Author responses to reviewers' comments of ACP-2020-1308 - Downscaling system for modelling of atmospheric composition on regional, urban and street scales

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We are grateful to the reviewers for critical and valuable comments. Below we provide the response to reviewer's comments and suggestions (with table and figures included in the Appendix A).

Reviewer #1

Question - Line 128. In the M2UE simulation, is the 500 m horizontal extent sufficient to represent the atmospheric environment of the street? I wonder if the airflow around the monitoring site is still substantially influenced by the boundary conditions. The extent of the airflow around the street that is largely affected by boundaries needs to be further investigated.

Answer: The M2UE computational domain was constructed following the COST Action 732 best practices and guidelines (see Franke et al., 2007) to ensure minimal influence of inflow/outflow boundaries on the airflow and pollution dispersion. Therefore, for the current micro-scale simulations with a steady-state RANS approach, the distance between buildings and inlet/outlet boundaries was equal to $5H_{max}$, where H_{max} = 20 m is the tallest building height. The distance between the tallest building and top boundary was $4H_{max}$.The computational domain could have been larger in extent, in particular, towards the outflow boundary. However, that would not satisfy the operational modelling system requirements because the total runtime interval of the entire modelling chain would exceed 12 hr. Therefore, the current micro-scale domain extent/size is an acceptable compromise between the best practices and guidelines as well as total runtime as requirements.

Hence, manuscript text was modified by adding the following sentences: "The horizontal and vertical extent of the computational domain is 500 x 500 x 100 m (detailed grid is shown in Figure A2). The distance between buildings in the centre of computational domain and inlet/outlet boundaries is $5H_{max}$, where H_{max} = 20 m is the tallest building height. The distance between the tallest building and top boundary was $4H_{max}$.Therefore, the current micro-scale domain extent/size is acceptable compromise between the best practices and guidelines (Franke et al., 2007) as well as total operational runtime (should not exceed 12 hr in order to satisfy modelling system requirements for the entire modelling chain)."

Question - Line 122. What chemical components and their reactions are included in the M2UE? Are the emission data used in the M2UE simulation equal to the emissions in the corresponding grids in the CMAx simulation? If not, how the difference between the emission data affects the simulation results?

Answer: The gas-phase chemistry mechanism (see Table A1, Appendix A) is mostly identical to the mechanism described by Stockwell and Goliff (2002) in Table 2. The only difference is the following additional chemical reaction: $SO_2 + OH \longrightarrow H_2SO_4 + HO_2$ with the rate parameter from Sander et al. (2006).

The emissions in large- and micro-scale models are different. The CAMx model uses annual emission inventory from TNO, which is pre-procced before simulations to account for monthly, weekly and diurnal variations. The M2UE model uses traffic counts measured at the Jagtvej street of Copenhagen in order to derive emissions, and therefore, are considered to be more accurate. Moreover, it would be rather crude to use TNO emissions for the micro-scale modelling as these do not account for a very local spatio-temporal features specific for this street.

Hence, manuscript text was modified by adding the following sentences: "The M2UE model is coupled with simplified atmospheric gas-phase chemistry mechanism. This mechanism is based on Stockwell and Goliff (2002) with extra chemical reaction included: $SO_2 + OH \longrightarrow H_2SO_4 + HO_2$. Full list of chemical reactions and corresponding rate parameter for this reaction are given in Table A1, Appendix A."

Line 131: "Note, the emissions utilized in large- and micro-scale models are different. The CAMx model uses annual emission inventory from TNO. It is pre-procced to account for monthly, weekly and diurnal emission variations. M2UE uses traffic counts measured at the Jagtvej street of Copenhagen to derive more accurate emissions (Figure A1) and hence, account for a very local spatio-temporal features specific for this street."

Question - Line 150. Are the inlet or outlet properties of each boundary fixed in the 48 h simulations? How many grids in HIRLAM-S03 and CMAx-04 are chosen to drive the M2UE model? Are the inlet/outlet properties derived from these coarse grids consistent with each other?

Answer: During each model integration cycle new boundary fields are read at 1-h interval, so the models retrieve updated meteorological and chemical fields from the previous low-resolution outer domains HIRLAM-T15 and CAMx-C20.

In order to drive the M2UE model, the output from the HIRLAM-S03 and CAMx-C04 models is linearly interpolated from four surrounding grids points into a grid point corresponding to the centre of the M2UE domain. The interpolated fields are used to derive the mean inlet conditions under the assumption of equilibrium boundary layer with power-law velocity profile and local equilibria assumption for turbulent parameters (Richards and Hoxey, 1993). As for the chemical fields the interpolated values are considered as the urban background concentrations. The outlet boundary condition are zero normal derivatives of all meteorological and chemical concentration variables corresponding to a fully developed and well-mixed flow. The above-mentioned boundary conditions follow the COST Action 732 best practises and guidelines (Franke et al., 2007) for micro-scale meteorological and atmospheric composition models and ensure consistency with each other.

Hence, manuscript text was modified by adding the following sentences:

Line 146, before "The forecast length of…": "For each integration cycle, new boundary fields are read at 1-h interval. So, the models retrieve updated meteorological and chemical fields from the previous low-resolution outer domains."

Line 150: "For the Jagtvej street domain inlet boundaries, the Dirichlet conditions with constant profiles of airflow characteristics (from HIRLAM-S03), averaged urban roughness and atmospheric composition fields (from CAMx-C04) were chosen to drive the M2UE model. In particular, the output from S03 and C04 was linearly interpolated from four surrounding grid points into a grid point corresponding to the M2UE domain. The interpolated fields were used to derive the mean inlet conditions under the assumption of equilibrium boundary layer with power-law velocity profile and local equilibria assumption for turbulent parameters (Richards and Hoxey, 1993). As for the chemical fields, the interpolated values were considered as the urban background concentrations. The outlet boundary condition is of the Neumann type with zero normal derivatives of all meteorological and chemical concentration variables corresponding to a fully developed and well-mixed flow. These above-mentioned boundary conditions follow the COST Action 732 best practises and guidelines (Franke et al., 2007) for micro-scale meteorological and atmospheric composition models and ensure consistency with each other."

Question - Line 175. Why do the authors select 2011 as the study period?

Answer: The year of 2011 was chosen because the research leading to the current results was a part of the FP7 EU project "Monitoring of Atmospheric Composition and Climate" (MACC; 2009-2011). This fact has been mentioned in the Acknowledgments section of the paper.

Question - Figure 4. Why only the NOx concentration is validated in the M2UE simulation? More chemical species are suggested to be evaluated against obervations.
For the M2UE modeling, simulation output is analyzed at only one site. Since the results of a single grid may not be enough to support the conclusion, it is recommended to add more analysis on the horizontal and vertical planes.

Answer: When the current results were obtained only the NOx was measured (apart from particulate matter) at the Jagtvej street measurement site. There are no measurements of ozone and carbon monoxide available for that time at this location. Previously, the M2UE model contributed to the COST Action 732 evaluation exercise, which was devoted to micro-scale models quality evaluation and assurance. Moreover, the dispersion patterns of chemical species in typical urban canyons were investigated in the previous studies (Franke et al., 2007; Schatzmann et al., 2010; Nuterman et al., 2010; Nuterman et al., 2011; Sabatino et al., 2011) and would not add value to this research. Since the model's dispersion capabilities were thoroughly tested, it seemed interesting and valuable to focus on operational aspects of the problem, and hence, to apply the CFD M2UE model using real time weather and atmospheric composition fields. Therefore, the purpose of the current paper is rather the concept proof (on possibility to run CFD type model operationally coupled with gas-phase chemistry) than rigorous full-scale evaluation of the proposed downscaling chain. To the best of the authors' knowledge, such attempts have not been practically done.

Hence, manuscript text was modified by adding the following sentences:
Line 202:"and benzene were measured on the street; ozone and carbon monoxide were not available for that time at this location)."
After line 131: "Previously, the M2UE model contributed to the COST Action 732 evaluation exercise. This exercise was devoted to micro-scale models quality evaluation and assurance. Moreover, the dispersion patterns of chemical species in typical urban canyons were investigated in the previous studies (Franke et al., 2007; Schatzmann et al., 2010; Nuterman et al., 2010; Nuterman et al., 2011; Sabatino et al., 2011) and would not add value to this research. Since the model's dispersion capabilities were thoroughly tested, it seemed interesting and valuable to focus on operational aspects of the problem, and hence, to apply the CFD M2UE model using real time weather and atmospheric composition fields. Therefore, the purpose of the current study is rather the concept proof (on possibility to run CFD type model operationally coupled with gas-phase chemistry) than rigorous full-scale evaluation of the proposed downscaling chain."

Question - Line 222 and Figure 4. Time-series data/figures of traffic volumes, emissions and boundary conditions are suggested to be provided. Do these data also show two peaks at 31 and 34 h? If so, the interesting difference between the observed concentrations and emissions may need to be discussed.

Answer: Time-series of M2UE boundary conditions are identical to O_3 and NO_x values from DK domain in Figure 4, because both nested M2UE domain and roof-level observation site are spatially located very close to each other and within one grid-cell of DK domain. As for the traffic volume at the Jagtvej street, it is identical to diurnal variations measured during the EU TMR TRAPOS project (Berkowicz et al., 2004; Berkowicz et al., 2006).
The emissions are shown in Figure A1, according to which only one concentration peak was observed during morning hours and also proven by street-level observations.

Hence, manuscript text was modified by adding the following sentences:
Line 196: "Due to the fact that the nested M2UE domain and roof-level observation site are spatially located very close to each other and within the same grid-cell of DK domain, the time-series of CFD boundary conditions are identical for O_3 and NO_x.

Line 140: The traffic volume at the Jagtvej street is similar to measured diurnal variations (Berkowicz et al., 2004; Berkowicz et al., 2006). The emissions are given in Appendix A (see Figure A1), where only one peak of concentration was observed during morning hours and also proven by street-level observations."

Question - Line 246. Typo "/Pearson".
Answer: The typo has been corrected.

Question - Line 247. Typo "domians/".
Answer: The typo has been corrected.

Question - Typos: "µg" instead of "ug".
Answer: The typos have been corrected.

Additional references

Berkowicz, R., Winther, M., Ketzel, M.: Traffic pollution modelling and emission data, Environmental Modelling & Software, 21, 454-460, https://doi.org/10.1016/ j.envsoft.2004.06.013, 2006.

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Sander, S. P., Friedl, R. R., Golden, D. M., Kurylo, M. J., Moortgat, G. K., Keller-Rudek, H., Wine, P. H., Ravishankara, A. R., Kolb, C. E., Molina, M. J., Finlayson-Pitts, B. J., Huie, R. E., and Orkin, V. L.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation Number 15, JPL Publication 06-2, Jet Propulsion Laboratory, Pasadena, CA, 2006.

Schatzmann, M., Olesen, H., Franke, J. (Eds.): COST 732 Model Evaluation Case Studies: Approach and Results, COST Office, ISBN: 3-00-018312-4, 2010.

Reviewer #2

Discussion section was more elaborated and improved.

Question - 1. Is there a double-counting of the urban processes in the CFD simulations, considering that those simulations are initialized with meteorological fields from HIRLAM model with activated BEP module?

Answer: There is no double-counting of urban process, since the BEP module was disabled during operational forecasting with HIRLAM-S03 domain. This fact has been mentioned in the lines 89-91.

Hence, manuscript text was modified by adding the following sentences:
Line 91: The urban effects were taken into account through roughness parameter and meteorological data assimilated from urban and suburban stations.

Question - 2. Are those emissions provided by TNO and used in CAMx simulations the most updated emissions for all the SNAPs?

Answer: For this year the EMEP emission inventory was available but at low resolution (0.5 x 0.5 deg.). The emission inventory (at resolution 0.125°×0.0625°) produced by TNO from official country-reported emission data from the year of 2005 was of a better quality. Despite the fact that the emission inventory was 6 years older than the simulations presented in the current research, the inventory had the finest spatial resolution available at that time. Therefore, we favoured TNO emissions since the goal of this study was the high-resolution air-pollution modelling.

Hence, manuscript text was modified by adding the following sentences:
Line 109 (end): Although, the EMEP emission inventory was also available, but at substantially lower resolution of 0.5 x 0.5 deg., and therefore, the TNO inventory was used.

Question - 3. Which kind of k-epsilon turbulence schemes are available in M2EU model? In addition, which schemes are available for meshing?

Answer: There are two types of turbulence closure schemes available in M2UE model, i.e. k-eps and cubic eddy-viscosity viscosity scheme by Craft et al., (1996). There is no any specific (advanced) meshing technique available in the M2UE model. An ordinary uniform or non-uniform regular (rectilinear) 3D grid with fictitious domain method (Aloyan et al., 1982; Vabishchevich, 1991) is used in the model.

Hence, manuscript text was modified by adding the following sentences:
Line 199: equations, k-eps (Launder and Spalding, 1974) and cubic eddy-viscosity (Craft et al., 1996) turbulence closure schemes, and …
Line 121 after … van Leer, 1974): "An ordinary uniform or non-uniform regular (rectilinear) 3D grid with fictitious domain method (Aloyan et al., 1982; Vabishchevich, 1991) is used in the model."

Question - 4. Authors mentioned that the horizontal and vertical extent of the computational domain is 500 x 500 x 100 m. There is a lack of information about the dimensions of the domain (e.g. height of the tallest building in the domain). Did the authors follow the COST Action 732 guidelines

Answer: The M2UE computational domain was constructed following the COST Action 732 best practices and guidelines (see Franke et al., 2007) to ensure minimal influence of inflow/outflow boundaries on the airflow and pollution dispersion. Therefore, for the current micro-scale simulations with a steady-state RANS approach, the distance between buildings and inlet/outlet boundaries was equal to $5H_{max}$, where H_{max} = 20 m is the tallest building height. The distance between the tallest building and top boundary was $4H_{max}$.The computational domain could have been larger in extent, in particular, towards the outflow boundary. However, that would not satisfy the operational modelling system requirements because the total runtime interval of the entire modelling chain would exceed 12 hr. Therefore, the current micro-scale domain extent/size is an acceptable compromise between the best practices and guidelines as well as total runtime as requirements.

Hence, manuscript text was modified by adding the following sentences:
"The horizontal and vertical extent of the computational domain is 500 x 500 x 100 m (detailed grid is shown in Figure A2). The distance between buildings in the centre of computational domain and inlet/outlet boundaries is $5H_{max}$, where H_{max} = 20 m is the tallest building height. The distance between the tallest building and top boundary was $4H_{max}$.Therefore, the current micro-scale domain extent/size is acceptable compromise between the best practices and guidelines (Franke et al., 2007) as well as total operational runtime (should not exceed 12 hr in order to satisfy modelling system requirements for the entire modelling chain)."

Question - 5. Authors should provide a figure plotting the mesh to be more specific about this information: 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 domains boundaries was used. How about the distance between the boundaries and the build-up area? Again, are you considering the COST Action guidelines or similar?

Answer: Detailed M2UE grid is included in Appendix A, Figure A2.

Hence, manuscript text was modified by adding the following sentences:
line 129 after "500 x 500 x 100 m": "(detailed grid is shown in Figure A2)."

Question - 6. 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). Therefore, I am assuming you are only considering the road traffic emissions for the M2EU simulations. Am I right?

Answer: It is correct, only the most significant pollution source in M2UE computational domain, i.e. traffic pollution, was considered. Road traffic emissions are included in Appendix A, Figure A1.

Hence, manuscript text was modified by adding the following sentences:
Adding to line 131: "M2UE uses traffic counts measured at the Jagtvej street of Copenhagen to derive more accurate emissions (Figure A1) and hence, account for a very local spatio-temporal features specific for this street."

Additional references

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Craft, T.J., Launder, B.E., Suga, K.: Development and application of a cubic eddy-viscosity model of turbulence, Int. J. of Heat and Fluid Flow, 17(2), 108-115, https://doi.org/10.1016/0142-727X(95)00079-6, 1996

Franke J., Hellsten, A., Schlünzen, H., Carissimo, B. (Eds.): Best Practice Guideline for the CFD Simulation of Flows in the Urban Environment: COST Action 732 Quality Assurance and Improvement of Microscale Meteorological Models, COST Office, ISBN: 3-00-018312-4, 2007.

Launder, B.E., Spalding, D.B.: "The numerical computation of turbulent flows", Computer Methods in Applied Mechanics and Engineering, 3(2), 269-289, https://doi.org/10.1016/0045-7825(74)90029-2, 1974

Vabishchevich, P.N.: The Method of Fictitious Domains in Problems of Mathematical Physics [in Russian], Moscow University, Moskva, 156pp., 1991.

Appendix A

Table A1: List of chemical reactions included as gas-phase chemistry mechanism in M2UE model

$NO_2 + hv \longrightarrow O(^3P) + NO$	$RO_2 + NO \longrightarrow NO_2 + HO_2 + HCHO$
$O_3 + hv \longrightarrow O(^1D) + O_2$	$CO + HO \longrightarrow HO_2 + CO_2$
$HCHO + hv \longrightarrow 2HO_2 + CO$	$HO + HC \longrightarrow RO_2 + H_2O$
$HCHO + hv \longrightarrow H_2 + CO$	$HO + HCHO \longrightarrow HO_2 + CO + H_2O$
$O(^3P) + O_2 \longrightarrow O_3$	$HO + NO_2 \longrightarrow HNO_3$
$O(^1D) + N_2 \longrightarrow O(^3P) + N_2$	$2HO_2 \longrightarrow H_2O_2 + O_2$
$O(^1D) + O_2 \longrightarrow O(^3P) + O_2$	$2HO_2 + H_2O \longrightarrow H_2O_2 + H_2O + O_2$
$O(^1D) + H_2O \longrightarrow 2OH$	$HO_2 + RO_2 \longrightarrow ROOH + O_2$
$HO_2 + NO \longrightarrow NO_2 + HO$	$2RO_2 \longrightarrow 2HCHO + HO_2$
$O_3 + NO \longrightarrow NO_2 + O_2$	$SO_2 + OH \longrightarrow H_2SO_4 + HO_2$

Chemical reactions and rate parameters are the same as in Stockwell and Goliff (2002), except chemical reaction ($SO_2 + OH \longrightarrow H_2SO_4 + HO_2$) with the rate parameter from (Sander et al., 2006):

$$k_0 = 3 \times 10^{-31} \times C_{air} \times (300/T)^{3.3}, k_\infty = 1.5 \times 10^{-12}$$

$$k = \frac{k_0}{1 + k_0/k_\infty} \times 0.6^{\left(1+[\log_{10}(k_0/k_\infty)]^2\right)^{-1}}$$

where T is temperature [K] and C_{air} is air concentration [molecules/cm^3].

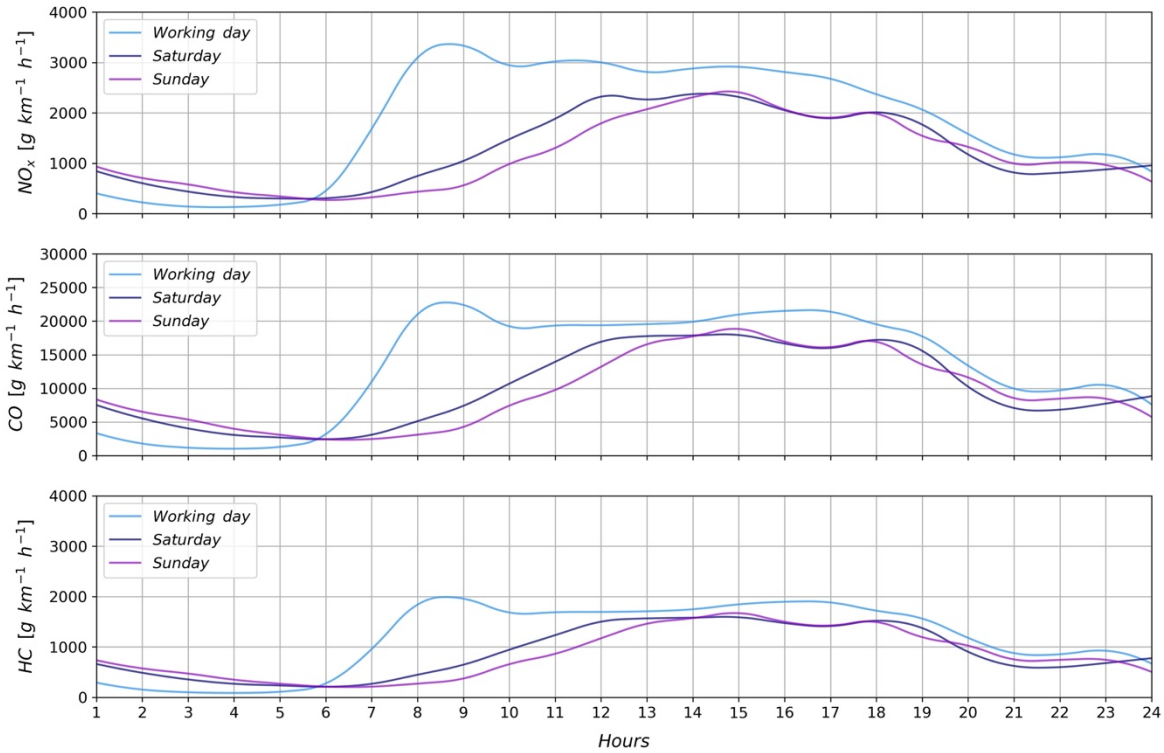

Figure A1: Time-series of diurnal cycle emissions on typical Saturday, Sunday and Working day of a week at the Jagtvej street, Copenhagen, Denmark.

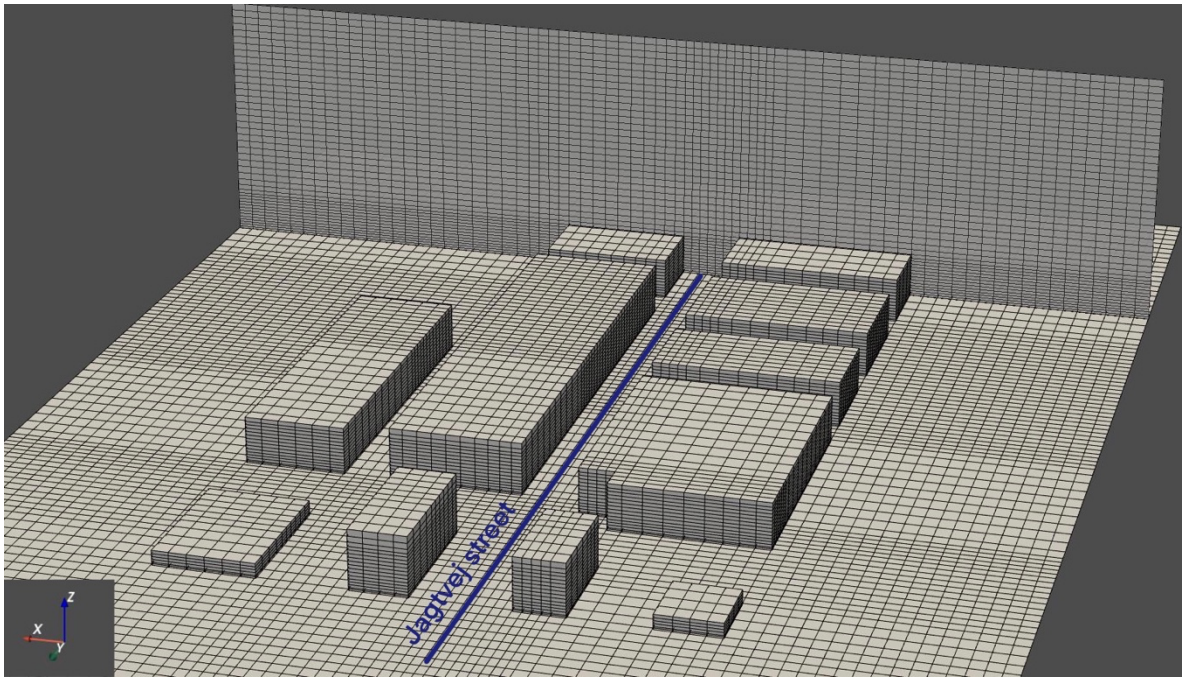

Figure A2: M2UE numerical grid of the Jagtvej street, Copenhagen, Denmark.