



Downscaling system for modelling of atmospheric composition on regional, urban and street scales

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10 **Abstract.** In this study, the downscaling modelling chain for prediction of weather and atmospheric composition is described and evaluated against observations. The chain consists of interfaced models for forecasting at different spatio-temporal scales and run in a semi-operational mode. The forecasts were performed for European (EU) regional and Danish (DK) sub-regional/urban-scales by the offline coupled numerical weather prediction HIRLAM and atmospheric chemical transport CAMx models, and for Copenhagen city/street scale - by the online coupled computational fluid dynamics M2UE model.

15 The results showed elevated NO_x and lowered O_3 concentrations over major urban, industrial and transport land/water routes in both the EU and DK domain forecasts. The O_3 diurnal cycle predictions in both these domains were equally good, although O_3 values were closer to observations for Denmark. At the same time, the DK forecast of NO_x levels was more biased (with better prediction score of the diurnal cycle) than EU forecast, indicating a necessity to adjust emission rates. Further downscaling to the street level (Copenhagen) indicated that the NO_x pollution was 2-fold higher on weekend and

20 more than 5 times higher during working day with high pollution episode. Despite of high uncertainty in road traffic emissions, the street-scale model captured well the NO_x diurnal cycle and onset of elevated pollution episode. The demonstrated downscaling system could be used in future online integrated meteorology and air quality research and operational forecasting, as well as applied for impact assessments on environment, population and decision making for emergency preparedness and safety measures planning.

25 1 Introduction

A progress in numerical weather and atmospheric composition modelling and continuously increasing supercomputing power make it possible to perform downscaling and nesting from the global to the local scales reaching necessary horizontal and vertical resolutions for a very detailed local meteorology and pollution forecasts. The global and regional scale Atmospheric Chemistry Transport (ACT) modelling systems actively developed and applied during the last decade. These

30 were developed and applied within the frameworks of multiple EU FP6, FP7 and H2020 Monitoring of Atmospheric



Composition and Climate (MACC) projects (Hollingsworth et al., 2008; Simmons, 2010; Peuch et al., 2014; Peuch et al., 2016). Such systems simulate mostly the regional background of air pollution, for instance, in the Copernicus Atmosphere Monitoring Service (CAMS; Grasso, 2017). These large-scale models with increased resolution have limited performance improvement for rural areas (Schaap et al., 2015), but have better modelling scores at reproducing spatio-temporal pollution
35 gradients in and near large urban areas. As a matter of fact, urban and street air pollution is usually several times higher than the pollution at regional scale over suburbs and rural areas and is mostly associated with both local emission sources (Falasca and Curci, 2018) and dominating urban weather conditions (González et al., 2018). Therefore, improvements in performance of high-resolution models for urban areas are closely linked to availability and quality of emission inventories at high spatio-temporal resolution as well as accurate simulation of urban meteorology (Mahura et al., 2008a; Mahura et al.,
40 2008b; Pepe et al., 2016).

Generally, within the deterministic modelling approach, there are two ways applicable for downscaling modelling. It can be performed with a single model capable of local grid refinement (Gettelman et al., 2018) or nesting of numerical grids (Petersen et al., 2005; Lauwaet et al., 2013). It can be also realised as a chain of different resolution models interfacing with each other (Temel et al., 2018; Veratti et al., 2020). In the latter case, the need of different models is justified by the fact that
45 mesoscale models cannot capture local scale processes accurately since the fine-scale flow patterns should be explicitly resolved rather than parameterized (Schlünzen et al., 2011; Ching, 2013). As for the air-quality prediction systems, an offline (Kukkonen et al., 2012) and online (Baklanov et al., 2014) approaches of coupling meteorological and chemical transport models have been commonly used. Each of these has its own advantages and limitations.

The goal of this paper is to demonstrate and evaluate applicability of the downscaling system coupled with computational
50 fluid dynamics model on an example of operational modelling of an acute air-pollution episode. This system consists of several models with nested numerical grids where meteorological and atmospheric composition prediction on regional- and sub-regional/urban-scales is performed. Three interfaced and coupled models – (i) numerical weather prediction (HIRLAM; Undén et al., 2002); (ii) atmospheric chemical transport (CAMx; Ramboll Environ, 2016; Amstrup et al., 2010a; Amstrup et al., 2010b); (iii) computational fluid dynamics (M2UE; Nuterman, et al., 2010; Sabatino, et al., 2011) – were used for
55 airflow and pollution prediction at city/street-scale (on example of Copenhagen, Denmark). In the Methodology section, we firstly describe the applied models and their configurations; and secondly - their interplay within semi-operational setup of the downscaling system. The Results and Discussion section presents the models' evaluation against two urban observation sites (at roof and street levels) as well as recommendations about possible improvements in downscaling system to achieve better prediction quality of forecasting at finest scales.

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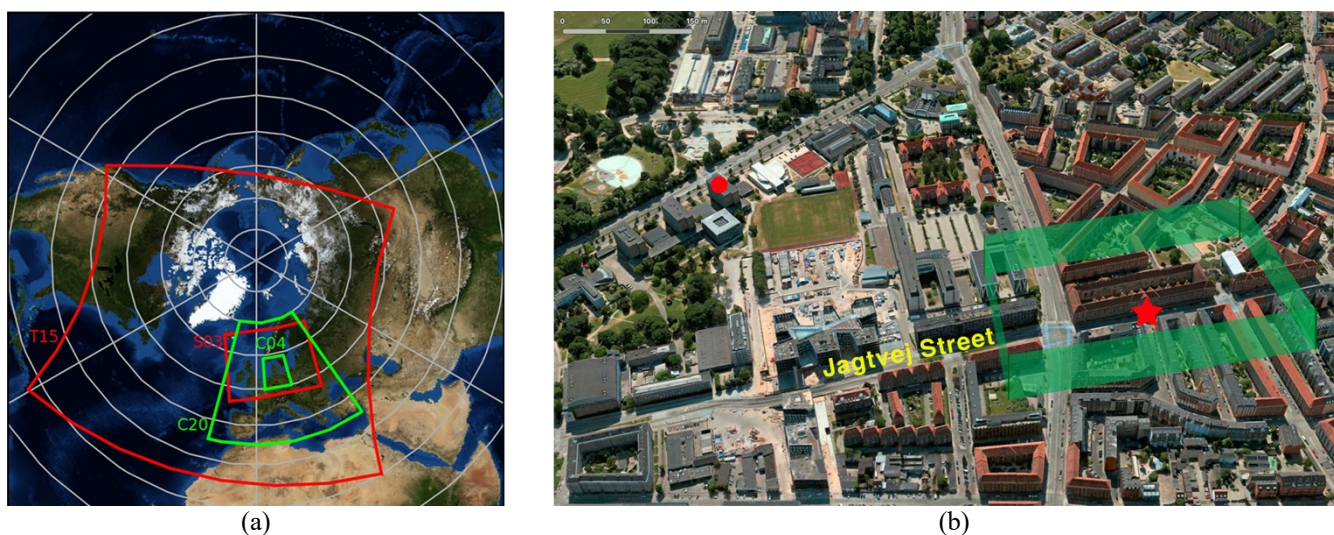


2 Methodology: downscaling model system

2.1 Description of models

HIRLAM

The Numerical Weather Prediction (NWP) model used in the current downscaling system is the DMI's version of High-Resolution Limited Area Model (HIRLAM; Undén et al., 2002; Petersen et al., 2005). It has basic components such as the hydrostatic semi-Lagrangian dynamical core, digital filtering initialization (Lynch and Huang, 1992), physical parameterization of radiation processes (Savijärvi, 1990), cloud-microphysics Soft Transition Condensation scheme (Sass, 2002), turbulence parametrization (Cuxart et al., 2000), and Interaction-Soil-Biosphere-Atmosphere surface scheme (ISBA; Noilhan and Planton, 1989). The ISBA scheme also includes the building effect parametrization (BEP; Martilli et al., 2002) module to account for effects associated with urban anthropogenic heat flux and roughness. The model is forced by meteorological lateral boundary conditions and 3D-VAR assimilated ground-based and satellite observation data (Gustafsson et al., 2001; Lindskog et al., 2001). The lateral boundaries are received every 6 h interval from the European Centre for Medium-Range Weather Forecasts (ECMWF) and had horizontal grid resolution of $0.15^{\circ} \times 0.15^{\circ}$.



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Figure 1: (a) operational and research modelling domains for European regional-scale (HIRLAM-T15+CAMx-C20) and sub-regional/urban Denmark scale (HIRLAM-S03+CAMx-C04) forecasts; (b) Nørrebro district of Copenhagen urban area with 2 air-quality monitoring stations, where red circle indicates a roof level air-quality observation at H.C. Ørsted Institute and red star indicates Jagtvej Street level observation; the green trapezoid shows M2UE modelling domain (extracted from © Apple Maps 2020).

In this study, the chosen modelling domains were used for operational numerical weather prediction at DMI. These two domains with crude (T15: $0.15^{\circ} \times 0.15^{\circ}$) and fine (S03: $0.03^{\circ} \times 0.03^{\circ}$) horizontal grids were applied for European regional and sub-regional/urban Denmark scale modelling (Figure 1a), correspondingly. In vertical, 40 hybrid pressure levels (starting



85 from 32 m above ground) were used in T15 domain and 65 such levels (starting from 12 m above ground) - in S03 domain. The upper boundary reached 10 hPa at the top of the atmosphere in both computational domains.

There are approximately 8 x 8 horizontal grids cells (each cell is about 3 x 3 km size) covering the Copenhagen metropolitan area in S03 domain. According to (Mahura et al., 2008b), the HIRLAM model with activated BEP module must have at least 4 times more grid cells to predict a significant effect of the city area on meteorology. Thus, the BEP module was disabled
90 during operational forecasting with S03 domain, considering the employed numerical grid as well as city size and urban characteristics of Copenhagen.

CAMx

The Comprehensive Air Quality Model with Extensions (CAMx; Ramboll Environ, 2016) is the finite volume ACT model
95 for regional- and urban-scales employed for air-quality forecasting in our downscaling system. An updated version of Carbon Bond IV (CB-IV) Mechanism (Gery et al., 1989) with improved isoprene chemistry (Yarwood et al., 2005) and 2-mode aerosol microphysics scheme were used in the current setup. The Tropospheric Ultraviolet and Visible radiation model (Madronich and Focke, 1998) was applied to calculate photolysis rate coefficients. Further details about gas-phase chemistry and aerosol microphysics together with wet (Seinfeld and Pandis, 2016) and dry (Wesely, 1989; Slinn and Slinn, 1980)
100 deposition schemes are described in the model's users guide (Ramboll Environ, 2016).

For this study, two computational domains (Figure 1a) were selected within the ACT model for modelling on regional- (C20: 0.2°×0.2°) and sub-regional/urban scales (C04: 0.04°×0.04°) forced by meteorological output (with a coupling interval of 1 hour) from HIRLAM-T15 and -S03 modelling domains, respectively. The vertical resolution of CAMx numerical grid is defined by the one of meteorological driver and therefore, corresponds to 25 HIRLAM hybrid pressure levels covering the
105 lowest 3 km of the troposphere. The chemical initial and boundary conditions for regional-scale modelling are represented by climatological mean values, and those for the sub-regional/urban scale modelling are obtained from the regional scale CAMx model output.

The emission rates were calculated from emission inventory provided by TNO (Kuenen et al., 2010). The inventory has longitude-latitude resolution of 0.125°×0.0625° and covers the entire Europe, Western Russia and Northern Africa. It
110 includes gases (NO_x , SO_2 , CO , $NM VOC$, NH_3 , CH_4) and lumped primary aerosols with diameters less than 2.5 μm and 10 μm . The emission rates are associated with different anthropogenic sources attributed to various anthropogenic activities according to the Selected Nomenclature for sources of Air Pollution (SNAP).

M2UE

115 For the city/street scale modelling, the Micro-scale Model for Urban Environment (M2UE) was developed and applied. It is a Computational Fluid Dynamics (CFD) code for airflow and pollution prediction in an urban environment (Nuterman et al., 2010), which is able to simulate a complex aerodynamics in heterogeneous urban canopy with penetrable (vegetation) and impenetrable (buildings) obstacles and traffic induced turbulence. The model includes three-dimensional system of



Reynolds', $k - \epsilon$ model of turbulence, and the 'advection-diffusion' equations to simulate atmospheric chemistry transport.
120 A numerical solution of governing equations is based on the fully implicit time advancing scheme and the finite volume
method (Patankar, 1980; Ilin, 1995; van Leer, 1974). The model is coupled with simplified atmospheric gas-phase chemistry
mechanism with 19 chemical reactions (Stockwell and Goliff, 2002). Such simple chemistry is dictated by the fact that the
model was run in a semi-operational mode, which implies relatively short forecasting time on available computer facility. In
the future, when more powerful supercomputers become available the mechanism could be extended or improved with more
125 comprehensive one.

The computational domain (a section of Jagtvej Street and surroundings) used in the current study is explicitly defined by
buildings, roads, vegetation of the Copenhagen metropolitan (Figure 1b) area obtained from the high-resolution Danish
Elevation Model dataset (Flatman et al., 2016). The horizontal and vertical extent of the computational domain is 500 x 500
x 100 m. The horizontal and vertical numerical grids with local refinement of grid-cells ranging from 1 m at the Jagtvej
130 Street to 5 m near the domain's boundaries was used. The Jagtvej Street emission inventory was derived from hourly traffic
counts (Berkowicz et al., 2004) and emissions for different types of road-vehicles (Chao et al., 2018).

2.2 Description of downscaling model system

In the developed downscaling model system (Figure 2), both the European regional (hereafter referred to as the EU) and the
sub-regional/urban Denmark scale (hereafter referred to as the DK) forecasts were performed by the off-line coupled
135 HIRLAM and CAMx models. After up-to-date meteorological data assimilation and boundary conditions from ECMWF
became available, the HIRLAM-T15 produced 48 h meteorological forecast for the EU domain. This NWP model was
always fully spun-up, because such forecast was performed in a continuous manner 4 times per day (at 00, 06, 12 and 18
UTC). Afterwards, the meteorological output was post-processed, interpolated and adapted to drive the CAMx-C20 model
with a spin-up time of 48 hour and the forecast length of 24 hour. The spin-up integration was the model's cold-start run
140 prior to the current forecasted day. The entire cycle of offline coupled HIRLAM-T15+CAMx-C20 modelling chain took
approximately 4.5 hour of CPU time.

As soon as the EU scale forecast is completed, the DK scale forecast of meteorology and atmospheric composition is
initiated. In general, the entire procedure of model runs and interplay is very similar to the EU modelling chain. However,
the differences were in boundary conditions, forcing and resolution of numerical grids. The HIRLAM-S03 meteorological
145 forecast was forced by outer model lateral boundaries, while the CAMx-C04 atmospheric composition forecast was forced
by meteorology from HIRLAM-S03 plus chemical boundary and initial conditions from CAMx-C20. The forecast length of
HIRLAM-S03 and CAMx-C04 runs was 36 h and 24 h, respectively. The forecast cycle used 4 h of CPU time since the DK
forecast initiation.

After the urban-scale forecast completed, the street-scale (hereafter referred to as the street) forecast is launched for a section
150 of Jagtvej Street of Copenhagen and surroundings. For the Jagtvej's domain inlet boundaries, the Dirichlet conditions with
constant profiles of airflow characteristics (from HIRLAM-S03) and atmospheric composition fields (from CAMx-C04)



were chosen to drive the M2UE model. The outlet boundary conditions are of Neumann type. The forecast for 24 h was performed after HIRLAM-S03+CAMx-C04 completed runs and it took ~1.5 h of CPU time. Since the M2UE model is very computationally expensive, the 24 h forecast was performed with 24 instant integration cycles forced by hourly HIRLAM-CAMx models' output. In this case, the spin-up time was just several minutes; so, such as for individual M2UE forecast. It is a reasonable approach of doing such the forecast, because the boundary conditions and emission rates for each integration cycle were constant and only the rapid-photochemical reactions of O_3 and NO_x were of principal interest in the study. Therefore, the air-flow regime was assumed to be steady during an instant integration cycle. The ratio of horizontal resolution of HIRLAM-S03+CAMx-C04 and M2UE-Jagtvej domains exceeds a permissible limit of 5 (Sokhi et al., 2018). However, the runtime of the entire modelling chain equals to 10 CPU hours, and adding an intermediate domain (or chain of domains) between these 3 model domains will obviously lead to increased runtime over 12 hours. Such large span of forecasting time is considered to be too large, taking into account the time constrains for operational tasks and cases when the models' rerun is required (not to mention pre-processing and post-processing the large amount of models' input and output). Thus, such downscaling is a trade-off between acceptable runtime and permissible resolution.

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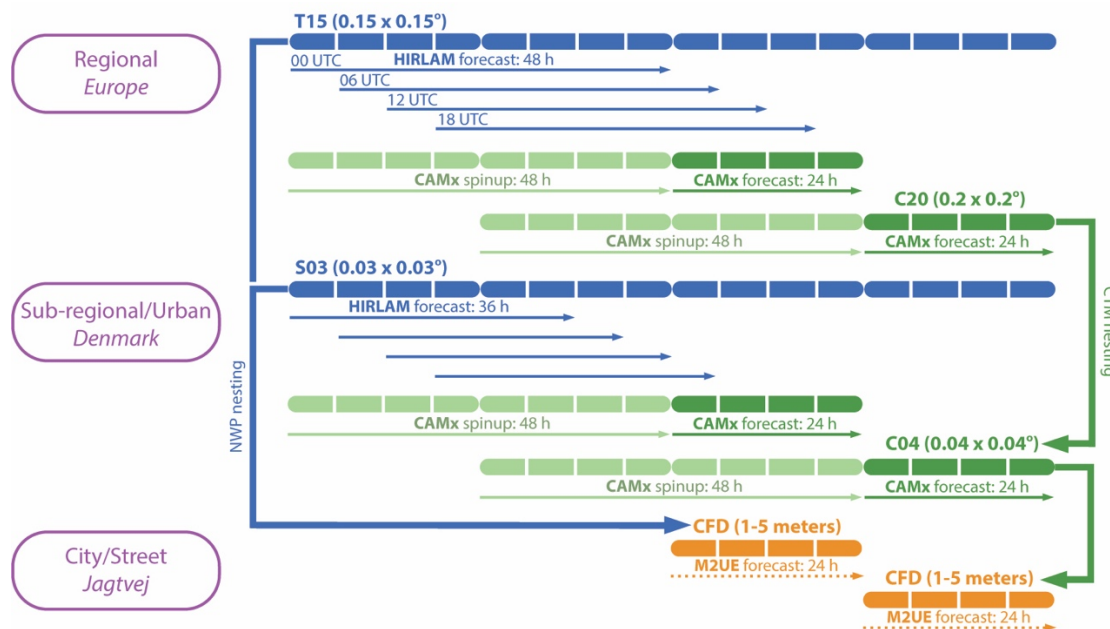


Figure 2: Downscaling modelling system: from the European regional-scale forecast (HIRLAM-T15+CAMx-C20) to the sub-regional/urban Denmark (HIRLAM-T03+CAMx-C04) and city/street scale for Copenhagen (CFD M2UE); the blue, green and orange horizontal bars indicate NWP HIRLAM, CTM CAMx and CFD M2UE forecasts, respectively; horizontal and vertical arrows indicate the forecasts' cycles and downscaling (dataflow), correspondingly.



3 Results and Discussion

The example of the downscaling modelling chain realised in this study in a semi-operational mode with coupled HIRLAM+CAMx+M2UE models is described and evaluated with focus on Denmark and Copenhagen for specific meteorological situation.

175 During 4-5 September 2011 the meteorological situation was the following. The cyclonic system originated over Iceland moved southward towards the British Islands, and then eastward towards the Jutland Peninsula of Denmark with gradually changing atmospheric pressure from 990 to 1010 hPa. The cold front associated with cyclone passed over UK and Denmark on these days. On 4th September morning, the cold front approached the northern part of the Jutland Peninsula, and then propagated towards the Zealand Island, and brought up to 10 mm of accumulated (6 hour) precipitation. Over Denmark, 180 during night-morning hours on 5th September, the precipitation increased on average up to 15-20 mm (with several local maxima up to 40 mm). During these days, on a diurnal cycle the air temperature's range was 18-24 °C and 12-18 °C (on 4th and 5th September, respectively) with further gradual cooling. The vertical sounding diagrams (Schleswig, Germany, 54.53° N, 9.55° E – the closest station to Denmark) showed the presence of the temperature inversion layer extended up to 1.5 km (at noon on 4th Sep) and reduced to 500 m altitude (at night on 5th Sep), and then a layer of smaller depth remained at top of 185 boundary layer at noon.

A near surface spatial distribution of O_3 and NO_x concentrations (Figure 3ab) within the EU domain is shown for 5th Sep 2011, at 10 UTC. As seen, the elevated NO_x concentration of up to 50 $\mu\text{g m}^{-3}$ was observed over urban, industrial and port areas of Denmark and neighbouring countries. In addition, the North Sea oil extraction and international shipping were other sources of elevated NO_x levels over the Danish territorial waters. The near surface O_3 concentration varied within the range 190 of 40-150 $\mu\text{g m}^{-3}$, with local minima over and downwind the areas of anthropogenic NO_x sources (Figure 3a) where ozone was depressed due to the NO_x titration.

As for the nested DK domain (Figure 3cd), it is seen from the near-surface wind and concentrations patterns that the mesoscale circulation as well as the local anthropogenic emission sources were resolved in greater details due to the finer S03-C04 horizontal resolution. Therefore, one can observe additional local concentration maxima of NO_x with higher levels 195 up to 250 $\mu\text{g m}^{-3}$ over Denmark. These were mostly localized near the same type of anthropogenic sources as the mentioned above in the EU domain. As the result, there were more O_3 depression spots including those over the northern Jutland Peninsula's highways over the territories of Denmark and Germany. However, the background values of the near surface ozone did not change significantly at large distances from the anthropogenic NO_x sources.

In Figure 4, the time-series of O_3 and NO_x observations provided by the Danish air-quality monitoring programme (Ellerman et al., 2012) and modelled concentrations by the downscaling system are presented. Those observations were performed by 200 automatic stations (Figure 1b) at the roof level of H.C. Ørsted Institute and at the Jagtvej Street (only NO_x , particulate matter and benzene were measured on the street). As seen in Figure 4a, the T15-C20 and S03-C04 results showed an ability to reproduce well the O_3 diurnal cycle ($EU_{R_p} = 0.81$ and $DK_{R_p} = 0.8$, with $p \ll 5\%$) for both domains at regional- and



sub-regional/urban scales. However, the forecasted O_3 at the EU scale was generally overestimated in comparison to the
205 modelling results at the DK scale ($EU_RMSE = 31$ vs. $DK_RMSE = 19$). Although, the NO_x levels were generally
overestimated in the DK scale forecast (Figure 4b) when compared to the EU scale forecast and observations ($EU_RMSE =$
 23 vs. $DK_RMSE = 47$), the diurnal cycle at the DK scale is better captured according to obtained Pearson correlation
values ($EU_R_p = 0.56$ vs. $DK_R_p = 0.69$). And it is particularly notable when the NO_x peak was observed during several
morning hours (on 5th Sep 2011, 07 UTC). This caused by the complex unfavourable meteorological conditions over the
210 Copenhagen metropolitan area and high emission rates mainly from intense morning traffic. The timing and levels of NO_x
peak were well captured by the DK scale forecast in contrast to the EU one, which poorly predicted it with slightly elevated
 NO_x values. Note, the O_3 depression at the same time, which was not captured by the EU air-quality forecast. Since the
primary sources of atmospheric nitrogen are anthropogenic emissions, its overestimated concentrations are rather attributed
to pre-processing and treatment of emission rates. It can be related to interpolation of original gridded emissions into the
215 meshes of ACT model, which is apparently insufficient, and therefore, some additional rescaling adjustments in terms of
emission rates and their time dynamics are required.

The diurnal cycle of NO_x concentrations observed and modelled for the Jagtvej Street is shown in Figure 4c. Following
analysis and calculated correlation value ($R_p = 0.66$), the street-scale M2UE model forecasted well the observed NO_x
diurnal cycle including the onset of elevated air pollution episode on 5th Sep (see forecast length 30-35 h). It corresponded to
220 the local time of 8-10 h of a typical working day (Monday) when the most intense road traffic is observed. However, the
model's quantitative estimate of concentration is substantially biased (with $RMSE = 103$) particularly during 5th Sep 2011.
In spite of the captured elevated NO_x levels, the model predicted two peaks at 31 and 34 h of forecast length and depression
at 32 h, while the time-series of observations showed only one peak at 32 h, which was approximately $200 \mu\text{g m}^{-3}$ higher
than the modelled peaks.

225 There are several reasons why the M2UE model was able to make the qualitatively good prediction in general but had
difficulties at capturing the elevated NO_x concentrations. First of all, it is the coupling interval span of the offline coupled
models (HIRLAM+CAMx), which plays an important role in constraining the influence of mesoscale disturbances on
evolution of atmospheric composition (Korsholm et al., 2011). It might give an offset in timing and position of the predicted
concentrations. As seen in Figure 4ab, the effect of that at the onset of the high air pollution episode (where its slight offset
230 of approximately half an hour) was observed, and then inherited by the nested micro-scale model. The second reason is that
the M2UE forcing was provided on an hourly basis by the HIRLAM-S03+CAMx-C04 modelling chain. Such forcing is
rather crude in terms of time and horizontal resolution for the CFD model capable to predict very fine spatio-temporal
turbulent flow scales occurring within meters and seconds. The third reason is an uncertainty in local road traffic emissions
used by the M2UE model, although some traffic count data and information about emissions from different types of vehicles
235 were available (Chao et al., 2018). Although those above-mentioned shortcomings, the presented downscaling modelling
system was able to produce good quality atmospheric composition forecasts across different spatial and temporal scales.

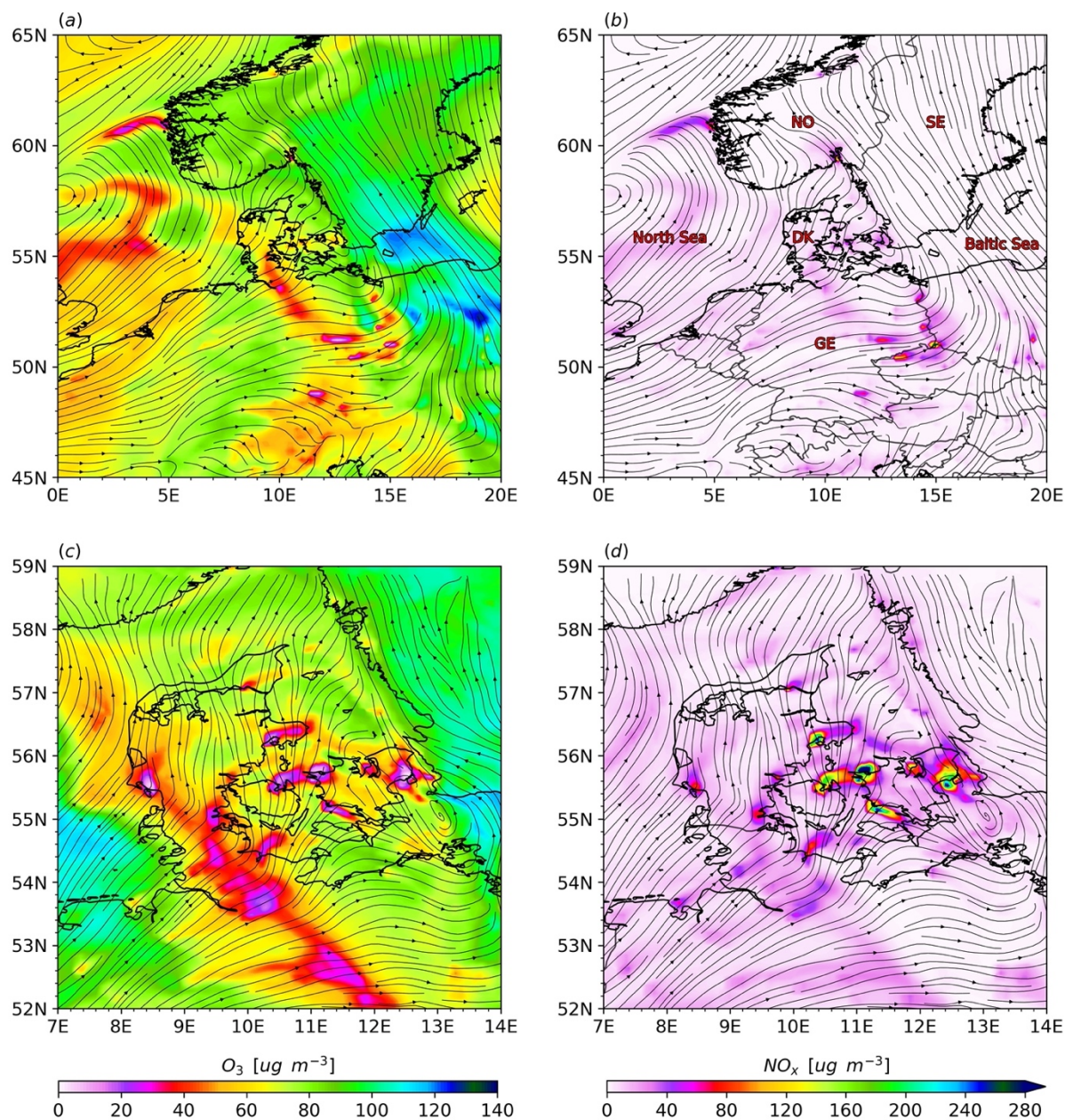
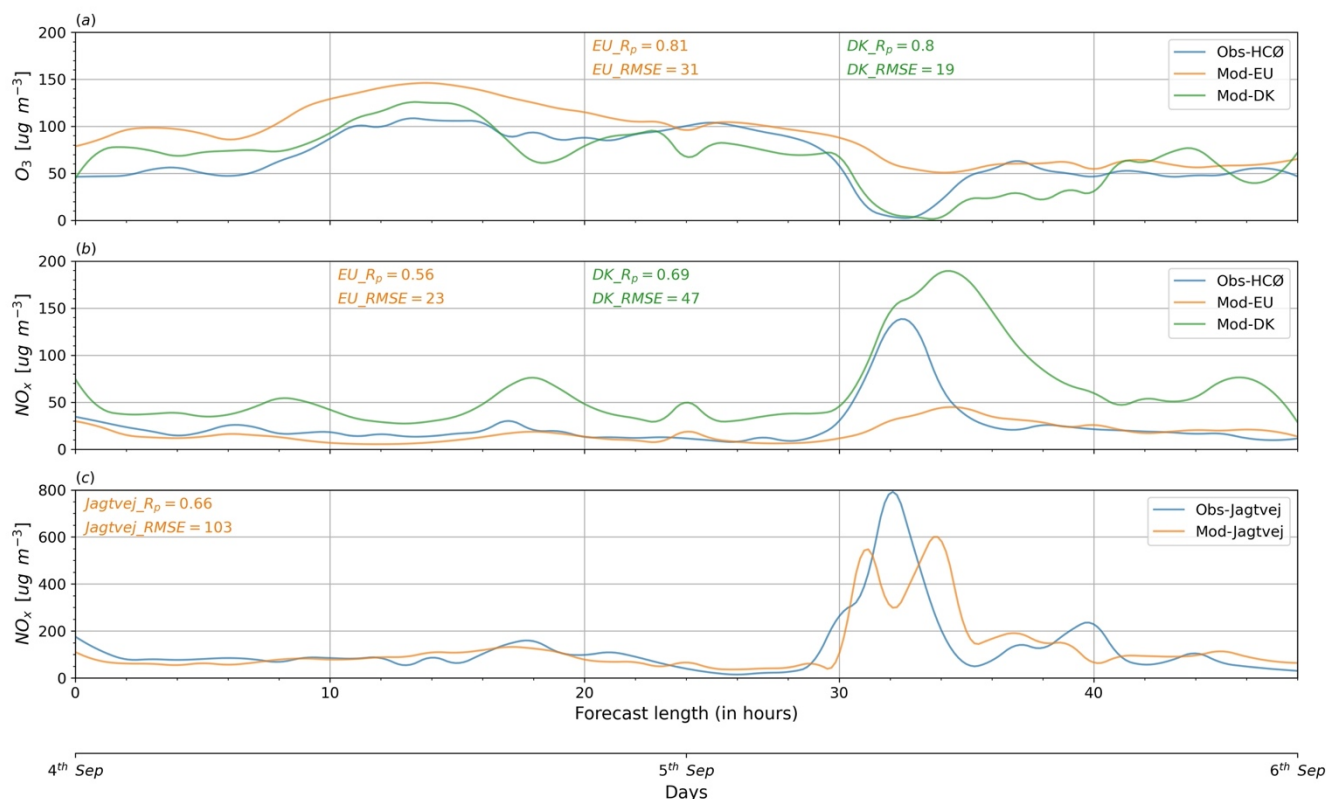


Figure 3: Simulation output on 5 Sep 2011, 10 UTC: HIRLAM-T15+CAMx-C20 results for concentrations in $[\mu\text{g m}^{-3}]$ of (a) O_3 and (b) NO_x within the European regional-scale domain and HIRLAM-S03+CAMx-C04 results for concentrations of (c) O_3 and (d) NO_x within the Denmark sub-regional/urban scale domain.



245 **Figure 4:** Time-series of observations at the building’s roof level vs. HIRLAM+CAMx+M2UE forecasts for (a) O_3 and (b, c) NO_x for the European, Denmark and Copenhagen modelling domains during Sunday-Monday 4-5 Sep 2011; (a, b) HCØ roof level observations of O_3 and NO_x vs. modelling results for EU and DK domains; (c) Jagtvej Street level observations of NO_x vs. M2UE /Pearson’s correlation R_p and root mean square error RMSE of modelled vs. observed concentrations for 3 domains/.

4 Conclusions

250 In this study, the downscaling modelling system for real time prediction of weather and atmospheric composition up to the street scale has been described and tested. It consists of several interfaced models. The forecasts were performed at the regional and sub-regional/urban-scales by the offline coupled operational numerical weather prediction HIRLAM and atmospheric chemical transport CAMx models and at the city/street scale by the online coupled computational fluid dynamics M2UE model. The downscaling system was tested for the Europe (EU), Denmark (DK) and Copenhagen’s street domains in a semi-operational forecasting mode and evaluated against existing observations for a high pollution episode of
255 4-5 September 2011.

The results of modelling showed elevated NO_x and lowered O_3 concentrations over major urban, industrial and transport land/water routes in both EU and DK scale forecasts. The comparison of these forecasts showed higher levels of NO_x and slightly lower O_3 in the DK domain because of higher NO_x emission rates and titration. The O_3 diurnal cycle predictions in both the EU and DK domains are equally good, although O_3 values were closer to observations for DK. At the same time,



260 the DK scale forecast of NO_x levels was more biased (with better prediction score of the diurnal cycle) than EU scale
forecast. Further downscaling to the street level indicated that the NO_x pollution (mainly from road traffic) was 2-fold higher
on weekend and more than 5 times higher during working day with high pollution episode. Despite of high uncertainty in
road traffic emissions, the M2UE model captured well the NO_x diurnal cycle and onset of elevated pollution episode.
265 However, in order to come to the final conclusion about the performance of individual system's components and the entire
downscaling chain, one needs to perform an evaluation for extended time period and additional measurement sites around
Denmark.

A potential improvement of such downscaling system can come from employing online coupled (instead of offline coupled)
mesoscale models. Such approach could help to minimize problems associated with offline coupling interval and therefore,
to give a better fit of modelling results to observations, and to better identify a timing and location of elevated pollution
270 episodes. As for the local-scale predictions, an intermediate additional nested domain between sub-regional/urban and micro-
scale runs for the Copenhagen metropolitan area could provide improvement for local scale airflow and pollution forecasting
scores. However, these will be conditioned on availability of a better-quality high-resolution emission inventory. The
demonstrated downscaling system with the suggested above improvements could be used in future online integrated
meteorology and air quality research and operational forecasting. Such system can be also applied for advanced planning
275 safety measures, post-accidental analysis, emergency preparedness and health/environment impact assessments.
Keeping in mind the main uncertainties (e.g., street-level emissions, increasing number of urban observations, etc.), there are
several possibilities to improve demonstrated urban / street level forecasts using different types of observations (e.g., from
remote sensing, crowd sourcing and citizen science) in urban areas. These observations and recently developing methods
such as the bias correction techniques, machine learning, artificial intelligence and neural networks can also improve air-
280 quality forecasting (see overview e.g., in Bai et al., 2018).

Code availability

The HIRLAM model source code is available under the HIRLAM consortium agreement (<http://hirlam.org>). The CAMx
model source code is an open-source software (can be downloaded from <http://www.camx.com>). The M2UE model source
code is available from the authors upon request.

285 Authors contribution

AB, AM designed the research; BA, RN created and setup integrated downscaling of the models; AZ developed local scale
gas-phase chemistry mechanism; RN performed models' evaluation; RN, AM and AB wrote the paper.



Competing interests

The authors declare that they have no conflict of interest.

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References

- Amstrup B., Baklanov, A., Feddersen, H., Lorenzen, T., Mahura, A., Nuterman, R., Weismann, J., Caian, M., Dumitrache, 300 R., Rada, C., and Craciunescu, V.: Core-downstream processing chain test cases. Evaluation of current R-ENS individual and ensemble forecasts in the Copenhagen and Bucharest areas, in EU FP7 MACC Report D_OINT_2.4.1-2, edited by: Baklanov, A., and Mahura, A., Danish Meteorological Institute, Copenhagen, 36 pp., 2010a.
- Amstrup B., Baklanov, A., Lorenzen, T., Mahura, A., Nuterman, R., Weismann, J., Banciu, D., Tascu, S., Pietrisi, M., Dumitrache, R., and Caian, M.: Core-downstream processing chain test cases. Setup of the two downscaling model 305 configurations, in EU FP7 MACC Report D_OINT_2.5.1-2, edited by: Baklanov, A., and Nuterman, R., Danish Meteorological Institute, Copenhagen, 18 pp., 2010b.
- Bai, L., Wnag, J., Ma, X., Lu, X.: Air Pollution Forecasts: An Overview, *Int. J. Environ. Res. Public Health*, 15, 780; doi:10.3390/ijerph15040780, 2018.
- Baklanov, A., Schlünzen, K., Suppan, P., Baldasano, J., Brunner, D., Aksoyoglu, S., Carmichael, G., Douros, J., Flemming, 310 J., Forkel, R., Galmarini, S., Gauss, M., Grell, G., Hirtl, M., Joffre, S., Jorba, O., Kaas, E., Kaasik, M., Kallos, G., Kong, X., Korsholm, U., Kurganskiy, A., Kushta, J., Lohmann, U., Mahura, A., Manders-Groot, A., Maurizi, A., Moussiopoulos, N., Rao, S. T., Savage, N., Seigneur, C., Sokhi, R. S., Solazzo, E., Solomos, S., Sørensen, B., Tsegas, G., Vignati, E., Vogel, B., and Zhang, Y.: Online Coupled Regional Meteorology-Chemistry Models in Europe, *Atmospheric Chemistry and Physics*, 14(1), 317-398, <https://doi.org/10.5194/acp-14-317-2014>, 2014.
- 315 Berkowicz, R., Britter, R., and Di Sabatino, S.: Optimisation of Modelling Methods for Traffic Pollution in Streets (TRAPOS), National Environment Research Institute, Roskilde, Denmark, 114 pp., 2004.



- Chao, E. L., Rosen, J. A., Hu, P. S., Schmitt, R., Sprung, M. J., Nguyen, L. X., Riley, D., Parker, K., Young, L., Zhang, J., Beningo, S., Chambers, M., Ford, C., Notis, K., Liu, M., and Smith-Pickel, S.: National Transportation Statistics, Bureau of Transportation Statistics, U.S. Department of Transportation, 469 pp., 2018.
- 320 Ching, J.: A perspective on urban canopy layer modeling for weather, climate and air quality applications, *Urban Climate*, 3, 13-39, <https://doi.org/10.1016/j.uclim.2013.02.001>, 2013.
- Cuxart, J., Bougeault, P., and Redelsperger, J.-L.: A turbulence scheme allowing for mesoscale and large-eddy simulations, *Quart. J. Roy. Meteor. Soc.*, 126, 1-30, <https://doi.org/10.1002/qj.49712656202>, 2000.
- Ellermann, T., Nøjgaard, J., Nordstrøm, C., Brandt, J., Christensen, J., Ketzler, M., & Jensen, S.: The Danish Air Quality Monitoring Programme. Annual Summary for 2011, DCE – Danish Centre for Environment and Energy, Aarhus: Aarhus University, 63 pp., <https://www2.dmu.dk/Pub/SR37.pdf>, 2012.
- 325 Falasca, S. and Curci, G.: High-resolution air quality modeling: Sensitivity tests to horizontal resolution and urban canopy with WRF-CHIMERE, *Atmospheric Environment*, 187, 241-254, <https://doi.org/10.1016/j.atmosenv.2018.05.048>, 2018.
- Flatman, A., Rosenkranz, B., Evers, K., Bartels, P., Kokkendorff, S., Knudsen, T., and Nielsen, T.: Quality assessment report to the Danish Elevation Model (DK-DEM), Agency for Data Supply and Efficiency, Copenhagen, 26 pp., 2016.
- 330 Gery, M., Whitten, G., Killus, J., and Dodge, M.: A photochemical kinetics mechanism for urban and regional scale computer modelling, *J. Geophys. Res.*, 94(D10), 12925–12956, <https://doi.org/10.1029/JD094iD10p12925>, 1989.
- Gettelman, A., Callaghan, P., Larson, V.E., Zarzycki, C.M., Bacmeister, J.T., Lauritzen, P.H., Bogenschutz, P.A., and Neale, R.B.: Regional climate simulations with the Community Earth System Model, *Journal of Advances in Modeling Earth Systems*, 10, 1245–1265, <https://doi.org/10.1002/2017MS001227>, 2018.
- 335 González, C.M., Ynoue, R.Y., Vara-Vela, A., Rojas, N.Y., and Aristizábal, B.H.: High-resolution air quality modeling in a medium-sized city in the tropical Andes: Assessment of local and global emissions in understanding ozone and PM10 dynamics, *Atmospheric Pollution Research*, 9(5), 934-948, <https://doi.org/10.1016/j.apr.2018.03.003>, 2018.
- Grasso, O.: Interim evaluation of Copernicus, Final report, Imelpgriuerie centrale, Luxembourg, 224 pp.,
340 <https://doi.org/10.2873/373088>, 2017.
- Gustafsson, N., Berre, L., Hörnquist, S., Huang, X.-Y., Lindskog, M., Navascués, B., Mogensen, K.S., Thorsteinsson, S.: Three-dimensional variational data assimilation for a limited area model. Part I: General formulation and the background error constraint, *Tellus A: Dynamic Meteorology and Oceanography*, 53A, 425-446, <https://doi.org/10.3402/tellusa.v53i4.12198>, 2001.
- 345 Hollingsworth, A., Engelen, R. J., Textor, C., Benedetti, A., Boucher, O., Chevallier, F., Dethof, A., Elbern, H., Eskes, H., Flemming, J., Granier, C., Kaiser, J. W., Morcrette, J.-J., Rayner, P., Peuch, V.-H., Rouil, L., Schultz, M. G., Simmons, A.



- J., and The GEMS Consortium: Towards a monitoring and forecasting system for atmospheric composition: The GEMS Project, *Bull. Amer. Meteor. Soc.*, 89, 1147–1164, <https://doi.org/10.1175/2008BAMS2355.1>, 2008.
- Ilin, V.: *Methods of Incomplete Factorization for Solving the Algebraic Systems*, Moscow: Fizmatlit, 286 pp., 1995.
- 350 Korsholm, U., Baklanov, A., and Sørensen, J.: Status and Evaluation of Enviro-HIRLAM: Differences Between Online and Offline Models, in *Integrated Systems of Meso-Meteorological and Chemical Transport Models*, edited by: A. Baklanov, A. Mahura, and R. Sokhi, 61-74, Springer, Berlin, 2011.
- Kuenen, J., van der Gon, H., Visschedijk, A., van der Brugh, H., Finardi, S., Radice, P., d’Allura, A., Beevers, S., Theloke, J., Uzbasich, M., Honoré, C., and Perrussel, O.: A Base Year (2005) MEGAPOLI European Gridded Emission Inventory
355 (Final Version), MEGAPOLI Scientific Report 10-17, DMI, Copenhagen, 39 pp., ISBN:978-87-993898-8-9, 2010.
- Kukkonen, J., Balk, T., Schultz, A., Baklanov, A., Klein, T., Miranda, A., Monteiro, A., Hirtl, M., Tarvainen, V., Boy, M., Sokhi, R., Lehtinen, K., Karatzas, K., San Jose, R., Astitha, M., Kallos, G., Schaap, M., Reimer, E., Jakobs, H., and Eben, K.: A Review of Operational, Regional-Scale, Chemical Weather Forecasting Models in Europe, *Atmospheric Chemistry and Physics*, 12, 1-87, <https://doi.org/10.5194/acp-12-1-2012>, 2012.
- 360 Lauwaet, D., Viaene, P., Brisson, E., van Noije, T., Strunk, A., van Looy, S., Maiheu, B., Veldeman, N., Blyth, L., de Ridder, K., and Janssen, S.: Impact of nesting resolution jump on dynamical downscaling ozone concentrations over Belgium, *Atmospheric Environment*, 67, 46-52, <https://doi.org/10.1016/j.atmosenv.2012.10.034>, 2013.
- Lindskog, M., Gustafsson, N., Navascués, B., Mogensen, K.S., Huang, X.-Y., Yang, X., Andræ, U., Berre, L., Thorsteinsson, S., Rantakokko, J.: Three-dimensional variational data assimilation for a limited area model. Part II:
365 Observation handling and assimilation experiments, *Tellus A: Dynamic Meteorology and Oceanography*, 53A, 447-468, <https://doi.org/10.3402/tellusa.v53i4.14578>, 2001.
- Lynch, P., and Huang, X.-Y.: Initialization of the HIRLAM Model Using a Digital Filter, *Mon. Wea. Rev.*, 120, 1019–1034, [https://doi.org/10.1175/1520-0493\(1992\)120<1019:IOTHMU>2.0.CO;2](https://doi.org/10.1175/1520-0493(1992)120<1019:IOTHMU>2.0.CO;2), 1992.
- Madronich, S., and Focke, S.: The role of solar radiation in atmospheric chemistry, in *Handbook of Environmental
370 Chemistry*, edited by Boule P., Springer-Verlag, New York, 1–26, 1998.
- Mahura, A., Leroyer, S., Baklanov, A., Mestayer, P., Korsholm, U., and Calmet, I.: Temporal and Spatial Variability of Fluxes in Urbanized Areas, *Urban Climate and Bioclimate*, 219–232, ISBN:978-83-7525-243-9, 2008a.
- Mahura, A., Petersen, C., Baklanov, A., and Amstrup, B.: Evaluation of Building Effect Parameterization Module for Urbanized Numerical Weather Prediction Modelling, *Urban Climate and Bioclimate*, 371–380, ISBN:978-83-7525-243-9,
375 2008b.
- Martilli, A., Clappier, A., and Rotach, M.: An urban surface exchange parameterization for mesoscale models, *Boundary-Layer Meteorology*, 104, 261-304, <https://doi.org/10.1023/A:1016099921195>, 2002.



- Noilhan, J., and Planton, S.: A simple parameterization of land surface processes for meteorological models, *Mon. Wea. Rev.*, 117, 536–549, [https://doi.org/10.1175/1520-0493\(1989\)117<0536:ASPOLS>2.0.CO;2](https://doi.org/10.1175/1520-0493(1989)117<0536:ASPOLS>2.0.CO;2), 1989.
- 380 Nuterman, R., Baklanov, A., and Starchenko, A.: Modeling of aerodynamics and pollution dispersion from traffic in the urban sublayer, *Math. Models Comput. Simul.*, 2, 738–752, ISSN: 2070-0482, 2010.
- Patankar, S.: *Numerical Heat Transfer and Fluid Flow* (1st Ed.), CRC Press, 214 pp., 1980.
- Pepe, N., Pirovano, G., Lonati, G., Balzarini, A., Toppetti, A., Riva, G.M., and Bedogni, M.: Development and application of a high-resolution hybrid modelling system for the evaluation of urban air quality, *Atmospheric Environment*, 141, 297–311, <https://doi.org/10.1016/j.atmosenv.2016.06.071>, 2016.
- 385 Petersen, C., Kmit, M., Nielsen, N., Amstrup, B., and Huess, V.: Performance of DMI-HIRLAM-T15 and DMI-HIRLAM-S05 and the storm surge model in winter storms, Technical Report 05-13, DMI, Copenhagen, 31 pp., ISSN:1399-1388, 2005.
- Peuch, V.-H., Engelen, R., Calnan, R., Lambert, J.-C., and de Rudder, A., and The MACC-II Consortium: Monitoring Atmospheric Composition and Climate II - Interim Implementation, Final Report, ECMWF, Reading, 137 pp., 2014.
- 390 Peuch, V.-H., Engelen, R., Calnan, R., Lambert, J.-C., and de Rudder, A., and The MACC-III Consortium: Monitoring Atmospheric Composition and Climate 3, Final Report, ECMWF, Reading, 148 pp., 2016.
- Ramboll Environ: *User's Guide - COMPREHENSIVE AIR QUALITY MODEL WITH EXTENSIONS* Version 6.40, Ramboll Environ, Novato, California, 283 pp., 2016.
- Sabatino, S. D., Buccolieri, R., Olesen, H., Rørdam, H., Ketzel, M., Berkowicz, R., Franke, J., Schatzmann, M., Schlünzen, K.H., Leidl, B., Britter, R., Borrego, C., Alexandre, C., Castelli, S.T., Reisin, T.G., Hellsten, A., Saloranta, J., Moussiopoulos, N., Barmpas, F., Brzozowski, K., Goricsán, I., Balczò, M., Bartzis, J.G., Efthimiou, G., Nuterman, R., and Starchenko, A.V.: COST 732 in practice: the MUST model evaluation exercise. *International Journal of Environment and Pollution*, 44(1/2/3/4), 403-418, <https://doi.org/10.1504/IJEP.2011.038442>, 2011.
- 400 Sass, B. H.: A research version of the STRACO cloud scheme, DMI Tech. Rep. 02-10, Danish Meteorological Institute, Copenhagen, 25 pp., ISSN:1399-1388, 2002.
- Savijärvi, H.: Fast radiation parameterization schemes for mesoscale and short-range forecast models, *J. Appl. Meteor.*, 29, 437–447, [https://doi.org/10.1175/1520-0450\(1990\)029<0437:FRPSFM>2.0.CO;2](https://doi.org/10.1175/1520-0450(1990)029<0437:FRPSFM>2.0.CO;2), 1990.
- Schaap, M., Cuvelier, C., Hendriks, C., Bessagnet, B., Baldasano, J.M., Colette, A., Thunis, P., Karam, D., Fagerli, H., Graff, A., Kranenburg, R., Nyiri, A., Pay, M.T., Rouil, L., Schulz, M., Simpson, D., Stern, R., Terrenoire, E., and Wind, P.: Performance of European chemistry transport models as function of horizontal resolution, *Atmospheric Environment*, 112, 90-105, <https://doi.org/10.1016/j.atmosenv.2015.04.003>, 2015.



- Schlünzen, K., Grawe, D., Bohnenstengel, S., Schlüter, I., and Koppmann, R.: Joint modelling of obstacle induced and mesoscale changes - Current limits and challenges, *Journal of Wind Engineering and Industrial Aerodynamics*, 99(4), 217-225, <https://doi.org/10.1016/j.jweia.2011.01.009>, 2011.
- 410 Seinfeld, J., and Pandis, S.: *Atmospheric Chemistry and Physics, From Air Pollution to Climate Change (2nd Ed.)*, John Wiley & Sons, New York, 1152 pp., 2016.
- Simmons, A.: Monitoring Atmospheric Composition and Climate, *Meteorology - ECMWF Newsletter No. 123*, 10–13, <https://doi.org/10.21957/vqcvmylg>, 2010.
- Slinn, S., and Slinn, W.: Predictions for particle deposition on natural waters, *Atmos. Environ.*, 24, 1013-1016, 415 [https://doi.org/10.1016/0004-6981\(80\)90032-3](https://doi.org/10.1016/0004-6981(80)90032-3), 1980.
- Sokhi, R., Baklanov, A., and Schlünzen, K. (Eds.): *Mesoscale Modelling for Meteorological and Air Pollution Applications*, Anthem Press, New York, 382 pp., <http://www.jstor.org/stable/j.ctv80cdh5>, 2018.
- Stockwell, W. R., and Goliff, W. S.: Comment on “Simulation of a reacting pollutant puff using an adaptive grid algorithm” by R. K. Srivastava et al. *J. Geophysical Research*, 107(D22), 4643, <https://doi.org/10.1029/2002JD002164>, 2002.
- 420 Temel, O., Bricteux, L., and van Beeck, J.: Coupled WRF-OpenFOAM study of wind flow over complex terrain, *Journal of Wind Engineering and Industrial Aerodynamics*, 174, 152-169, <https://doi.org/10.1016/j.jweia.2018.01.002>, 2018.
- Undén, P., Rontu, L., Järvinen, H., Lynch, P., Calvo, J., Cats, G., Cuxart, J., Eerola, K., Fortelius, C., Garcia-Moya, J. A., Jones, C., Lenderlink, G., McDonald, A., Mc-Grath, R., Navascues, B., Nielsen, N. W., Øidegaard, V., Rodriguez, E., Rummukainen, M., Rööm, R., Sattler, K., Sass, B. H., Savijärvi, H., Schreur, B. W., Sigg, R., The, H., and Tijm, A.: 425 HIRLAM-5 Scientific Documentation, Tech. rep., The HIRLAM project, Norrköping, Sweden, 2002.
- van Leer, B.: Towards the Ultimate Conservative Difference Scheme. II. Monotonicity and Conservation Combined in a Second Order Scheme, *J. Comput. Phys.*, 14, 361–370, [https://doi.org/10.1016/0021-9991\(74\)90019-9](https://doi.org/10.1016/0021-9991(74)90019-9), 1974.
- Veratti, G., Fabbi, S., Bigi, A., Lupascu, A., Tinarelli, G., Teggi, S., Brusasca, G., Butler, T.M., Ghermandi, G.: Towards the coupling of a chemical transport model with a micro-scale Lagrangian modelling system for evaluation of urban NO_x levels 430 in a European hotspot, *Atmospheric Environment*, 223, 117285, <https://doi.org/10.1016/j.atmosenv.2020.117285>, 2020.
- Wesely, M.: Parameterization of Surface Resistances to Gaseous Dry Deposition in Regional-Scale Numerical Models, *Atmos. Environ.*, 23, 1293-1304, [https://doi.org/10.1016/0004-6981\(89\)90153-4](https://doi.org/10.1016/0004-6981(89)90153-4), 1989.
- Yarwood, G., Rao, S., Yocke, M., and Whitten, G.: Updates to the Carbon Bond chemical mechanism: CB05, RT-04-00675, ENVIRON International Corporation. Novato, CA: Yocke & Company, 161 pp., 2005.