Author responses to editor's 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 editor for critical and valuable comments. Below we provide the response to editor's comments and suggestions.

Comment 1. One of the referees is very critical about the publication of your paper. The main critics are listed below. Could you put your work in perspectives to the works of Kwak et al. (2015), Khan et al. (2021), José et al. (2021)?

Answer: Indeed, there are several studies by Kwak et al. (2015), Khan et al. (2021), José et al. (2021), which demonstrated the atmospheric composition modelling with downscaling from regional to street scale. Amongst these only one study (José et al., 2021) used the micro-scale model in an operational mode. But this model has very basic chemistry scheme predominately applicable for cold seasons. The others did not consider an operational aspect and/or unlikely to be able to employ their micro-scale models in operational mode. The operational runtime constraints will not allow doing that because the complexity of gas-phase chemistry mechanism (Kwak et al., 2015) or requirements for numerical grid resolution in large eddy simulation models (Khan et al., 2021).

Hence, the manuscript text was modified in the following lines

Line 48: "Currently, there are several studies describing and evaluating systems capable of downscaling modelling of weather and atmospheric composition from regional to micro-scales. Amongst these the study by José et al. (2021) performed operational micro-scale simulations, but this model has very basic chemistry scheme predominately applicable for cold seasons. The others did not consider an operational aspect and/or unlikely to be able to run their micro-scale models in operational mode. The operational runtime constraints will not allow doing that because the complexity of gas-phase chemistry mechanism (Kwak et al., 2015) or requirements for numerical grid resolution in large eddy simulation models (Khan et al., 2021).

Line 349: Khan, B., Banzhaf, S., Chan, E. C., Forkel, R., Kanani-Sühring, F., Ketelsen, K., Kurppa, M., Maronga, B., Mauder, M., Raasch, S., Russo, E., Schaap, M., and Sühring, M.: Development of an atmospheric chemistry model coupled to the PALM model system 6.0: implementation and first applications, Geosci. Model Dev., 14, 1171-1193, https://doi.org/10.5194/gmd-14-1171-2021, 2021.

Line 355: Kwak, K.-H., Baik, J.-J., Ryu, Y.-H., Lee, S.-H.: Urban air quality simulation in a high-rise building area using a CFD model coupled with mesoscale meteorological and chemistry-transport models, Atmospheric Environment, 100, 167-177, https://doi.org/10.1016/j.atmosenv.2014.10.059, 2015.

Line 398: San José, R., Pérez, J.L., Gonzalez-Barras, R.M.: Assessment of mesoscale and microscale simulations of a NO2 episode supported by traffic modelling at microscopic level, Science of The Total Environment, 752, https://doi.org/10.1016/j.scitotenv.2020.141992, 2021.

Comment 2. Furthermore, as the coupling to gas-phase chemistry seems to be an essential part of this work, could you add a comparison to NO2 measurements? The referee suggests that the comparison to NOx only and at only one site is not strong enough to validate the model.

Answer: The comparison to NO_2 measurements was added to the manuscript for each used air-quality model in the downscaling chain.

Hence, the Fig. 4 was replaced by

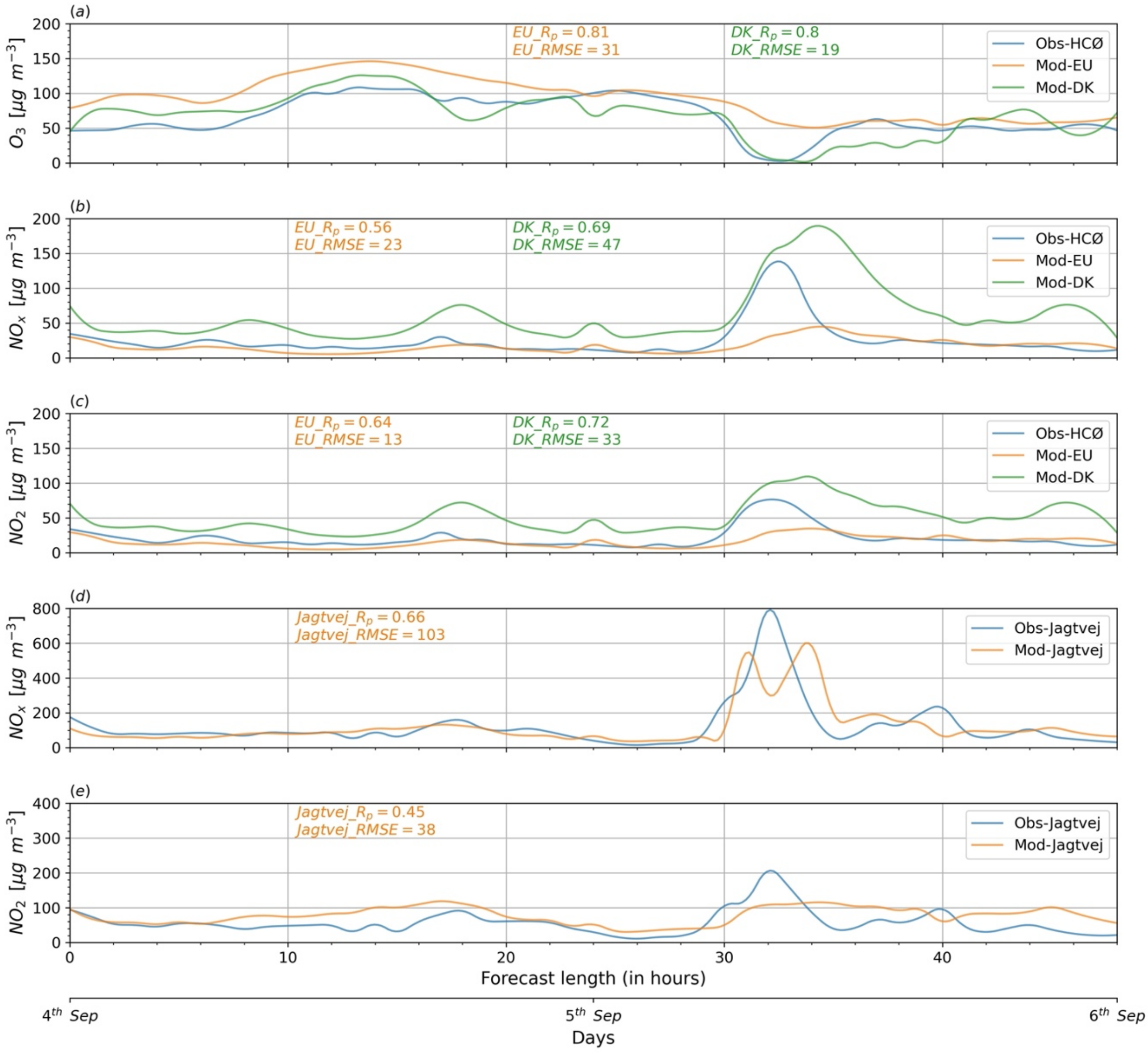

Figure 4: Time-series of observations vs. HIRLAM+CAMx+M2UE forecasts for (a) O_3, (b, d) NO_x and (c, e) NO_2 for the European, Denmark and Copenhagen modelling domains during Sunday-Monday 4-5 Sep 2011; (a, b, c) HCØ roof level observations of O_3, NO_x and NO_2 vs. modelling results for EU and DK domains; (d, e) Jagtvej Street level observations of NO_x and NO_2 vs. M2UE /Pearson correlation R_p and root mean square error $RMSE$ of modelled vs. observed concentrations for 3 domains/.

and the manuscript text was modified in the following lines

Line 17: "… forecast of NO_x and NO_2 levels …"

Line 21: "… and NO_2 diurnal cycles …"

Line 157: "… photochemical reactions of O_3, NO_x and NO_2 were of …"

Line 158: "… time-series of CFD boundary conditions are identical for O_3, NO_x and NO_2."

Line 199: "… time-series of O_3, NO_x and NO_2 observations …"

Line 201: "… only NO_x and NO_2, particulate matter …"

Line 205: "Although, the NO_x and NO_2 levels were generally overestimated in the DK scale forecast (Fig. 4bc) …"

Line 207: "… ($EU\_RMSE = 23$ vs. $DK\_RMSE = 47$ for NO_x and $EU\_RMSE = 13$ vs. $DK\_RMSE = 33$ for NO_2)…"

Line 208: "… ($EU\_R_p = 0.56$ vs. $DK\_R_p = 0.69$ for NO_x and $EU\_R_p = 0.64$ vs. $DK\_R_p = 0.72$ for NO_2)."

Line 208: "… when the NO_x and NO_2 peaks were observed …"

Line 210: "The timing and levels of NO_x and NO_2 peaks were…"

Line 212: "… it with slightly elevated NO_x and NO_2 values."

Line 217: "The diurnal cycles of NO_x and NO_2 concentrations observed and modelled for the Jagtvej Street are shown in Fig. 4de."

Line 218: "… values ($R_p = 0.66$ and $R_p = 0.45$ for NO_x and NO_2, respectively), …"

Line 218: "… observed NO_x and NO_2 diurnal cycles …"

Line 221: "… estimate of NO_x concentration …"

Line 224: "Note, the model also exhibited elevated NO_2 levels (with RMSE=38) during the high air pollution episode with the concentrations underestimated."

Line 226: "… the elevated NO_x and NO_2 concentrations …"

Line 229: "As seen in Fig. 4abc, the effect of …"

Line 260: "… forecast of NO_x and NO_2 levels …"

Line 263: "… the NO_x and NO_2 diurnal cycles …"

Comment 3. The "possibility to run CFD type model operationally coupled with gas-phase chemistry" has been proved by many researches, such as Kwak et. al., (2015), José et. al., (2021) and Khan et. al., (2021). They adopted mesoscale models (e.g., WRF-chem, CMAQ, COSMO) and CFD models (e.g., PALM, MICROSYS) to simulate real world atmospheric environment with gas phase chemistry (including chemistry components such as NO, NO2, O3, CO, …).

Answer on this comment as on the comment 1: Indeed, there are several studies by Kwak et al. (2015), Khan et al. (2021), José et al. (2021), which demonstrated the atmospheric composition modelling with downscaling from regional to street scale. Amongst these only one study (José et al., 2021) used the micro-scale model in an operational mode. But this model has very basic chemistry scheme predominately applicable for cold seasons. The others did not consider an operational aspect and/or unlikely to be able to employ their micro-scale models in operational mode. The operational runtime constraints will not allow doing that because the complexity of gas-phase chemistry mechanism (Kwak et al., 2015) or requirements for numerical grid resolution in large eddy simulation models (Khan et al., 2021).

Comment 4. Valid modeling settings and reliable evaluation are the basis of operational modeling. In this paper, (1) the boundary conditions are "read at 1-h interval", (2) the total emission values of the whole CFD domain are not equal to the emission values of the corresponding CMAx grid, (3) the horizontal extend is only 500 m, (4) evaluation only conducted on NOx at only one site. Comparatively, the aforementioned studies are more reliable than this work in terms of modeling and evaluation.

Answer:

(1) To our knowledge most national meteorological services/institutes run their regional or limited geographical area operational models with output frequency of 1 hour. Since the goal of this study is to demonstrate and test the operational system in the context of current operational practices in the numerical weather prediction and atmospheric composition modelling, the local-scale forecast was also forced with 1-h interval boundary conditions from the meso-scale model.

(2) The anthropogenic emission inventories for most regional-urban air quality models represent annually accumulated fluxes from various sources. Usually, these are redistributed over months, weeks (working days and weekends) and hours with corresponding coefficients. Therefore, these emissions are less accurate than those obtained from local traffic counts. Moreover, the studies by Kwak et al. (2015), Khan

et al. (2021), José et al. (2021) adopted a similar approach to our approach for local scale emissions using either emission models or traffic counts.

(3) The selected street (for M2UE model) domain is rather typical street canyon configuration and a typical section (block) of the lengthy Jagtvej Street. In such configuration the bulk wind direction and speed as well as buildings surrounding the street have the most significant effect on air-flow and traffic pollution dispersion (Karra et al., 2017; Schatzmann et al., 2010).

(4) The comparison to NO_2 measurements was added to the manuscript for each used air-quality model in the downscaling chain.

References

Karra, S., Malki-Epshtein, L., Neophytou, M. K.-A.: Air flow and pollution in a real, heterogeneous urban street canyon: A field and laboratory study, Atmospheric Environment, Volume 165, 2017, Pages 370-384, https://doi.org/10.1016/j.atmosenv.2017.06.035.

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