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

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Version 1.1, 20/03/2026

Summary

This document presents a comprehensive set of recommendations for using microscale air quality models to estimate long-term pollutant concentrations at very high spatial resolution in urban areas. It aims to improve air quality assessments in urban hotspots, where pollutant concentrations can vary spatially over just a few meters. The present guidelines were developed by the members of WG4 on Microscale Modelling within FAIRMODE (Forum for Air Quality Modelling in Europe), based on the results of an extensive intercomparison exercise involving multiple microscale dispersion models, as well as on the results from several research projects carried out by the members of WG4.

1. Introduction

Over the past few decades, European cities have made significant progress in improving air quality to protect human health. Despite progress, several cities are still facing acute air pollution episodes, with various urban areas frequently exceeding European air quality standards and the guidelines established by the World Health Organization (WHO, 2021) (EEA, 2023). The new EU directive introduces stricter pollutant concentration thresholds, which are likely to result in more and larger areas exceeding the limits, further emphasizing the need for effective measures. Within urban areas, the highest pollutant concentrations are usually found in traffic hotspots due to high vehicle emissions and the presence of buildings that limit transport and dispersion, which give rise to strong gradients of pollutant concentrations. Therefore, developing appropriate abatement strategies requires a proper assessment and modelling of such concentration gradients.

Numerical models play a fundamental role in the assessment of air pollution mitigation strategies, prior to implementation (Miranda et al., 2015; Borge et al., 2018; Vivanco et al., 2021,). Air quality models typically cover distinct spatial and temporal scales depending on the purpose of the application. For compliance purposes, Chemical Transport Models (CTM) have been widely used at the regional scale (Vivanco et al., 2009; Martin et al., 2014). However, their calculation grid spacing above 1 km does not resolve, for example, the high concentration gradients that occur in the vicinity of road sources at the microscale, which remain the dominant source of NO_x, black carbon (BC), and ultrafine particles (UFP) in urban areas. In many cases, the representative spatial scale of urban hotspots can be as small as a few meters, depending on the pollutant, its urban background contribution, and the characteristics of the hotspot. For example, NO_2 usually exhibits the largest concentration gradients; however, other pollutants, like PM2.5, can also show pronounced spatial variations. Therefore, CTM models are not suited to evaluate the concentration levels and the gradients found in hot spots. Hence, microscale air quality modelling is needed to best simulate the spatial distribution of the pollutant concentrations at very high resolution. Factors that affect the dispersion at this spatial scale must be included in the modelling explicitly or implicitly. These factors include urban structures (like building layouts and roads) as well as processes that describe how they affect wind patterns and turbulence. Additionally, processes such as chemistry and deposition, which can alter pollutant concentrations at short spatial/temporal scales, should be accounted for, where relevant. This type of modelling is increasingly used in the policy context of the Ambient Air Quality Directives (AAQDs) (EC, 2008, 2024), driven by increased focus on urban air quality. Microscale modelling helps locate and explain the causes of pollution hotspots. Additionally, it can be used to determine exceedance areas and test specific measures to mitigate or even avoid problems when used in the urban planning phase.

FAIRMODE (Forum for Air Quality Modelling in Europe) brings together air quality modelers and groups to exchange knowledge, experiences, and results from air quality modelling. Its goal is to support the harmonized usage of air quality modelling for air quality across Member States, for air quality assessment and management within the context of the AAQD. Within FAIRMODE, several working groups (WG) have been created to develop best practice guidance for several aspects of air quality modelling. WG4 deals with microscale modelling in the context of the AAQDs, 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 estimate long-term average concentrations and other AAQD indicators (e.g., percentiles). This involves the comparison of different microscale models to evaluate their suitability for air quality assessment and planning within the framework of the AAQDs.

So far other best practice guidelines have developed but mostly focused on CFD simulations of urban environments, where the model setup is relatively complex. They focus mostly on CFD-RANS models. The COST 732 action released well-known guidelines for CFD simulation of flows in the urban environment (Franke et al, 2007, 2011). However, other guidelines are available, such as those of Tominaga et al. (2008) and Blocken (2015). These guidelines provide advice about the modelling setup, including recommendations for the domain size, mesh features, etc., to ensure that the fluid equations are solved correctly. For example, the numerical domain should be large enough that the boundaries will not affect results in the study area, and the top of the computational domain should be at least 5 H_{max} higher than the tallest building, where H_{max} is the height of the tallest building (Franke et al, 2007). The computational grid must be designed in such a manner that the errors introduced by the numerical discretization are not large. Therefore, a grid sensitivity test must be carried out to determine whether the numerical mesh used is appropriate. A full discussion of existing guidelines for all aspects of CFD simulations is beyond the scope of this report. However, it is recommended that CFD modelers read carefully and follow the recommendations of the above-mentioned guidelines.

The first WG4 activity was to compare methodologies to derive long-term pollutant concentration indicators. This led to the identification of several microscale modelling best practices for air quality assessment in the context of the AAQDs.

Therefore, the main objective of this document is to present a list of recommendations for using microscale air quality modelling for air quality assessment. Evidence to support these recommendations is given in the results of the above-mentioned model intercomparison exercise, joint WG discussions, and individual WG4 members' research. Details of this model intercomparison exercise can be found in Martín et al. (2024, 2025). The guidance given here focuses mainly on pollutants emitted by traffic in streets, such as NO_2. The majority of the recommendations are also broadly applicable to PM2.5 and other pollutants such as BC and UFP; however, for these pollutants, other sources (e.g. domestic heating, industries, or ports) and physical processes (e.g. plume rise) may need to be included in the modelling framework with sufficiently high resolution.

2. Types of microscale air quality models

Microscale air quality models are models that can simulate processes at very high spatial resolution in urban environments to provide air pollutant concentrations and gradients at street scale. There are several types of microscale air quality models. Five main groups can be distinguished:

- Computational Fluid Dynamics (CFD) models
- Gaussian models
- Lagrangian models
- Street-network models
- Artificial intelligence (AI)/Machine Learning (ML)/ Artificial Neural Networks (ANN) models.

This document guides the use of air quality models and associated methodologies to estimate long-term pollutant concentrations at very high spatial resolution in urban areas. Therefore, it is important to consider the model and the associated post-processing methodology together. Following this idea, hereafter, the more general term "*modelling system*" will be used. It is defined in FAIRMODE (2025) as "*A chain of models and submodels, including all necessary input data, and any post-processing*". One example of a "modelling system" is a CFD model simulating representative meteorological scenarios combined with postprocessing methodologies to compute monthly or annual pollutant concentration distributions over a specific spatial domain.

2.1 Types of models:

2.1.1. Computational Fluid Dynamics (CFD) models

At the microscale, Computational Fluid Dynamics (CFD) models have been widely used to assess pollutant dispersion within street canyons (Santiago et al., 2007; Reiminger et al., 2020a; Santiago et al., 2021; Lin et al., 2023; Wang et al., 2023). CFD models can accurately simulate turbulent flow dynamics and the resulting dispersion by solving the Navier–Stokes equations and explicitly representing the complexity of the built environment. RANS (Reynolds-Averaged Navier-Stokes) and LES (Large Eddy Simulations) are the types of CFD models more frequently used for simulating the air quality in street-canyons. The main difference between these two CFD approaches is in the treatment of turbulence. In RANS simulations, an integral approach for the whole turbulence spectrum is considered, and turbulence closure schemes like k-ε or k-ω are necessary. This makes RANS computationally cheaper and faster but less accurate in capturing detailed, unsteady turbulent structures. In contrast, LES explicitly resolves the unsteady large turbulent eddies (the most energy-containing structures), while smaller eddies are modeled as in RANS. LES provides higher accuracy in capturing transient and complex flow behavior, but the simulations are much more computationally expensive than RANS (Blocken, 2018).

There are some limitations associated with CFD models, for example, they require large computational resources to perform long-term simulations. CFD modelling results are typically available for short periods, such as a single day or a few hours (Amorim et al., 2013; Sanchez et al., 2017, Rafael et al., 2018; Rivas et al., 2019). Additionally, a few CFD models (Sanchez et al., 2016, 2021; Reiminger et al., 2024) take into account the short-time scale NOx chemical reactions (NOx-O3 photostationary state and more complex schemes), or the particle dynamics (Lin et al., 2023, Lin et al., 2024a, Lin et al., 2024b). In some approaches, NO_2 is simulated as a non-reactive pollutant (Santiago et al, 2017). This approach seems to be more applicable for winter episodes, as the NOx-O3 reactions are much less effective due to the low solar radiation and temperature conditions. Some CFD models apply NO_2/NOx parameterizations such as Bächlin (2008) and Derwent (1996) to estimate NO_2 concentrations after simulating NOx dispersion (see, for example, Jurado et al (2023), Reiminger et al (2024, 2025)).

These limitations make applications associated with air quality legislation compliance challenging because there is a requirement for microscale model outputs to be aggregated to longer temporal scales, typically a year.

Some attempts have been made to derive long-term averages of pollutant concentrations in urban hotspots using CFD models. Parra et al. (2010) presented an early approach to the methodology for the derivation of long-term averages of NOx and PM10 concentrations based on a steady-state Reynolds-Averaged Navier–Stokes equations (RANS) and standard k-ε turbulence model. CFD simulations were performed for a set of 16 different inlet wind directions (corresponding to 16 wind rose sectors) over a real urban area, for two winter months, neglecting chemical reactions. Santiago et al. (2013), Santiago and Martín (2015), and Santiago et al (2017) applied an extension of the Parra et al. (2010) methodology using a weighted-average approach (WA CFD-RANS) to estimate the time evolution of pollutant concentrations using a sequence of steady-state RANS simulations, adjusting the simulated atmospheric parameters to the actual conditions at hourly frequency. NO_x maps were reconstructed using CFD simulations for different meteorological conditions covering several months or one year, assuming non-reactive pollutants and negligible thermal effects. Sanchez et al (2017) generated long-term average NO_x concentrations applying the same weighted-average methodology but using meteorological inflow conditions from a mesoscale model. Rivas et al (2019) presented annual average NO_2 and NO_x concentrations over an entire city applying the WA CFD-RANS methodology. Vranckx et al. (2015) simulated the impact of trees on the dispersion of elemental carbon and PM10 in urban street canyons using the CFD OpenFOAM model. CFD simulations were performed for ten vegetation settings and a range of wind directions. The simulation results were combined using meteorological statistics and the effects of seasonal leaf loss, to determine the annual average effect of trees in street canyons. Lastly, Reiminger et al. (2020b) recently suggested a new methodology to compute long-term average concentrations based on the continuous interpolation of wind rose data through a double sigmoid function. This methodology was then optimized by Jurado et al. (2021) to minimize the number of wind direction sectors used while maintaining accuracy.

Considering methodologies based on CFD simulations of scenarios, several studies (Borge et al., 2018; Santiago et al., 2020; Reiminger et al., 2020c and 2024) found that hourly concentration patterns are affected by thermal effects (stable and unstable conditions), and non-neutral CFD simulations (urban surface heat fluxes and/or non-neutral inlet profiles for wind flow) are needed to capture these concentration maps. However, the use of simulated CFD scenario-based approaches for considering non-neutral CFD for retrieving long-term averaged concentrations implies a large increase in the number of simulated scenarios. Not only for different wind directions, but also for different atmospheric stabilities. However, there are simple ways to consider thermal effects with simulated CFD scenarios-based approaches. Sanchez et al. (2017) found that using friction velocity (instead of wind speed) as a reference velocity to normalize the concentration improved the prediction of hourly concentrations during low wind speed conditions. Consequently, increase the accuracy of long-term averaged concentrations. On the other hand, the results of the WG4 FAIRMODE IE (Martín et al., 2024; 2025) and previous studies (Parra et al., 2010; Santiago et al., 2017; Sanchez et al., 2017; Rivas et al., 2019) show that the long-term averaged concentrations computed using methodologies based on CFD simulations of neutral atmospheric scenarios are consistent with experimental values recorded at air quality monitoring stations and passive samplers distributed throughout the study area. Nevertheless, more studies are needed to investigate this issue.

2.1.2. Gaussian models

Gaussian models (Oliveira et al., 2021, Rafael et al., 2021; Carruthers et al, 2001; Zhong et al, 2021; Hamer et al, 2020; Hooybergs et al, 2022) have been routinely used for regulatory purposes in assessing the impacts on local and urban air quality of pollution sources. They are not computationally demanding and can produce fast and reliable answers in operational setups that are accessible to a wide range of users. They can be coupled with other models, such as weather prediction models and CTMs.

Gaussian models perform calculations at hourly resolution, allowing straightforward calculations of AAQD metrics. The models include parameterizations (e.g., in terms of wind meandering) that correspond to an hourly averaging time. The models commonly use spatially homogeneous wind speed and turbulence boundary layer profiles to drive dispersion, although some models account for flow variations relating to building density and in-canyon effects. Gaussian models have limitations in low wind speed conditions. Specifically, the mean wind speed must be larger than the turbulence, so that diffusion in the downwind direction is negligible in comparison with advection. Notwithstanding, the influence of stagnation conditions can be taken into account through coupling with CTMs. Gaussian models commonly account for simple NO_x chemistry (Smith et al, 2017, and Carruthers et al, 2017).

In contrast to CFD models, Gaussian models do not explicitly solve the fluid equations to calculate the effects of the buildings on air flow, turbulence, and hence dispersion. When modelling the urban environment, parametrizations are used to account for such effects, thus approximating pollution distribution. Hood et al (2020) describe an advanced street canyon module, integrated within an extensively used Gaussian model, which accounts for a wide range of canyon geometries and includes six component sources to represent different effects of street canyons on the dispersion of road traffic emissions. As with other dispersion modelling approaches, Gaussian models are dependent on the reliability of the meteorological and emission data used, but on the quality of the parametrizations for street-canyon effects as well.

2.1.3. Lagrangian models

Lagrangian models simulate air pollutant dispersion through virtual particles, each representing a small amount of the mass of the released substance. The average motion and diffusion of the particles are determined by the local wind, computed using a microscale meteorological model, and by the velocities derived from solving the Langevin stochastic differential equations, respectively. These equations can accurately reproduce the statistical characteristics of the turbulent flow. For example, Veratti et al. (2020), Villani et al. (2021), and Barbero et al. (2021) reconstructed the air quality in urban areas with the modeling suite PMSS, which couples a terrain-following 3D diagnostic mass-consistent model and a Lagrangian Particle Dispersion Model. In particular, the meteorological model could be run solving the momentum equations (averaged Navier Stokes equations), initialized with the standard diagnostic solution (Carissimo et al., 2021). Some Lagrangian models also include simple NOx chemical schemes such as the case of the GRAL-C model (Oettl and Uhrner, 2011; Alessandrini and Ferrero, 2009).

2.1.4. Street-network models

Street-network models (Kim et al. 2018, 2022, Soulhac, 2011) simulate streets explicitly, allowing for transport of pollutants between the streets and the urban background above each street, as well as transport of pollutants from one street to another. In these models, the transfer of pollutants between streets and urban background has been parameterized using CFD modelling (Maison et al. 2022a, 2022b). The location of each street, as well as length, mean height, and width must be specified. Emissions and deposition of the different pollutants are considered, as well as chemistry and aerosol dynamics. Some models of this type are SIRANE (Soulhac, 2011) or MUNICH (Kim et al, 2018). The Model of Urban Network of Intersecting Canyons and Highways (MUNICH) has been widely used coupled to different chemistry transport models, such as CHIMERE and Polair3D for applications over European cities (Lugon et al. 2021a, 2021b, 2022, Sarica et al. 2023b, 2024, Park et al. 2024, Sartelet et al. 2025, Squarcioni et al. 2025), and other CTMs over other cities (Wang et al. 2023b, Tonoli Cevolani et al. 2024). The coupling between regional and street-scale modelling allows for a multi-scale representation from the regional to the street scale of the different pollutants. Concentrations are calculated at hourly resolution, allowing straightforward calculations of AAQD metrics. For fast-running applications of street-network models, concentrations are assumed to be homogeneous in each street segment. However, the street segments may also be discretized vertically (Sarica et al. 2023a). Additionally, the influence of trees, particularly their aerodynamic effects within street canyons, may also be taken into account (Maison et al., 2024).

2.1.5. Artificial Intelligence (AI)/Machine Learning (ML)/ Neuronal Networks (ANN) models

Recently, the potential of using Artificial Intelligence (AI)/Machine Learning (ML)/Neuronal Networks (ANN) models to model the dispersion of air pollution in urban areas has been investigated with the use of a convolutional neural network (CNN) based algorithm trained on CFD results (Jurado et al., 2022). The model then demonstrated its computational efficiency on a larger scale, allowing real-time modeling at the scale of the city without compromising micro-scale phenomena, such as street canyon effects, which are generally neglected in larger scale models, or, at least, modeled through additional street canyon models (Jurado et al., 2023). As in the case of the CFD models, these models can use NO_2/NO_x parameterizations (Bächlin or Derwent) to estimate NO_2 concentrations from simulated NO_x concentrations.

2.2. Computational resources and run time

CFD models are usually the most demanding because they solve the Navier-Stokes equations numerically, including the dispersion of pollutants and chemistry in some cases. CFD requires very high-resolution grids, with cell size on the order of meters. Long-term unsteady-state CFD simulations required to calculate annual pollutant concentration metrics for direct comparison with the AAQD are very computationally demanding. However, some procedures for faster computing have been developed for estimating long-term (annual) pollutant concentrations based on a set of steady-state CFD simulations. These methods offer significant benefits in terms of computational resources. However, CFD remains the most computationally intensive compared to other modelling approaches. Gaussian modelling seems to be the least computationally demanding, followed by AI and Lagrangian models. Table 1 presents an indication of the computational resources and run times for the different models used in the FAIRMODE WG4 intercomparison exercise for Antwerp.

Table 1. Computational resources and running times for some of microscale modelling systems used for the FAIRMODE WG4 Antwerp Intercomparison Exercise

TYPE	MODEL	GRID SIZE/ nº cells/ resolution	CPUS	RUNNING TIME
CFD-RANS STEADY	STAR-CCM	1x1 km2 1.2 M (at surface level) 1 m	64 cores Intel(R) Xeon(R) Gold 6254 CPU @ 3.10GHz	0.5 days approx. for each scenario.
CFD-RANS STEADY	OPEN FOAM /VITO	1.5 ×1.5Km2 19M cells 1 m (near walls) at least	32 CPU (specs = Intel(R) Xeon(R) CPU E5-2620 v4 @ 2.10GHz)	1.3 days (per wind direction scenario), total 21 days for 16 scenarios
CFD-RANS STEADY	OPEN FOAM /AIR&D	1.3X1.3Km2 16M cells 0.5 m (near walls) at least	30 CPU processors Intel Xeon Gold 6126 2,60 GHz	Around 3 days a simulation (one meteorological scenario): total 54 days for 18 scenarios
CFD-RANS STEADY	OPEN FOAM /SZE	2.6x2.6 km2 3.3M 2m	8 node x (2 x 64) core AMD EPYC 7702 at Hawk,	Almost 1 day per wind sector scenario Total 15.7 days for 16 scenarios
CFD-RANS STEADY	ADREA	1x1 km2 2.5M cells 5 m	8 processors Haswell - Intel(R) Xeon(R) E5-2660v3 2.6Ghz	At least 1 day per run (one for each wind sector scenario) Total > 32 days for 32 scenarios
CFD-LES	WRF/ Chem - PALM4U	1X1 km2 2.8M cells 5m	400 Intel Xeon Platinum 8160 24C processors at 2.1 GHz	11 hours per simulated day.
GAUSSIAN	ADMS-URBAN	7.8x7.8 km/ …/ 0.3-25m	No HPC required	
GAUSSIAN	ATMO-STREET	Full Antwerp City/…/ 10m	No HPC required	
GAUSSIAN	EPISODE	1x1 km2/ 2.5K cells 20m	No HPC required	
LAGRANGIAN	PMSS	0.8x0.8 km2 71289 cells (only surface level) 3m	26 CPU Intel(R) Xeon(R) CPU E5-2698 v4 @ 2.20GHz	25 min per simulated day Total 6 days for a full year simulation
Artificial Intelligence/ Machine Learning		1.3 ×1.3Km2 Nº of cells not relevant 1 m at least	10 CPU processors Intel Xeon Gold 6126 2,60 GHz for the pre-processing tasks and 1 GPU GTX 1080 Ti for the model to run	around 1 h a simulation (one meteorological scenario): total including pre and post processing = 55h (all scenarios)

3. FAIRMODE WG4 Guidelines

3.1. Requirements for information to be provided by the modelling systems

It is first necessary to define what type of information the microscale air quality modelling systems need to provide. One of the main advantages of the microscale air quality models over measurement datasets is the detailed spatial (usually in 3D) estimates of pollutant concentrations, which capture the strong gradients at the street scale. Hence, microscale models should provide the following information for air quality assessment:

a. Spatial distribution of pollutant concentration metrics over the study area, for example, as georeferenced air pollution map(s). Metrics presented in this way can include the annual mean concentrations (to be compared with annual limit values) or other indicators such as percentiles of hourly or daily concentrations (for comparison with the number of exceedances allowed by the AAQDs).
b. The spatial distribution of pollutant concentration metrics has to be provided at pedestrian level and/or at the height of the inlet of measuring devices in air quality stations. Heights of 1.5 to 3 m are recommended.
c. The study area must be sufficiently large to include all potential urban hot-spots and meet numerical simulation requirements (see Franke et al, 2007, 2011 in the case of CFD modelling).
d. Detailed information describing the urban geometry and distribution of emissions in the vicinity of any potential hotspots is required. Care should be taken when deciding upon the emissions dataset resolution, for example, the number of road sources to include in the inventory. Microscale models generate very high-resolution outputs, but pollution maps may be misleading if insufficient emission sources are used as input to modelling. Emissions are discussed further below.
e. The horizontal spatial resolution of the concentration maps should be sufficiently fine to include at least 3 grid points perpendicular to the street. However, for CFD simulations, the internal calculation grid resolution must be finer, following the recommendation of Best Practice Guidelines of COST732 (Franke et al., 2007). Based on the FAIRMODE WG4 IE results, in the case of wide avenues or roads, the horizontal resolution should not be larger than 10 m. However, considering that there are both wide and narrow streets in the majority of modelling domains (some more than 40m wide, and others less than 15 m wide), the output grid resolution should be less than 5 m to be sure that all concentration gradients are properly represented.
f. Regular output grids are preferable for graphical presentation. If models generate outputs on irregular grids, interpolation methods can be used to generate regular gridded outputs. The resolution must be similar to or coarser than the resolution of the irregular grid used in the model simulations. In this case, care should be taken when selecting not only the interpolation algorithms, but also the parameters that are used as input to the

calculations. Models that explicitly account for the presence of urban structures, such as buildings, do not generate outputs over the whole model domain.

g. Concerning the domain and grid configuration, the CFD model simulations must also follow the recommendation from specific best practice guidelines, such as those from COST action 732 (Franke et al. 2007, 2011) or others referred to in section 3.

3.2. Recommendations on the pollutant emission data requirements

Pollutant emissions inventory is a key input to air quality modelling. The modelling systems have to represent emissions of volume, area, line, and point source types. However, it is challenging to estimate very detailed emissions data for all sources in an urban area. Generally, traffic count data and/or traffic model output are available for main avenues, streets, and roads. For minor roads, aggregated emissions estimates (for example, at 1 km resolution) may be available, and calculations from these data may be needed to estimate the emissions for these roads. Emissions data for other source sectors, such as commercial and domestic sources, may also be available at coarse resolution, or as point sources in the case of industrial stacks. Emission inventory computation and validation is the focus of FAIRMODE WG7 on emission inventories. Here, some general recommendations are provided that relate specifically to microscale modelling:

a. The emission data must include NO_x and PM2.5. In case of needing explicit NO_2 emissions data, the NO_2 emissions (and it is not defined explicitly in the emission data) may be specified as a sector-average proportion of NOx emissions that is NO_2. For models that account for short-timescale chemical reactions, emission data from ozone precursors, such as VOC, are usually required. In such cases, background ozone concentration estimates are also required as input to the models.

b. The emission data will correspond to all the relevant sources located in the domain at every grid cell affected by area or point sources or at every street/lane segment in case of traffic emissions

c. In the case of NO_x, NO_2 and PM2.5, the emission sources to be considered are primarily traffic. However, other sources such as domestic heating, industries, ports, or traffic non-exhaust PM emissions must be considered, depending on the study area or pollutant of interest.

d. In the case of traffic emissions, the emission data must include all roads, even the smaller ones. In wide streets, avenues, or roads with several lanes, the traffic-related emission data should preferably be provided separately for each lane if possible. For small streets with lower emissions, less detailed information, for example, representation as diffuse sources in a grid can be used. Where traffic emissions are unavailable, proxies such as traffic intensity/congestion can be used (Santiago et al., 2017 and 2024). Emissions of NOx, NO2, BC, and PM2.5 may be estimated from the number of vehicles passing in the streets, and knowledge of the traffic fleet (Ibarra-Espinosa et al. 2018). For particles, traffic emissions must include exhaust and non-exhaust emissions.

e. For sources other than traffic, the level of spatial disaggregation should reflect the relative magnitude of the emissions. Emission height information must be provided in any case. In the cases of emissions from stacks, in addition to location and stack height data, the gas temperature and flow rate must be required to allow plume rise computation.
f. The temporal resolution of the emission data should be hourly at least. Nevertheless, annual emission data are much more usual than hourly or daily data. Hourly/daily data can be easily estimated using temporal profiles. They (at least, for road sources) should quantify seasonal, day-of-the-week and hour-of-the-day variations to facilitate the calculation of hourly emission data for model simulations of air pollution on an hourly basis. Temporal emissions variations from other source sectors should be allowed for in the modelling where these sources have relatively large emissions and/or where temporal variations are significant.

3.3. Recommendations on specifications of meteorological input data

Meteorological data are needed by the microscale models to provide inlet boundary conditions in the case of the CFD models, or to more generally represent atmospheric stability and synoptic conditions for other types of models. This information should be representative of the modelled domain and can be obtained from two main sources:

a) Nearby meteorological stations. The station should not be sheltered by nearby buildings or urban obstacles, nor should it be placed too far from the area of interest. An urban background location close to the domain being modelled, as used in the WG4 FAIRMODE IE (Martín et al, 2024) and in other works (e.g., Rivas et al., 2019), may be appropriate. The minimum data requirements are hourly wind speed and direction, and temperature. However, additional information about solar radiation (to estimate the atmospheric stability), cloud cover, and humidity are common requirements or recommendations for many models. Further information, such as heat fluxes or vertical profiles of wind and temperature, can be used as input to some models, but such data are rarely available.
b) Mesoscale meteorological modelling output. Meteorological models such as WRF can provide very detailed meteorological parameters in 3D with a horizontal resolution of 1x1 km^2 and a vertical resolution of several meters covering the modelling domain or city. The accuracy of such modelled meteorological data should be quantified before use, e.g., through validation using measured meteorological datasets. The minimum information required by the models is wind speed and direction, and temperature on an hourly basis. Vertical profiles of these variables may be required by some models. Including information about turbulence (TKE, etc) may be useful. The use of wind flow and turbulence profile data output from mesoscale meteorological models in CFD model simulations has been shown to improve performance (Santiago et al., 2020). Additionally, it is possible that in the summertime, simulations with solar radiation could improve the results of some models, when solar radiation rate is important (Reiminger et al., 2024). However, it needs more

investigation. In contrast, Martin et al. (2024) demonstrated that it is sufficient to derive annual mean concentrations through simulated CFD scenarios corresponding to neutral atmospheric conditions. In addition, meteorological variables (wind direction and a reference velocity) from mesoscale meteorological simulations used as input should be from the top of the urban canopy (above roof level) (Sanchez et al., 2017) to be representative of the regional meteorological conditions. The main disadvantage of using mesoscale meteorological modelling is that these data are less accurate than measured values. However, model data is a more comprehensive data source, for example, providing vertical profiles and additional parameters that are not usually recorded, such as turbulence variables. In the case of CFD scenario-based approaches, such datasets can help improve modeled concentration estimates. For example, using the friction velocity as the reference velocity may provide better outcomes than using only wind speed (Sanchez et al., 2017). Further details are provided in Section 4.5.

3.4. Recommendations on specifications of background pollution data

Background pollution can represent a significant portion of the observed pollutant concentration at urban hot-spots. The background information used for microscale modelling should be representative of the contributions from pollutant sources not included in the microscale simulations. This information can then be easily added to the microscale model outputs to provide a more accurate estimate of the total concentration at a hot-spot. There are two main options for obtaining background pollution:

a. Using measurements from one or more nearby urban background (UB) stations (Santiago et al., 2017; Sanchez et al., 2017). UB concentration data can vary considerably with wind direction (Pineda Rojas et al., 2020), so using multiple stations is advisable. Hourly pollutant UB concentrations measured must only correspond to sources that are not explicitly accounted for in the model domain. The contribution from local sources, such as traffic, must be minimal to avoid indirectly double-counting emissions. This UB station requirement may be difficult to fulfil or difficult to verify. The station should be located inside the modelling domain or adjacent to it. In case of UB stations located outside the domain, it may be important to account for the time delay related to advection of air masses from the UB station to the modelled domain boundary to compute correctly the hourly background pollutant concentrations (Rivas et al, 2024). This is particularly relevant when the measurement location is several km away.
b. Using outputs from larger-scale air quality models (CTM models). The advantage of this approach is that CTM models provide spatially resolved (roughly 1x1 km^2 resolution) information about the spatial distribution of pollution. The accuracy of background concentrations obtained from models also depends on the accuracy of the model itself. Validated mesoscale models must be used, and bias correction might be necessary. Hourly background concentration data is required for all the modelled domains. Outputs

from CTM models, such as CHIMERE, CMAQ, and WRF-Chem, are usually suitable due to their accuracy. Additionally, models that rely on smart geo-spatial interpolation of the background stations, such as the RIO model (Janssen et al., 2008) can be used. The RIO model was used in the WG4 Intercomparison Exercise (Martín et al., 2024, 2025) due to its computational efficiency and accuracy. It is essential to minimize the potential double-counting of local emission sources (e.g., traffic-related emissions) when combining outputs from the microscale model with those from the model used to estimate background concentrations. 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. In the case of the RIO model, double-counting corrections might also be needed. The use of tagged local city contributions from a CTM may be another option.

3.5. Recommendations on the suitable modelling system for air quality assessment at microscale

The different types of models used for local-urban microscale were described in Section 2. There are several model applications, such as air quality assessment, planning, or forecasting. However, this guidance document is focused on the use of modelling systems for air quality assessment. With this objective in mind, the FAIRMODE WG4 intercomparison exercise generated results from all types of models. The datasets were analyzed and compared with observations of NO_2 concentrations recorded in an urban district of Antwerp. Martín et al (2024, 2025) present a detailed discussion of the intercomparison exercise outcomes. The second paper focuses on model performance in relation to the prediction of limit value exceedances and spatial representativeness areas. Thus, as said in the Introduction Section, it is important to highlight that most of the evidence base for the recommendations presented here regarding urban microscale modelling system suitability primarily relates to microscale modelling of NO_2 concentrations that arise from road traffic. However, the FAIRMODE WG4 members’ expertise can support the recommendations for other pollutants or sources.

The general conclusion was that the models representing in detail more relevant processes for the street scale usually predict a more realistic spatial distribution of atmospheric pollutant concentrations. This is the case of the modelling NO_2 at the urban microscale and assumes that the input data have sufficient quality. The results suggest that the impact of the buildings on the wind-flow is one of the more relevant aspects in the dispersion process

In more detail for NO_2, the intercomparison exercise results suggest that modelling systems should account for street canyon effects when strong geometrical-driven spatial gradients are expected, since they can magnify the hot-spot. The Gaussian models with street-canyon parameterizations are able to reproduce many features of the spatial distribution of NO_2.

However, Gaussian models without street-canyon parametrization cannot reproduce these gradients and are therefore not recommended for use. Nevertheless, they can potentially be used solely for initial screening of possible hot-spots locations, when high-resolution emission data are available. Street-network models, which did not take part in the intercomparison exercise, when integrated with CTMs, can represent the urban spatial gradients of NO_2 or other pollutants such as PM2.5, UFP or BC (as shown in the RI-Urbans Project) throughout the city, particularly when coupled with a chemistry module. However, gradients inside the streets cannot be well represented because they assume homogeneous concentrations along each street segment. The AI (trained with CFD simulations) and Lagrangian models, accounting for building explicitly, generated NO_2 concentrations with quite similar accuracy to those generated by CFD, but in a faster way. Nevertheless, the highest accuracy is obtained by several CFD-based modelling systems.

However, a notable drawback of the CFD models is the large computational load (see Table 1). This can be mitigated by applying methodologies for retrieving the long-term averages of pollutant concentration from the scenario simulations. Those methodologies have been documented (Santiago et al., 2017; Sanchez et al., 2017; Rivas et al., 2019; Reiminger et al., 2020b; Jurado et al., 2021; Santiago et al., 2024, for example). They rely on simulating (steady-state) scenarios corresponding to inlet wind direction sectors under neutral stability atmospheric conditions. Jurado et al. (2021) showed that for a wind sector approach, homogeneous discretization is better on average than prioritizing wind directions with the highest frequencies. The WG4 FAIRMODE IE (Martin et al., 2024) found that the wind sector approaches yield as good results as the full-year/month unsteady CFD-RANS simulations. The results of this IE indicate that 8 wind sectors are likely to be sufficient, but the exact number will depend on the urban morphology, the pollutant source geometry and relative position to building layout and the wind rose (Jurado et al., 2021). More studies for other conditions are needed to reach more consolidated conclusions.

As said in previous sections (Section 2), the inclusion of thermal processes in CFD simulations could improve the CFD simulations. However, it implies considering more meteorological scenarios that cover different atmospheric stabilities, which would significantly increase the computational time. However, several studies have shown that using wind sector scenarios assuming neutral conditions yields good annual results as required for air quality assessment under the AAQDs. Therefore, further research is needed to investigate this issue to provide a final recommendation.

As explained in Section 2, atmospheric chemistry is easier to represent in the street-network and Gaussian models due to their algebraic formulations. For CFD models, accounting for chemical reactions is not straightforward, and can significantly increase the computational load. However, some CFD models have been developed including some simple chemical schemes (Sanchez et al., 2016 and 2021; Reiminger et al., 2024). Lagrangian models can also use simple chemical schemes with a relatively short demand for computation time (Oettl and Uhrner, 2011; Alessandrini and Ferrero, 2009).

A simple approach to accounting for NOx chemistry in models that do not allow chemical reactions is to model NO_x as a non-reactive pollutant and to use the ratio NO_2/NOx to transform NO_x to NO_2. The ratio NO_2/NO_x can be obtained from:

a) Data recorded at the air quality monitoring stations (Rivas et al., 2019)
b) Outputs of CTM mesoscale models (Santiago et al., 2022; 2024)
c) Using the Bachlin or Derwent parameterizations (Reiminger et al., 2024; Jurado et al., 2023).

However, the ratio of NO_2/NO_x varies spatially (and very quickly away from roads). Therefore, the use of a single value for the whole domain is not correct (as in case a) and b)). Moreover, the ratios obtained from a CTM model (urban scale) may not be representative for street canyon situations.

Other modelling methods that avoid explicit NOx chemistry calculations include hourly parametrizations, for instance using hourly O_3 values and direct emissions of NO_2; $NO/NO_2/O_3$ relationships from local curbside monitoring stations; or parameterizations derived from street scale models.

At this point, it is difficult to make a recommendation regarding the appropriate chemical formulation because more studies are needed.

To provide rule-based guidelines for selecting models, we followed the initial structure proposed by Haeger-Eugensson et al (2021). The results from the IE presented by Martin et al (2024) were used to corroborate this structure, along with the expert opinion of the WG4 members. Additionally, AI (trained with CFD) and Lagrangian models were added to the guidelines following the IE results. Accordingly, as the street-network models did not participate in such an intercomparison exercise, they were not included in these recommendations. Presently, a new intercomparison exercise is being carried out, in which the street-network models are participating along with the other modelling system types. It does not mean that such modelling systems are not adequate for microscale modelling. When it finishes, a new version of this guidance document will be prepared with updated recommendations for all modelling system types, including street-network models.

Considering the results up to date, it can be proposed that:

- For no adjacent or complex buildings (few buildings):
    - Low concentrations and low local emissions: Use simple Gaussian models (Figure 1)
    - High concentrations and/or high local emissions: Use simple Gaussian or Gaussian models with street-canyon parametrizations (Figure 2).

- For adjacent regular and irregular buildings:
    - Symmetric street-canyon and no contribution from nearby large roads (Figure 3):
        - Low local emissions and concentrations: Advanced Gaussian modelling systems, with parameterizations for asymmetric street-canyon can be used
        - High emissions and concentrations: Advanced Gaussian modelling systems, with parameterizations for asymmetric street-canyon can be used. However, expert judgment is required to evaluate whether more complex modelling systems based on CFD, AI (trained with CFD), and Lagrangian models are necessary.
    - More complex street-canyon (asymmetric and/or pollution coming from nearby large roads) (Figure 4): CFD, AI (trained with CFD), and Lagrangian modelling are recommended. Nevertheless, expert judgment or validation may be used to evaluate whether advanced Gaussian modelling systems, with parameterizations for asymmetric street-canyon, are appropriate to use.
- For very complex urban configurations which strongly affect the wind flows and turbulence (blocks or large areas with complex buildings with strong variations in building heights; multiple street junctions; tunnel outlets; relevant street vegetation) (Figure 5): CFD-based modelling systems must be used. Other model systems based on AI (trained with CFD) or Lagrangian models can be used following appropriate on-site validation with observations. Advanced Gaussian modelling systems with suitable street-canyon parametrizations could be used only for preliminary screening to detect hotspots in street canyons. More complex models, that explicitly resolve wind flows, would be required to get more reliable estimates of the pollutant concentrations and their spatial distribution in such complex areas.

This workflow for selecting the suitable models is summarized in Figure 6. Whenever possible, the modelling system to be applied should always be evaluated with on-site experimental data (see section 4.7).

Figure 1. 2D and 3D examples of urban configuration with few and no complex buildings (images from Google Earth).

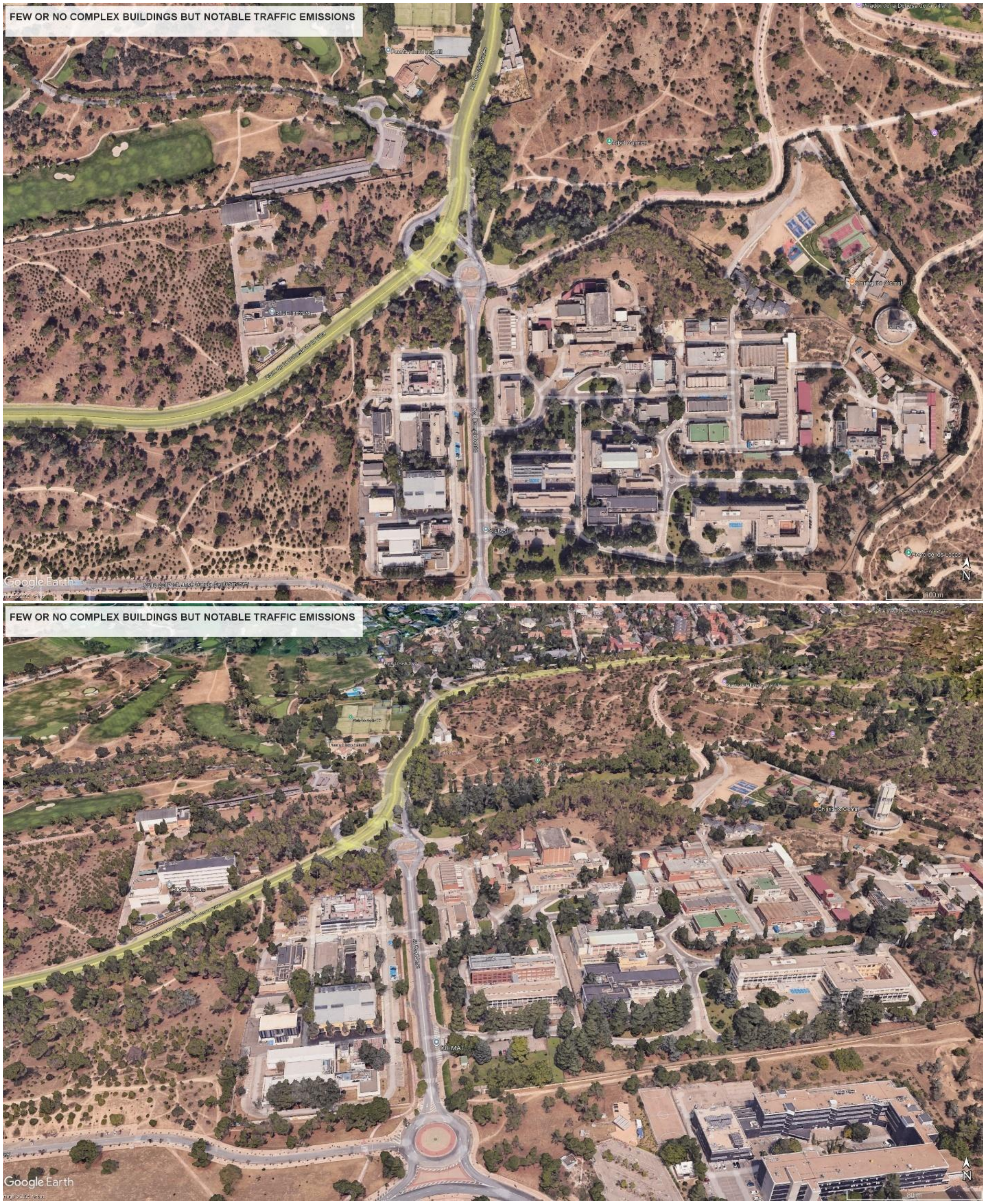

Figure 2. 2D and 3D examples of urban configuration with few and no complex buildings and high local emissions (images from Google Earth).

Figure 3. 2D and 3D examples of urban configuration with regular and irregular buildings without high local emissions (images from Google Earth).

Figure 4. 2D and 3D examples of urban configuration with regular and irregular buildings with high local emissions (images from Google Earth).

Figure 5. 2D and 3D examples of a very complex urban configuration (images from Google Earth).

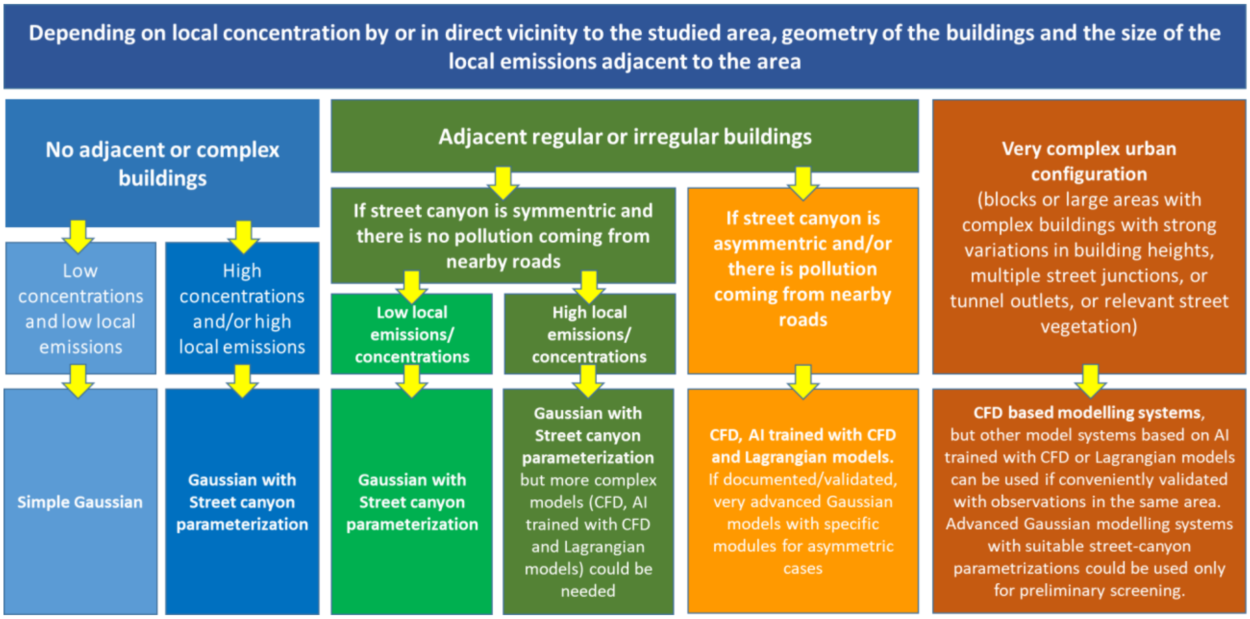

Figure 6. Workflow based on Haeger-Eugensson et al (2021) and Martín et al (2024,2025) to choose microscale air quality modelling systems depending on the urban configuration, pollutant concentrations, and emissions

3.6. Recommendations on the estimation of limit values exceedances and spatial representativeness areas

Studies carried out in the FAIRMODE WG4 (Martín et al, 2025) have shown that microscale air quality modelling systems are good at predicting NO_2 limit value exceedances (LVEA) and the spatial representativeness (SRA) areas of urban air quality stations. Small SRA (low concentration tolerances or traffic stations) are more difficult to predict. Guidance on how to compute LVEA and SRA can be found in Stijn Janssen et al. (2023) and FAIRMODE (2025).

The CFD-based modelling systems seem to provide more consistent results when predicting LVEA and SRA. Furthermore, unsteady full-month CFD simulations do not seem to provide significantly better results than the scenario CFD simulation methodologies. AI trained with CFD models and Lagrangian models (in this order) also achieved good results. Finally, the Gaussian models benefit significantly from street canyon parameterization when predicting SRA and LVEA. For a background station, these Gaussian models with parameterization deliver similar values for LVEA and SRA. However, the SRA for the traffic station is smaller, and in this case, the Gaussian models with street canyon parameterization do not show such good performance. Generally, the Gaussian models appear to overpredict the SRA. Gaussian models without street-canyon parametrization yield the worst results of LVEA and SRA.

In summary, the workflow for selecting the most suitable modelling system to be used for estimating the LVEA and SRA could be the same as shown in Figure 6. However, more studies should be done to further generalize this conclusion.

As the modelling results can have a significant bias with respect to the observations, several bias correction methodologies were applied to compare potential improvements in LVEA and SRA. The proposed bias correction methods for NO_2 are summarized here based on Martin et al. (2025):

- ***Modeled data modified using the averaged sampler bias (ASBC).*** Modeled concentrations at the sampler's locations are modified using the average bias of the monthly NO_2 concentration over all the samplers.

$$B = \overline{C_{MS} - C_{OS}}, \quad MSBC_S = C_{MS} + B$$

  where C_{MS} is the concentration predicted by a modelling system at the sampler site *S*, C_{OS} is the concentration measured by the sampler *S*, *B* is the mean bias of the predictions of a modelling system, and $MSBC_S$ is the bias-modified concentration at the sampler site *S*.

- ***Modelled data modified using reference station bias (MSBBG for background station, MSBTF for traffic station).*** Modelled data at each sampler location are corrected based on bias at a station location using the difference of monthly NO_2 concentration prediction of the modelling system at each station location with respect to the observed data to modify all the sampler estimates from each modelling system. It can be done for the background and traffic stations, respectively.

$$\Delta C_{BGS} = C_{MBGS} - C_{OBGS}; \quad MSBBG_S = C_{MS} + \Delta C_{BGS}$$

$$\Delta C_{TFS} = C_{MTFS} - C_{OTFS}; \quad MSBTF_S = C_{MS} + \Delta C_{TFS}$$

  where C_{MBGS} is the predicted concentration at the background station *BGS*, C_{MTFS} is the same but at the traffic station *TFS*. C_{OBGS} is the concentration measured at the background station *BGS,* while C_{OTFS} is the observation at the traffic station *TFS.* $MSBBG_S$ and $MSBTF_S$ are the modified concentrations at the sampler location *S* by the background and traffic station, respectively.

- ***Modelled data modified using linear regression*** (*Ax+B*). The linear regression functions were computed for every concentration data set of the modelling systems with the observed concentrations from the samplers. The slopes *A* and the intercepts *B* were computed for every modelling system.
- ***Modelled data modified using linear regression with intercept zero*** (*Ax*). The coefficients *A* were computed for every modelling system as in the former case.

However, it was not possible to determine what model data correction could be suitable because there is no clear tendency to improve the raw data. It seems to slightly depend on the modelling system type, but it could be very particular to the case studied. Surely, further studies with other urban configurations should be conducted.

3.7. Model Uncertainty and Evaluation

Regardless of the level of complexity, every model should be evaluated with field data to determine the expected level of uncertainty. Ideally, the evaluation should be done over the same area. When this is not possible, the modelling system should be evaluated under similar urban configurations.

Concerning the criteria that a model is fit for purpose, no recommendations can be given besides those already existing in the CFD community. However, there is the possibility to use the criteria developed in WG2 and adopted by the new AAQD (2024). This follows the Model Quality Indicators to define if a model reaches the Model Quality Objective. However, further studies should be done about the availability of suitable measured data tailored to evaluate micro-scale models. In particular, how many measuring points are needed for a correct model evaluation at this level of spatial resolution. Additionally, investigate whether some specific statistical metrics are preferred for urban microscale modelling. All of these will be tackled in the coming years, and future intercomparison exercises. The resulting conclusion will be incorporated into the new versions of this Guidelines document.

Model uncertainty is an important issue that must be addressed in subsequent versions of this guidance. Additional studies are needed to investigate the sources of uncertainties (representation of chemistry, turbulence in CFD modelling, spatial resolution, emissions, meteorology, modelling approach, etc) and to explore methods to estimate them.

4. Conclusions

Micro-scale air quality modelling systems provide added value on top of the measurements by resolving strong spatial gradients at street level. To be suitable for micro-scale air quality assessment, these models should deliver high -resolution concentration maps at pedestrian height, considering relevant representation of urban geometries, emissions and meteorological conditions. In case of CFD modelling systems, compliance with established CFD best practices guidelines is essential.

High-quality emission inventories for NO_2 and particles are crucial of model reliability. Traffic emissions should be well represented, including minor roads, lane-level detail where relevant, and both exhaust and non-exhaust particle emissions. Other sources (domestic, industrial, ports, etc.) should be included where significant, with appropriate spatial and vertical disaggregation. Hourly temporal resolution is required, typically derived from annual inventories using representative temporal profiles.

Meteorological input data must be representative of the modelling domain and provided at least hourly information. Both measured data from suitable undisturbed weather stations and outputs from validated mesoscale meteorological models are acceptable, with the latter offering advantages in terms of spatial coverage and vertical profiles despite lower accuracy.

Background pollution represents an important contribution to urban hot-spot concentrations and but double-counting needs to be avoided. This can be achieved using nearby urban background measurements or validated regional/urban CTM outputs.

Regarding model choice, evidence from the FAIRMODE WG4 intercomparison exercise and current state of the art, shows that models explicitly accounting for building effects yield the most realistic street-scale concentration patterns. CFD-based models deliver the highest accuracy but are computationally demanding. However, this limitation can be mitigated with wind-sector scenario approaches. Lagrangian models and CFD-trained AI models offer a promising compromise between accuracy and computational efficiency. Gaussian models are suitable only when enhanced with street-canyon parameterizations and mainly for simpler urban configurations or preliminary screening. A detailed scheme to select the type of modelling is proposed in Figure 6.

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