness = 0.1
- Pollutant dispersion
 - Emission: line source of NOx
 - Passive scalar model (linear advection-diffusion) for NOx (no reaction is computed)
 - Eddy diffusivity is a function of PBLH (PBL height) and nu_t (turbulent viscosity):
 D = D0 + m*PBLH*nu_t, m=0.03 is calibrated according to the validation results of May 6 (other formulas were tested as well, e.g. D as function of radiation, nu_t and Sc_t)
 - Post-processing forNO2 at time t_i and vertex x_j:
 - NO2(t_i, x_j) = NOx_simulated(t_i, x_j) * [NO2 / NOx](t_i, x_j)_measured-at-UBstation
 - NO2-sampler: NO2-average in time and in space near sampling points (within 5m distance)
- Computer: 8 node x (2 x 64) core AMD EPYC 7702 at Hawk, HLRS (Stuttgart)
- Runtime: 67 mins (IE-step 1), 23 hours 48 mins (IE-step 2)





CFD modelling to retrieve annual metrics

- Main modelling assumptions (neutral stability simulations, neglecting NOx chemistry)
- Steady-state simulations

VADIS	OpenFOAM
RANS	RANS
Steady	Steady
No chemistry	No chemistry
Regular and structured mesh	Unstructured Mesh
Turbulence closure scheme k- ϵ standard	Turbulence scheme k-ε

M1: Typical days

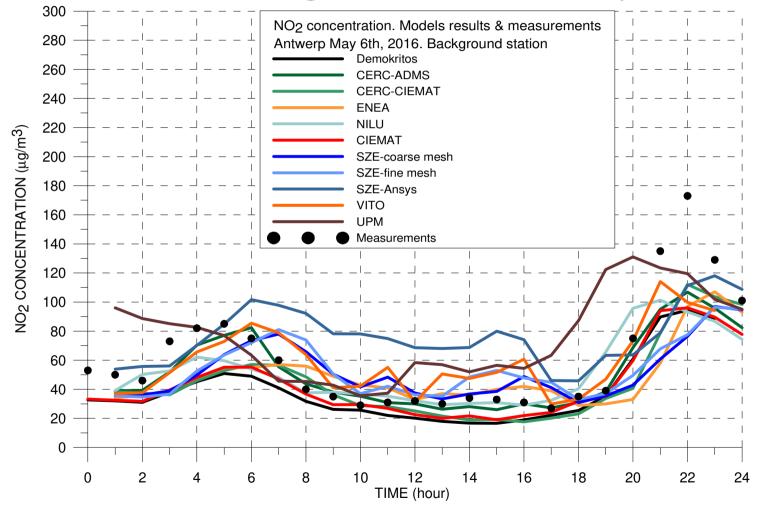
• Weighting factors from a set of air quality measurements

M2: Look-up table method

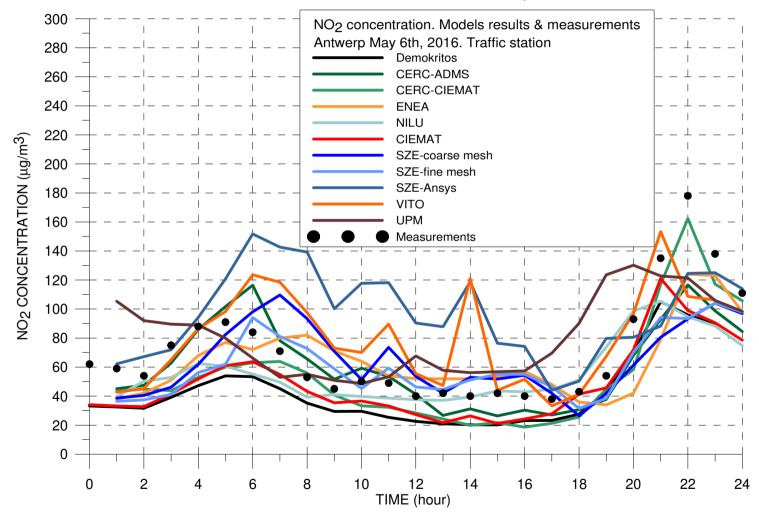
- Representative meteorological data: wind frequencies up to 75%
- Representative emission scenarios:
 - 3 5 scenarios

First look at the results

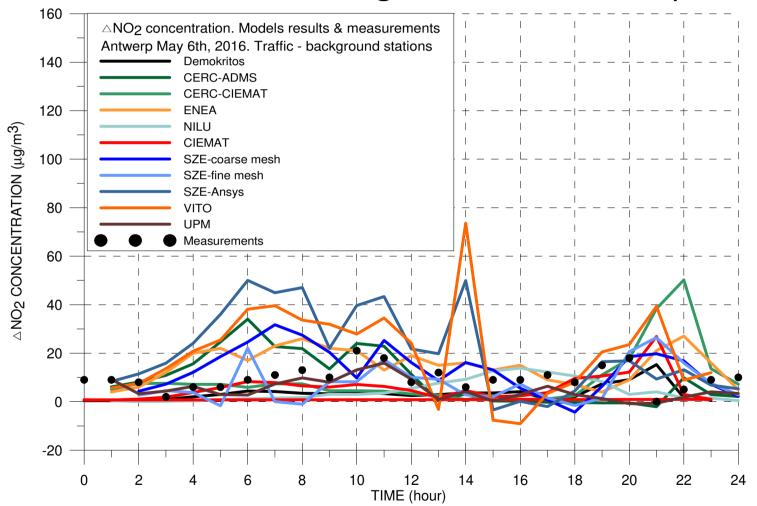
Step 1. Time series background station. May 6th, 2016



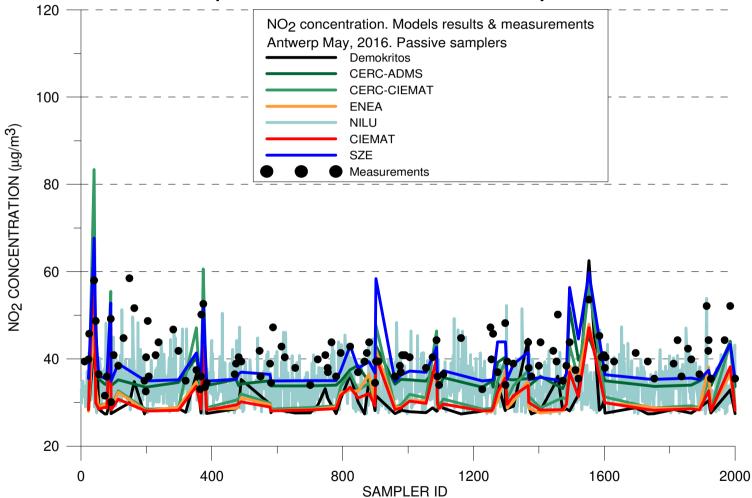
Step 1. Time series traffic station. May 6th, 2016



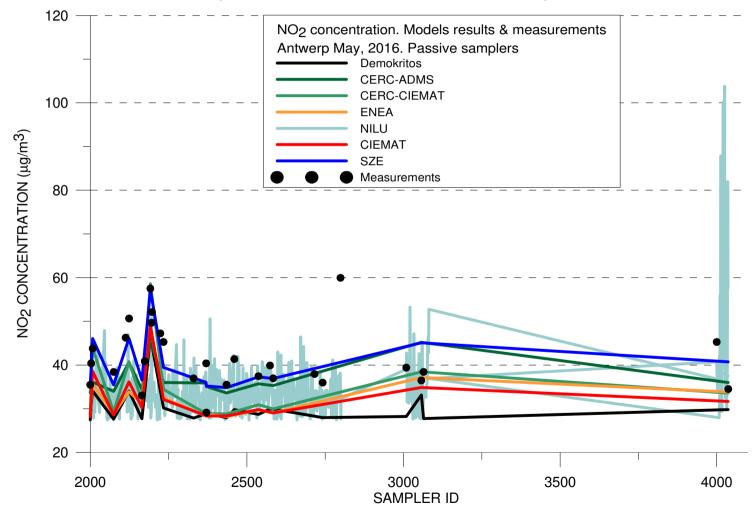
Step 1. Time series traffic – background stations. May 6th, 2016



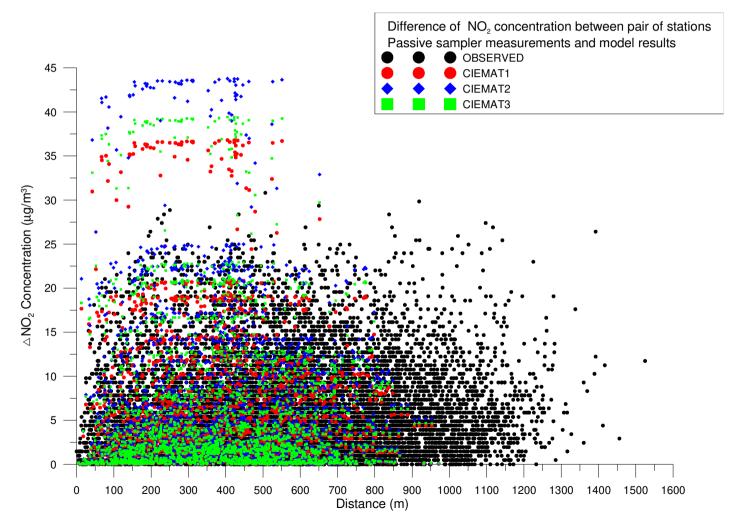
Step 2.1. Passive sampler location data. May 6th, 2016



Step 2.1. Passive sampler location data. May 6th, 2016



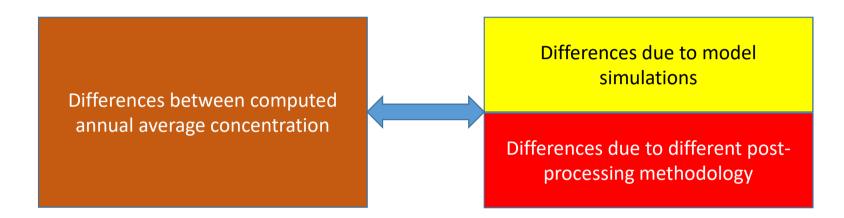
Step 2.1. Delta concentration vs distance. May 6th, 2016



FAIRMODE Forum for air quality modelling in Europe

Discussion

How can we validate the approaches?



How to separate both contributions?

Outcome of HARMO20 SS1 (June 15th, 2021)

- Discussion about the RIO model background data and emission data.
- Spatial intercomparison using the DeltaBM tool (remember presentation of Kees Cuvelier in the hackathon of December 2020). Very useful
- Spatial intercomparison using a big number of virtual sensors (apart of real samplers and stations). Need more discussion.
- Model vs Observed concentrations (time series, scatter plots, statistics, etc)
- Interesting to investigate how models describes the concentration difference (delta) between the traffic and background station.
- Applying concentration threshold? Maybe not suitable.
- Using MQI and Delta Tool? Not possible except in the case of AQ stations during the complete 2016 but there are no model results in this case.

How to evaluate and inter-compare the results provided by the participants?

Model results compared with AQ stations data (May 6th case)

24 pairs of data per station, two stations

PROPOSAL:

- Statistical comparison with observations of concentration and delta (trafficbackground stations):
 - Correlation, RMSE, NMSE, FAC2, BIAS, Normalized BIAS, etc
 - Other statistics? Other techniques?
 - Concentration threshold? Discriminating for low, medium and high concentrations?
- Graphical analysis of concentration and delta concentration:
 - TIME SERIES,
 - SCATTER PLOT,
 - BOX PLOT,
 - Others?

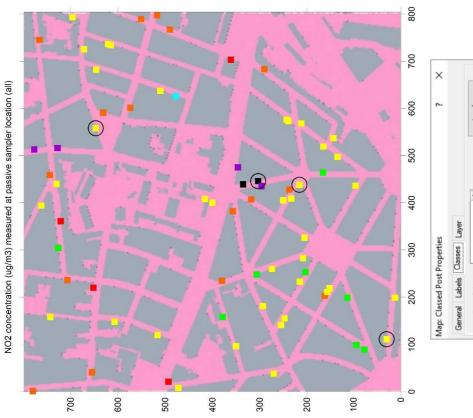
How to evaluate and inter-compare the results provided by the participants?

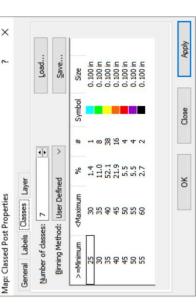
Comparison with passive samplers' data (April 30 – May 28 case)

73 passive samplers, NO₂ average concentration (April 30 – May 28). PROPOSAL:

- Statistical comparison with observations of concentration and delta (pairs of samplers):
 - Correlation, RMSE, NMSE, FAC2, BIAS, Normalized BIAS, etc
 - Other statistics? Other techniques?
 - Concentration threshold? Discriminating for low, medium and high concentrations?
 - Discriminating by sampler height? For surface concentration, use only samplers deployed at floor 0 and 1
- Graphical analysis of concentration and delta concentration (pairs of samplers):
 - TIME SERIES,
 - SCATTER PLOT,
 - BOX PLOT,
 - VARIOGRAM,
 - Concentration map with model result and sampler observation?
 - Others?







How to evaluate and inter-compare the results provided by the participants?

Intercomparison among models results. (campaign period, complete 2016) PROPOSAL:

• Kees software for spatial comparison

- Comparison grid point to grid point:
 - Spatial correlation?? Need of using a common grid?
 - Statistics of differences among models results (mean of differences, standard deviation)?
 - Other statistics?
 - Intercomparison only for areas with concentration above a threshold?
- Additional graphical analysis:
 - Map of mean and standard deviation of differences among models??
 - VARIOGRAM for every concentration fields provided by the models?? <u>Huge volume of data</u> (>10¹⁰data/model)

FAIRMODE



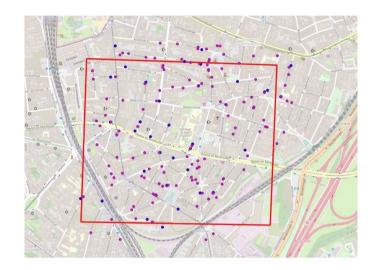
Case/domain/city for IEs

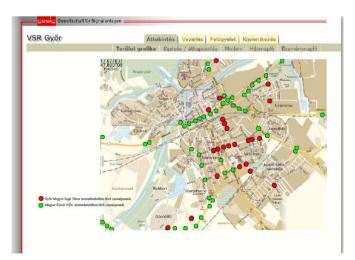
Antwerp (Belgium). Area around a traffic station.
 2021 current intercomparison exercise

2. Győr (Hungary)2022 next intercomparison exercise

- Proposed by Zoltán Horváth (SZE).
- Data from meteorological stations, AQ microsensors and AQ stations
- Real-time emission data for traffic.
- CFD model simulations for the entire year (but need several months of computing)

Who are interested in participating?





WRAP UP

- Most of the groups sent their results.
- Presentations of methodologies of every group were done
- Very preliminary plots of the analysis of results for STEP1 and 2.1 were presented.
 - Time series for one day episode (concentrations and delta concentration), STEP 1
 - Concentration vs samplers, variogram, STEP 2.1
 - General underprediction in peaks concentrations,
- Long discussion on several topics.

WRAP UP Discussion

- Atmospheric stability by the models. Most considered neutral stability. Low correlation between stability and NO2 concentration.
- Some inconsistencies between concentration data of AQ stations and RIO background data.
 - Background station is not in fact background (affected by others sources (residential)?).
 - Use other background station as background data instead of RIO (difficult to selected other station, better to keep on using RIO)
- Some questions on wind speed data.
- Agreement with the proposed methodology for analysis of the results, but several recommendations were done:
 - As there are no emission data in some small streets affecting to model outputs, better discard (or separated analysis) samplers of such streets for analysis of results.
 - Effect of a near highway (East) can affect the model results if it was not taken into account.
 - Make analysis by type of model/methodologies, by type of input data (wind direction, etc), use of chemistry or not in modelling, etc.
 - Not clear that use of thresholds could be useful in this case.
 - In the case of groups computing hourly concentrations along all 20166, good to compare percentiles of model concentrations with AQ stations data.
 - Use of variograms or semivariograms for the STEP 2.1 (only with samplers locations) is good idea, not for gridded data.
 - Good to compute spatial correlations when possible.
 - Good to use the Delta BM tool (Kees Cuvelier)

Next steps

- Receiving some pending model/methodologies results from some groups. → Soon
- Work on statistical intercomparison
 Next 4 months ??
- Possible Hackathon

 end 2021 or January 2022??
- Presentation of results
 February/March 2022 (Plenary meeting)??
- Submission of paper to Journal
 Spring 2022??
- New exercise for Gyor Case. → Mid 2022??