WG4. Best practice guidelines for air quality modelling at microscale for regulatory purposes

Fernando Martín and José Luis Santiago (CIEMAT)

WG4 Microscale Modelling - FAIRMODE

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WG4 – 1st session agenda

- General information of the Guidelines Document and Description of received feedbacks to the Questionnaire (15')
- Discussion about Terminology Questions (20')
- Discussion about General Questions (80')
- Discussion of some Specific Questions if time permits.

Introduction

- WG4 deals with microscale modelling in the context of the AAQD, i.e. air quality modelling at very high spatial resolution in urban environments, where local hotspots occur.
- One of the main goals of the WG4 is to test the robustness of developed methodologies to retrieve long-term averaged concentrations, and other AAQD indicators (e.g., percentiles), applying microscale models, and, overall to discuss the ability of microscale models to be used for air quality assessment and planning in the framework of the AAQD.
- The WG4 first activity was to perform an intercomparison exercise of methodologies to derive long-term pollutant concentration indicators. This allows the identification of several microscale modelling best practices for microscale air quality assessment in the context of the AAQD.
- The main objective of this document is to show a list of recommendations for using local-urban scale models for air quality assessment (mainly, annual average concentrations) using the results of the above-mentioned model intercomparison exercise.

Index of the Guidelines Document

1. Introduction
2. Types of local-urban microscale models
3. Review of the available guidelines for air quality modelling at microscale
4. Guidelines provided by the FAIRMODE WG4

Types of local-urban microscale models

- Computational Fluid Dynamics (CFD) models.
  - Unsteady long term simulations
  - Steady-state simulations of scenarios + methodology for retrieving long-term concentrations
- Gaussian models
- Lagrangian models
- Artificial intelligence (AI) trained with CFD simulations

Review of the available guidelines for air quality modelling at microscale

- In the case of CFD simulations for urban environments several best practice guidelines have been elaborated. Mostly, they are focus on CFD-RANS models.
  - The COST 732 action released a well-known guideline for the CFD simulation of flows in the urban environment (Franke et al, 2007, 2011).
  - Other ones such as those of Tominaga et al. (2008) and Blocken (2015).
  - Denby (2011) FAIRMODE Guide for NO2 modelling (need to be included)
- These guidelines provide information about the modelling setup describing recommendations for the domain size, mesh features, etc. to guarantee that the fluid equations are numerically solved in a correct way. For example:
  - The numerical domain should be large enough that the boundaries will not affect results in the study urban area
  - The computational grid has to be designed in such a manner that the errors introduced by the numerical discretization are not large (grid sensitivity test)

Guidelines provided by the FAIRMODE WG4

1. Requirements on the type of information to be provided by the models.
2. Recommendations on the pollutant emission data requirements
3. Recommendations on specifications of meteorological input data
4. Recommendations on specifications of background pollution data
5. Type of applications and best modelling approach for that specific application
6. Recommendations on the estimation of limit values exceedances and spatial representativeness area

Questionnaire

- General questions (8)
- Terminology questions (2)
- Specific questions for every group of recommendations (33)

- *Feedback from 11 persons/groups*
- *Now, we are going to discuss some questions (mostly General and Terminology).*

- *Hackathon for discussing the Guidelines Document (feedbacks) by late November-early December.*
- *2nd round of review of the Guidelines Document and responding to the questionnaire. Deadline for feedback, November 1st, 2024*

Terminology questions

2. Do you agree with this definition of the microscale air quality models for urban areas:

"Local-urban microscale air quality models are the models, which are able to simulate the main processes of the pollutants in the streets of an urban environment at very high spatial and time resolution being able to provide detailed information on how the pollutants are distributed inside the streets."?

- YES. **4 votes**
- YES, but… **6 votes**
- NO, **1 vote**

Terminology questions: *2. Yes, but…*

A. Simplified definition: *Local-urban microscale air quality models simulate the key processes of pollutant dispersion in urban streets, providing detailed information on pollutant distribution with very high spatial and temporal resolution.*

B. *To remove the explicit references to 'streets', in the domain there can be squares, roundabouts, open spaces.*

C. *No mention of flow resolved model and we can include Gaussian models.* It is so.

D. Change the word *"time resolution"* for *"temporal resolution"*

E. Rewording*: Local-urban microscale air quality models are dispersion models, which are able to simulate the relevant processes of air pollutants in question in an ~~streets~~ urban environment at very high spatial and time resolution to provide concentrations of these pollutants at street scale*

F. Reserve the "urban street canyon" part as an example of what a microscale model can do. Models of this type can also be applied to industrial area. Suggest: *Local-urban microscale air quality models are the models, which are able to simulate the main processes of the pollutants at very high spatial and time resolution, for example in the streets of an urban environment, being able to provide detailed information on how the pollutants are distributed inside the streets.*

Terminology questions: 2.

- Proposal:

Microscale air quality models simulate the processes relevant at very high spatial-temporal resolution in urban environments to provide air pollutant concentrations and its gradients at street scale

Terminology questions

1. What is your preference for naming the microscale air quality models for urban areas?

a. Local-urban microscale models. **3.5 votes**

b. Street-urban microscale models. **0 votes**

c. Microscale models. **5 votes**

d. Street-scale models. **1.0 vote**

e. Other? urban microscale air quality models. **1 vote**

f. Not answer **1 vote**

General Questions (1)

QUESTION	ANSWERS' SUMMARY
1. What is your global opinion about this guidelines draft?	**Mostly good,** only one said: Not ready for publication
2. Do you miss some key point in this guidelines draft?	**NO, but some suggestions:** • Include list of examples of CFD models and applications, differences LES-RANS, • Include key point of other guides, (*specific question 1.e*) • Extension to other pollutants (PM2.5,…) and other sources (domestic, …) (*partly to be discussed in specific questions 2.a and 2.b*)
3. Do you think the structure of the guidelines draft is suitable?	**Mostly YES,** but 1 said need of a table of contents and list of abbreviations
4. Would you change some the order of the contents?	**Mostly NO**
5. Would you remove any part or section?	**Mostly NO, but somebody suggest to remove**: • Bias correction part • Section 6 related to LVEA y SRA

General Questions (2)

QUESTION	ANSWERS' SUMMARY
6. Would you extent any part or section?	**4 said NO but others suggest to extend:** • Background concentrations section (discuss in specific questions Block 4) • Differences RANS-LES (VITO) (see question 2) • Include a summary of the FAIRMODE report on NO2 modelling (2011) (Chemistry topics) (partly related to specific question 5.h) • Define maximum spatial and temporal scale, computational resources required and availability of high resolution emission data? • Extension to other pollutants (PM2.5,…) and other sources (domestic, …) (see general question 2)
7. Would you shorten any part or section?	**9 NO, 2 not answered**
8. Other comments or suggestions	• Correct typos, writing, etc • Some references are missed (CERC,UA, IVU, …) • Include other pollutants (PM2.5, PM10), other sources (domestic, industrial,…) (see general question 2) • Extend list of needed meteo data (specific questions block 3 on meteo data) • Include discussion on model/input uncertainties and how to manage them (UOWM).

Some suggestions for General Questions (1)

- **Include list of examples of CFD models and applications**
- In other FAIRMODE Guidance reports there are lists of models.
- For example, in "*Denby et al. 2011. Guide on modelling Nitrogen Dioxide (NO2) for air quality assessment and planning relevant to the European Air Quality Directive. Result of activities in the FAIRMODE Working Group 1. Version 4.6. ETC/ACM Technical Paper 2011/15*" (see table).
  - *Do you think it could be needed?*
  - *Can it be interpreted as "recommended models"?*

Table 3. Table showing a number of street canyon models used in Europe. When available the model names are linked to the EEA Model Documentation System (MDS). Often these models may be imbedded within modelling systems.

Model (MDS link)	Comments/description	Links to documentation, validation and inter-comparison studies
OSPM	Operational street-scale model, based on a combined plume and box model.	Berkowicz (2000, 2008)
AEOLIUS	Based on OSPM but with some adaptations. Used in the UK.	Buckland (1998)
IMMIS^{cpb}	for the calculation of complex individual case studies and short term calculations of air pollutant's transmission in street canyons	http://www.ivu-umwelt.de/e
SEP_SCAM	A combined plume and box model	Papathanassiou et al. (2008)
CAR II (SRM-1)	Developed by TNO and applied in URBIS, The Netherlands. Highly parameterised model for a range of street canyon configurations (annual means only). Also known as SRM-1, legislated as the standard calculation method (1) in The Netherlands near roads (< 60 m). Access through a web based version available.	(van den Hout, 1988), den Boeft et al. (1996), Wesseling and Sauter (2007) http://wetten.overheid.nl/BWBR0022817/ http://car.infomil.nl/Login/Login.aspx?ReturnUrl=%2fScenarios%2fNew.aspx
ADMS-Roads	Multiple source Gaussian model with street canyon module based on OSPM methodology.	www.cerc.co.uk/environmental-software/ADMS-Roads-model.html
MSS (Micro Swift_Spray)	Multiple source Lagrangian Particle Dispersion Model (MicroSpray) applicable at microscale with obstacles	www.aria-net.it www.aria.fr Tinarelli *et al.*, 2007, 2009
WINMISKAM	Three-dimensional prognostic flow model coupled with an Eulerian dispersion model.	Olesen, H.R., Berkowicz, R., Ketzel, M., Løfstrøm, P. (2009) http://www.lohmeyer.de/eng/Software/default.htm
PROKAS_B	Precalculated results (nondimensionalized) of the microscale flow- and dispersions model WINMISKAM for 21 building patterns are used for the calculation of complex individual case studies of air pollutant's transmission in street canyons	http://www.lohmeyer.de/eng/Software/default.htm Flassak, Th., Bächlin, W., Bösinger, R. (1996)

Some suggestions for General Questions (2)

- **Describe differences LES vs RANS.** Both CFD approaches are cited at section, when describing the CFD models: *"…RANS (Reynolds-Averaged Navier-Stokes) and LES (Large Eddy Simulations) are the more frequent type of CFD models used for simulating the air quality in street-canyons…".:*
    - *Include a short description of RANS and LES?*
    - *Refer to some book, paper or report for description and details?*

Some suggestions for General Questions (3)

- **Include the key points or a summary of the recommendations of other Guidelines Documents (such as COST 732, FAIRMODE NO2, or others).**
- It is related to Specific question 1.e.
- *The answer to this question of the questionnaire was:*
  - *Only refer to the document: 3*
  - *Include a summary of the main recommendations: 6*
  - *What is your opinion?*
  - *Many guides are for the CFD modelling.*
  - *We probably need to provide a lot of technical details about CFD simulations in the summary ➔ How many detail would be needed to avoid excessively longer document?*

Some suggestions for General Questions (4)

- **Extension to other pollutants (PM2.5, PM10, …)**
- It is related to Specific question 2.a.
- Some people suggests to extend the scope to PM (mainly PM2.5, but also PM10):
  - The intercomparison exercise (IE) of Antwerp was done for NO2 (long-term averages) and for traffic emissions (dominant in the case of NO2)
  - The recommendations of our document is based mainly in the results of that IE.
  - *Could we do recommendations for other pollutants besides NO2?*
  - *PM2.5 could be primary and secondary, very important chemical process, other sources, etc. Therefore, could we provide only suggestions for PM2.5 modelling instead of recommendations?*

Some suggestions for General Questions (5)

- **Extension to other sources (domestic, …)**
- It is related to Specific questions 2b.
- Some people suggests to extend the scope to Domestic (heating), and Industrial sources:
  - The IE of Antwerp was done for traffic emissions (along road emissions) and for NO2.
  - Other sources must be located in the building in the roofs, stacks, etc
  - The recommendations of our document is based mainly in the results of that IE.
  - *Should we do recommendations for other sources besides traffic?*

Some suggestions for General Questions (6)

- **Include a summary of the FAIRMODE report on NO2 modelling (Denby et al., 2011) (Chemistry topics, but others related to fit-to-purpose, etc)**
- The part on chemistry is related to Specific questions 5.h.
- We have to review the main outcomes and recommendations of that Guide to:
  - Be summarized in WG4 document
  - Update recommendations related to urban microscale models
- *Do you agree?*

Table 1. Fitness for purpose matrix for dispersion models. Shown are the four major model types (columns) and applications (rows). Fitness for purpose is indicated by colour and appropriate comments. Green = 'fit for purpose'; Orange = 'conditionally applicable'; Purple = 'not fit for purpose'.

Model types and applications	Gaussian models	Lagrangian particle models	Obstacle resolving Eulerian models (CFD)	Terrain resolving Eulerian models
Open roads			No obstacles, computationally expensive	Unresolved
Street canyon	In combination with parameterised wind field model	In combination with parameterised wind field model	Computationally expensive	Unresolved
Urban scale	Requires homogenous meteorology	Computationally expensive	Not computationally feasible	
Regional scale	Requires homogenous meteorology	Computationally expensive	Not computationally feasible	

Table 9. Fitness for purpose matrix for NO_2 chemical schemes. Shown are the major chemical scheme types (columns) and spatial scales (rows) for both assessment and planning applications. Fitness for purpose is indicated by colour and appropriate comments. Green = 'fit for purpose'; Orange = 'conditionally applicable'; Purple = 'not fit for purpose'.

Chemical schemes and applications	Empirical schemes	Photo-stationary and ozone limiting schemes	Distance from source and mixing schemes	Reduced photochemical schemes	Full photochemical schemes
Assessment					
Street level	Given sufficient observations	Overestimates NO_2 in the presence of ozone		Difficult to apply at this scale. CFD only	Only reduced schemes necessary
Urban scale	Given sufficient observations	Suitable for winter or low hydrocarbons			
Regional scale				Missing significant chemistry	

Some suggestions for General Questions (7)

- **Define:**
  1. **maximum spatial and temporal scale?**
  2. **computational resources required?**
  3. **availability of high resolution emission data?**
- 1. Depends on your computational resources. Agree?
- 2. We need the modelers send to us information about the minimum needed computational resources (for example, for the Antwerp case). Agree?
- 3. We have the question block 2 of the Specific question section. We can discussed latter in a hackathon

Some suggestions for General Questions (8)

- **Include discussion on model/input uncertainties and how to manage them (UOWM).**
- *What can we tell about it?*
- *How to compute the uncertainties?*
- *How to separate the model uncertainties from the input (emission or meteorology, for example) uncertainties?*
- *Does the uncertainty comply with the AAQD requirements?*

Specific questions (1.a)

Requirements on the type of information to be provided by the models

1.a. Can we extend the methodologies for annual averages to other indicators (percentiles related to allowed number of exceedances of hourly/daily limit values)? YES OR NOT. EXPLAIN, How?

- For Gaussian and Lagragian models: YES
- For CFD:
  - Future work
  - Using the hourly time series. Not checked yet.
  - "The hourly concentrations for the whole year should be the primary aim the model used. These hourly data will be used to obtain other indicators often dependent of the pollutant under consideration and the corresponding health or other limits. The annual average, the hourly sigma, the peak value as well as the hourly pdf within the year probably will be enough for any other indicator needed" (UOWM).
- **Should we only include suggestions? Must it be checked with additional studies?**

Specific questions (1.b)

Requirements on the type of information to be provided by the models

1.b. The **domain** must be large enough to include all the expected size of the urban hot-spot. Usually, this **domain** should cover an area of at least 100x100 m2. Do you agree?

Error: "**Study Area**" instead of **"domain".**

Numerical domain (BPG) > built area > Study Area

- Not important for Gaussian models.
- 1 km x 1km (typical resolution of urban mesoscale simulations).
- 500 m x 500m
- Size should be related to the size of hotspot.
- AAQD, sampling points should be representative for a street length of at least 100m.
- **Should we include a recommendation of the minimum size or not? Can we provide typical sizes of other studies?**

Specific questions (block 2)

Recommendations on the pollutant emission data requirements

a. **Emission data** has to correspond to the **NOx and PM2.5**, which are the more problematic pollutants at street level, especially NO2. In the case of models using some chemical mechanism, emission data from precursors of ozone, such as **VOC** should be needed. In this case, ozone concentrations must be also provided as **background pollution data**. Do you agree?

b. The **emission sources** to be considered are traffic mainly, which is the main cause of the high air pollution at streets. However, other sources from domestic/residential sector has to be taken into account but located at the building roofs where stacks are located. Do you agree?

c. **The emission data has to cover all the streets**, even the smaller ones. Do you agree?

d. In wide streets or avenues or roads with several lanes, the **traffic-related emission** data have preferably to be provided **disaggregated for every lane**. For small street with low pollutant emission, perhaps less detailed information such as diffuse sources in a grid could be desirable. Do you agree?

e. The emission data will consist of annual total emissions from traffic and other relevant sources at every grid point or street/lane segment. In case of traffic emissions in every street are not available, **proxies such as traffic intensity** can be used (Santiago et al., 2017 and 2024). Do you agree?

f. **Temporal profiles** for all the type of sources considering the seasonal, weekly and daily emission variation must be available in order to provide good hourly emission data for the models simulations air pollution on hourly basis. Do you agree?

Specific questions (block 2)

Recommendations on the pollutant emission data requirements

Main aspects to be discussed (Answers):

- **Emissions** for all pollutants involved including background concentration. Also NO2/NOx emission ratio. Comments?
- **Emission sources**:
  - **Traffic emissions and other sources** (domestic heating specially for PM2.5, ports), non-exhaust emissions for PM2.5, etc…
  - **Difficulties: Are these data available? How should this be implemented in simulations (height of emissions)? Using background concentrations? Are additional studies needed?** Related to the question about whether this guide will be only focused on NO2 (and some suggestions of other pollutants). Relation with WG7?
- **Traffic emissions in all streets**: Yes, but some suggestions.
  - Emission in smaller streets with some simplifications and only if concentration in the study area is affected.
- **Traffic emissions:**
  - As better as possible (availability).
  - Hourly temporal profiles are needed.

Specific questions (block 3)

Recommendations on specifications of meteorological input data

a. For **nearby meteorological station data**, the needed information should be wind speed and direction, and temperature on an hourly basis, at least. Do you agree?

b. **Mesoscale meteorological model** should provide a very detailed 3D information of the meteorological parameters with a resolution of 1x1 km2 and several meters in vertical covering the modelling domain or city. Do you agree?

c. The **type of information required by the models** are wind speed and direction and temperature on an hourly basis. Vertical profiles of these variables could be required by some models, including information about turbulence (TKE, etc) information could be useful. Do you agree?

d. For CFD simulations, hourly modelled concentrations are better predicted using wind flow and turbulence profiles from mesoscale meteorological simulations (Santiago et al., 2020). However, to retrieve annual mean concentrations through simulated CFD scenarios-based approaches, neutral profiles are usually employed and meteorological variables (wind direction and reference velocity) from mesoscale simulation used as input should be taken at the top of the canopy (above roof level) (Sanchez et al., 2017). Do you agree? **Do we need to use non-neutral profiles for retrieving annual average concentrations**?

Specific questions (Block 3)

Recommendations on specifications of meteorological input data

Main aspects to be discussed (Answers):

This information should be representative of the domain being modelled:

- **Meteo data from stations**: Wind speed, wind direction, temperature, heat fluxes, solar irradiation (determine atmospheric stability), cloud cover, RH.
- **Data from mesoscale meteo models**:
  - Yes, but some comments about:
    - like meteorological measurements from outside an urban area, mesoscale data may not be representative of urban flow. What is your opinion?
    - How to interpolate or how to do the nesting. Taking the input at the roof level?
    - Ideal. Fit microscale domain to a mesoscale cell. What is your opinion?
  - Type of data: wind speed, wind direction, atmospheric stability, TKE. For some approaches, (Gaussian models (ADMS, AERMOD) and CFD methodologies) vertical profiles of some variables can be useful. What is your opinion?
  - Non-neutral conditions:
    - For Lagrangian and Gaussian. No problem.
    - For CFD, to investigate the impact of non-neutral conditions for retrieving annual average and hourly concentrations. Generally, neutral simulations work well for anual concentrations but it should be investigated for hourly concentrations. What is your opinion?

Specific questions (block 4)

Recommendations on specifications of background pollution data

a. **Using data from a nearby urban background station** (Santiago et al., 2017; Sanchez et al., 2017). The hourly pollutant concentration measured in such station have to be only due to sources non-modelled in the domain and the contribution from very local sources such traffic has to be very little in order to avoid a contribution in the domain, which could be indirectly a double counting of the emission from local sources. This requirement could be quite difficult to fulfil (or difficult of verifying) for the urban background station. It can be important to account for the delay of arriving air masses from the urban background air quality station to the modelled domain boundary, when the station is several km away to compute correctly the hourly pollutant concentrations (Rivas et al, 2024). Do you agree?

b. **Using outputs from larger scale air quality models**. The advantage of this approach is a good estimate of the spatial distribution of the background concentrations due to the city or urban area can be available with good spatial (1x1Km2) and time (hourly) resolution. This can be done, for example, with models CTM models such as CHIMERE, CMAQ, WRF-Chem or with models, which also processes (interpolates) the information from measurement stations such as the RIO model. The RIO model have been generally used in the WG4 Intercomparison Exercise with quite results resulting as very appropriate to use, but in some cases, data from WRF-Chem were used as background concentration with rather good results as well. Do you agree?

c. It is important that **the double counting of local emission** (e.g., traffic emissions) in both models (microscale model and the model used for background calculations) should be minimized. Therefore, methodologies for avoiding it must be applied. For example, the use of CTM concentrations above the rooftop could be used for estimating the background concentrations. Santiago et al. (2022) and (2024) used concentrations at 1.5 Hmax (being Hmax the height of the tallest building in the study area) from a mesoscale CTM simulation. Do you agree? Do you have something to add?

Specific questions (block 4)

Recommendations on specifications of background pollution data

Main aspects to be discussed (Answers):

Background concentrations used in the microscale modelling should be representative of the concentrations from unmodelled pollutant sources in the microscale simulations

Do you agree?:

- **Data from urban background stations**: Yes, but… (1 answer NO)
  - Difficult to avoid double counting the contribution from certain local sources.
  - Depending on wind direction.
  - Using outputs from larger scale air quality models is preferred.
  - Should we provide recommendations for the characteristics of background stations that can be used?
- **Data from larger scale air quality models**: Yes (1 answer, NO, only support 4D models as WRF-CHEM)

  Some comments about:
  - Important avoid double counting (importance of wind direction) Should we provide some recommendations how to avoid it?
  - Preferred option for almost all participant. Different successfully experiences with different models (RIO, FARM, CHIMERE, CMAQ…).
  - Recommendations for the type of larger scale air quality model? Recommendations for how to deal with CTM mesoscale models for background (3D map of concentrations and different resolutions)?