Authors' Response:

Manuscript Title: Development and application of a multi-scale modelling framework for urban high-resolution NO_2 pollution mapping

Discussion Link: https://acp.copernicus.org/preprints/acp-2022-371/#discussion

Revision notes:

Reviewers' comments are in blue italic type.
Authors' responses are in indent and in black normal font.
Revisions in the manuscript are in indent red normal font.

Content

Response to Editor's Comments

For the next revision, please add the name of the corresponding author into the line 9 (title page of the *.pdf manuscript file). 2. Regarding the figures #11: with the next revision, please check if a copyright statement/image credit is required and add it to the figure caption, if applicable. If you are the originator, you can just inform us via email.

Response:

Thanks for reminding. We have added the name of the corresponding author and a copyright statement/image credit in the manuscript.

Revisions in Manuscript:

(1) Line 9.

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(2) Figure 11.

Figure 11: Spatial distribution of monthly averaged NO2 concentrations from (a) CMAQ model and (b) CMAQ-RLINE_URBAN model (© OpenStreetMap contributors 2020. Distributed under the Open Data Commons Open Database License (ODbL) v1.0).

Response to Reviewers #2's Comments

Summary

The revised version has been much improved. All my concerns on the previous version have been addressed properly and quite clearly. I only have a few further minor comments to be considered.

Response:

Thank you very much to give us comments. We believed all the concerns you mentioned at this time were addressed in this revision.

Question 1

Line 153-155. Apart from the general description of the emission inventory, some quantities (e.g. total emission or emission factors) about the emissions for the simulation period would be helpful.

Response:

Thanks for your advice. We totally agreed, and the description about the emission amount and the main contribution of vehicle types has been added in the **Materials and Methods**.

Revisions in Manuscript:

(1) Materials and Methods, Line 158-160.

The daily averaged NO_x emission from on-road vehicles in Beijing in 2019 was estimated to be 136.0 Mg, of which emissions from heavy duty vehicles and heavy duty trucks accounted for 31% and 34%, respectively.

Question 2

It is suggested to add the running cost for the hybrid model CMAQ-RLINE_URBAN for the 50 m x 50 m resolution run, which may guide the future development towards higher resolutions at the street scale.

Response:

Thanks for your advice. In the base scenario CMAQ-RLINE_URBAN, in the hybrid model, the local meteorological field should be calculated separately according to the location of road and receptor points, thus the average simulation duration per unit hour is about 3.9 hours, and can reach 4.8 hours at night when the atmospheric stability is high and the results were difficult to convergence. The running cost has been added in **Conclusion and Discussions**.

Revisions in Manuscript:

(1) Conclusion and Discussions. Line 534-536.

At present, the execution time during 1 h running CMAQ-RLINE_URBAN over the urban domain was about 3.9 hours in average, which reached 4.8 hours at night due to the difficulty of convergence in the condition of the high atmospheric stability.

Question 3

Health impact of NO2 pollution (to be linked with population data and health data) could be added into the future research.

Response:

Thanks for your advice. This has been added in **Conclusion and Discussions**.

Revisions in Manuscript:

(1) Conclusion and Discussions. Line 554-555.

The high resolution NO_2 concentration map was benefit for the estimation of human health risks induced by the air pollution at the street level in future researches.

Response to Reviewers #4's Comments

Summary

This work presents a Multi-scale system to predict NO2 at high-spatial resolution. The system combines mesoscale results (CMAQ) with a Gaussian dispersion solver (RLINE). The study deals with the coupling between these two scales. The main innovation is the approach to derive local wind velocity within street canyons. The idea of using CFD simulations to train machine learning models to improve classic Gaussian Dispersion models is interesting and timely. However, some points of the current methodology need to be clarified before publication.

Response:

Thank you very much for spending time to give us so many constructive comments. Upon learning through them, we improved our manuscript. We try our best to address all the concerns in this revision, where more details about the methodology was introduced and clarified.

Question 1

As stated in the manuscript, ML methods estimate "the wind vector along X-axis and Y-axis at different heights within the street canyon respectively". However, where is this vertical profile located within the street canyon? Are the edges of the canyon affecting the profile? Are 3D CFD simulations justified?

Response:

Thanks for your question. We apologized that the description of the wind vector used in the ML method was unclear. Here, the wind vector used in the ML method is the average velocity of all horizontal CFD grids at same the height within the street canyon. For example, if there are 100 CFD grids at the height of 1.5 m within the street canyon, the wind vector was the average of predictions of these all grids. Therefore, the influence of edges of the canyon on the wind profile is included in predictions from ML method. We have revised the description of the wind vector along X-axis and Y-axis in the manuscript for better understating.

For 3D CFD simulations, the configurations refer to the CFD guideline (Tominaga et al., 2008; Franke et al., 2011) and previous studies (Hang et al., 2012; Hang et al., 2010), and the performance of the simulation is validated by wind tunnel data (Brown et al., 2001; Hang et al., 2010) (Figure S3), thus we believe the 3D CFD simulations are justified.

Revisions in Manuscript:

(1) Materials and Methods. Line 287-288.

The V_x and V_y were the average of all velocities along X or Y axis over the same horizontal profile at a specific height within the street canyons.

Question 2

In RLINE, a single wind speed value is associated with each line source. Could you please clarify in the manuscript how this wind speed has been derived for the different presented approaches (CMAQ-RLINE, CMAQ-RLINE-Urban-nc, CMAQ-RLINE-Urban).

Response:

Thanks for your advice. As we have introduced in the manuscript (Line 137-140), the wind at the top of street canyon was provided by the WRF for all scenarios (CMAQ-RLINE, CMAQ-RLINE-Urban_nc, and CMAQ-RLINE-Urban), and the wind environment of each road were obtained separately from WRF model according to the road location. The difference between different scenarios is the wind speed within the street canyon. For CMAQ-RLINE and CMAQ-RLINE-Urban_nc, the wind profiles within the street canyon are calculated by the MOST theory. For CMAQ-RLINE_URBAN, the wind profile within the street canyon is calculated by MLSCF. We have added this description in the manuscript for better understanding.

Revisions in Manuscript:

(1) Materials and Methods. Line 338-341.

Although the wind environment for each road at the top of the canyon was provide by the WRF model in all scenarios, the calculation of wind profile within the street canyon was different. It was estimated based on the MOST theory in the CMAQ-RLINE and CMAQ-RLINE_URBAN_nc rather than that from the MLSCF in the CMAQ-RLINE_URBAN.

Question 3

How intersections of two different street-canyons are treated.

Response:

Thanks for your question. The main simulation is based on the RLINE model, which is a Gaussian line source dispersion model rather than a street box model such as the SIRANE and MUNICH model. The description of the RLINE model has been introduced in **Line 122-127** in the manuscript. Therefore, the calculation of intersection between different road is not involved and each street canyon is treated as a single source in simulation.

Question 4

The heat flux condition of the vertical mixing parametrization is different from the one presented in Benavides et al. Also, Benavides's parametrization was adjusted to work with MOST estimation of surface wind speed. How is this parametrization still valid when using a different surface wind speed approach?

Also, to compute the ratio WSsfc/WSbh for the vertical mixing parametrization, how is WSsfc computed along the canyon, given that the ML surrogate provides a single vertical profile?

Response:

Thanks for questions. Firstly, when the background concentration mixing ratio (fac_{bg}) was calculated, actually we changed the threshold of heat flux from 0.3 to 0 compared with the Benavides's study. The transition value of 0.3 in Benavides's study is set to consider the impact of Urban Heat Island (Kheirbek et al.) effect, which is already considered in the UHI scheme of our hybrid model. Therefore, this change was aim to avoid the double-counting of impacts from the UHI effect, which was added into the description of the vertical mixing parametrization in **Supplement Section S2**.

Whether in our hybrid model or Benavides's study, we both assumed that the ratio of wind speed near the surface and the top of street can be used as a proxy parameter to characterize the turbulence intensity which influenced the vertical mixing of background concentrations in canyons. Although we use a different wind profile approach in street canyons compared with that in the Benavides's study, the basic theory of the vertical mixing of background concentrations in canyons was unchanged. Therefore, we believed that this parametrization still valid in our hybrid model.

We apologized again for the missing understanding of the output from MLSCF scheme, which is explained in the answer of **Question 1**. So WSsfc was the same at a specific height and canyon rather than different along the canyon,

Revisions in Manuscript:

(1) Supplement Section S2. Vertical mixing scheme

The transition value of H_u changed from 0.3 to 0 in this research compared with the Benavides's study in order to avoid the double-counting of impacts from the UHI effect.

Question 5

To fairly assess the ML performance, data from a velocity profile for a given set of predictors (Vbgx, Vbgy, z/H, Hl/Hr, H/W,L/W) should not be split between training and test sets. Then for the testing, the ML models will predict the entire velocity profile without seeing any other data point from this profile. This more restrictive data splitting will estimate better the performance in unseen street canyons.

Response:

Thank you for advice. According to the train strategy you proposed, we think you are concerned about the generalization ability of the machine learning model. There is no doubt that the training strategy you proposed will make the performance of the model acceptable in unseen street canyon. Although we split training and test sets randomly in this study, the sample in the test set with specific height in the specific canyon was never included in the training set. Therefore, the generalization ability of our model is believable, and has been validated in **Figure 5**. This figure showed the comparison between observations and predictions from MLSCF in two CFD validation cases, where the geometry of canyons and background wind were never included in the training sets of MLSCF, and the acceptable model performance were shown.

Question 6

How does this approach account for all non-local vehicle emissions?

Response:

Thanks for your question. As the statement in our manuscript (Line 162 to 165), the impact of all non-local vehicle emissions has been involved in the background concentrations simulated by CMAQ-ISAM model, in which the emissions were divided into mobile and other four emission groups to trace their contributions separately. The detailed configuration of CMAQ-ISAM model has been already introduced in our previous study (Lv et al., 2020).

Revisions in Manuscript:

(1) Materials and Methods. Line 162-164.

These background concentrations were simulated by CMAQ-ISAM model, in which the emissions were divided into local mobile and other four emission groups to trace their contributions separately, so the influence if non-local emission could be considered.

Question 7

Is the building geometry constraining the Gaussian dispersion?

Response:

Thanks for your question. In our hybrid model, the building geometry influenced the wind in street canyons using the MLSCF scheme, and also the surface roughness length as well as the atmospheric turbulence intensity using the z_0 scheme. Therefore, the building geometry influenced the Gaussian dispersion indirectly.

Question 8

A maximum of 1e4 iterations in the CFD solver are considered to avoid extra CPU time. From the full 1600 CFD simulations, what percentage did not reach the convergence conditions described in the paper?

Response:

Thanks for your question. As shown in the Figure below, most simulation cases (54.6%) met the convergence criteria (10^{-5}). The median residual error of continuity equation, velocity in X direction, velocity in Y direction, velocity in Z direction, k and ε are 1.0×10^{-5}, 8.5×10^{-7}, 8.5×10^{-7}, 4.1×10^{-7}, 3.4×10^{-6} and 5.4×10^{-6}, respectively, indicating that the overall model performance is acceptable. However, the residual error of continuity equation was relatively large, the number of cases with residuals greater than 10^{-5} and 10^{-4} accounts for 45.4% and 1.5% respectively. Particularly, when the external wind was parallel to the street and L/H was large, more iteration steps are required for the velocity in street canyons become a steady state, which should be improved in the future. And now we have added a brief description of the convergence conditions in the manuscript.

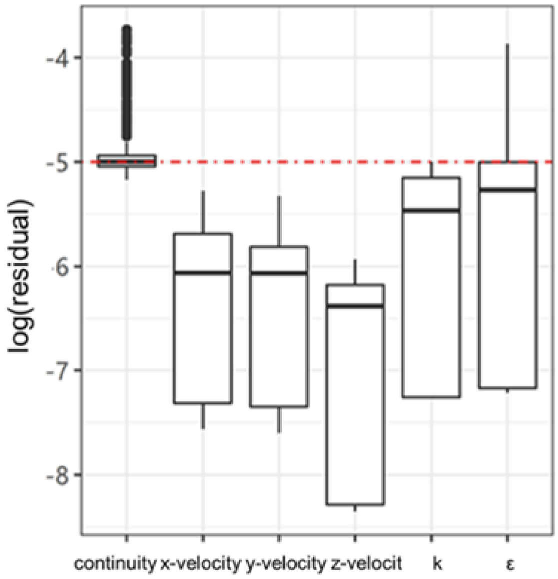

Figure. Residual distributions of each parameter in 1600 CFD simulation scenarios

Revisions in Manuscript:

(1) Materials and Methods. Line 226-230.

About 54.6% of cases met the convergence criteria, and the median residual values of continuity equation, velocity in X axis, velocity in Y axis, velocity in Z axis, k and ε were 1.0×10^{-5}, 8.5×10^{-7}, 8.5×10^{-7}, 4.1×10^{-7}, 3.4×10^{-6} and 5.4×10^{-6}, respectively, indicating the overall model performance was acceptable.

Question 9

What are the CFD mesh refinements criteria? The CFD mesh should be refined close to walls to capture strong velocity gradients, and it does not seem to be the case.

Response:

Thanks for your question. In the CFD validation (Section 2.2.3), we identify the influence of different minimum sizes of hexahedral cells near wall surfaces (fine: 0.1m, medium: 0.2m, and coarse: 0.5m) with an expansion ratio of 1.1 on the predicted velocity to an expansion ratio of 1.1, and we find different grid resolutions used in simulations would not obviously affect the predicted results (Figure S3). Therefore, the minimum size of hexahedral cells near wall surfaces was 0.5 m with an expansion ratio of 1.1 is applied to save the computing cost (**Line 259-260**).

Question 10

The described boundary conditions are not in accordance with Fig. 2. Also, please report the number of CFD mesh points and simulation time.

Response:

Thanks for your advice. We apologized that the distance between UCL and the domain top was wrong in the manuscript. We have revised its description in the manuscript.

The mesh number of 80 (5×4×4) CFD models is shown in the Table below. The average mesh number of 80 street canyon models is 136,7965.

Table. The mesh number of 80 CFD models

ID	Hl/Hr	H/W	L/H	Hl	Hr	W	L	Cells
1	0.50	0.25	3	14	28	84	63	1433054
2	0.50	0.25	5	14	28	84	105	1540924
3	0.50	0.25	10	14	28	84	210	1681155
4	0.50	0.25	20	14	28	84	420	1832173
5	0.50	0.50	3	14	28	42	63	1330574
6	0.50	0.50	5	14	28	42	105	1430044
7	0.50	0.50	10	14	28	42	210	1559355
8	0.50	0.50	20	14	28	42	420	1698613
9	0.50	1.00	3	14	28	21	63	1236634
10	0.50	1.00	5	14	28	21	105	1328404
11	0.50	1.00	10	14	28	21	210	1447705
12	0.50	1.00	20	14	28	21	420	1576183
13	0.50	2.00	3	14	28	11	63	1168314
14	0.50	2.00	5	14	28	11	105	1254484
15	0.50	2.00	10	14	28	11	210	1366505
16	0.50	2.00	20	14	28	11	420	1487143
17	0.75	0.25	3	18	24	84	63	1332478
18	0.75	0.25	5	18	24	84	105	1433068
19	0.75	0.25	10	18	24	84	210	1563835
20	0.75	0.25	20	18	24	84	420	1704661
21	0.75	0.50	3	18	24	42	63	1257204
22	0.75	0.50	5	18	24	42	105	1330108
23	0.75	0.50	10	18	24	42	210	1450735
24	0.75	0.50	20	18	24	42	420	1580641

25	0.75	1.00	3	18	24	21	63	1150088
26	0.75	1.00	5	18	24	21	105	1235728
27	0.75	1.00	10	18	24	21	210	1347060
28	0.75	1.00	20	18	24	21	420	1466956
29	0.75	2.00	3	18	24	11	63	1118508
30	0.75	2.00	5	18	24	11	105	1167088
31	0.75	2.00	10	18	24	11	210	1271660
32	0.75	2.00	20	18	24	11	420	1403380
33	1.00	0.25	3	21	21	84	63	1168566
34	1.00	0.25	5	21	21	84	105	1256796
35	1.00	0.25	10	21	21	84	210	1371495
36	1.00	0.25	20	21	21	84	420	1495017
37	1.00	0.50	3	21	21	42	63	1085118
38	1.00	0.50	5	21	21	42	105	1166508
39	1.00	0.50	10	21	21	42	210	1272315
40	1.00	0.50	20	21	21	42	420	1386261
41	1.00	1.00	3	21	21	21	63	1008624
42	1.00	1.00	5	21	21	21	105	1083744
43	1.00	1.00	10	21	21	21	210	1181400
44	1.00	1.00	20	21	21	21	420	1286568
45	1.00	2.00	3	21	21	11	63	952992
46	1.00	2.00	5	21	21	11	105	1023552
47	1.00	2.00	10	21	21	11	210	1115280
48	1.00	2.00	20	21	21	11	420	1214064
49	1.33	0.25	3	24	18	84	63	1332478
50	1.33	0.25	5	24	18	84	105	1433068
51	1.33	0.25	10	24	18	84	210	1563835
52	1.33	0.25	20	24	18	84	420	1704661
53	1.33	0.50	3	24	18	42	63	1257204
54	1.33	0.50	5	24	18	42	105	1330108
55	1.33	0.50	10	24	18	42	210	1450735
56	1.33	0.50	20	24	18	42	420	1580641
57	1.33	1.00	3	24	18	21	63	1150088
58	1.33	1.00	5	24	18	21	105	1235728
59	1.33	1.00	10	24	18	21	210	1347060
60	1.33	1.00	20	24	18	21	420	1466956
61	1.33	2.00	3	24	18	11	63	1118508
62	1.33	2.00	5	24	18	11	105	1167088
63	1.33	2.00	10	24	18	11	210	1271660
64	1.33	2.00	20	24	18	11	420	1403380
65	2.00	0.25	3	28	14	84	63	1433054
66	2.00	0.25	5	28	14	84	105	1540924
67	2.00	0.25	10	28	14	84	210	1681155

68	2.00	0.25	20	28	14	84	420	1832173
69	2.00	0.50	3	28	14	42	63	1330574
70	2.00	0.50	5	28	14	42	105	1430044
71	2.00	0.50	10	28	14	42	210	1559355
72	2.00	0.50	20	28	14	42	420	1698613
73	2.00	1.00	3	28	14	21	63	1236634
74	2.00	1.00	5	28	14	21	105	1328404
75	2.00	1.00	10	28	14	21	210	1447705
76	2.00	1.00	20	28	14	21	420	1576183
77	2.00	2.00	3	28	14	11	63	1168314
78	2.00	2.00	5	28	14	11	105	1254484
79	2.00	2.00	10	28	14	11	210	1366505
80	2.00	2.00	20	28	14	11	420	1487143

We apologize for the fact that the simulation time of CFD is not recorded. However, the iteration number of each simulation is recorded. The distribution of iteration number of 1600 simulations is shown in the Figure below. The average of that is 4443.

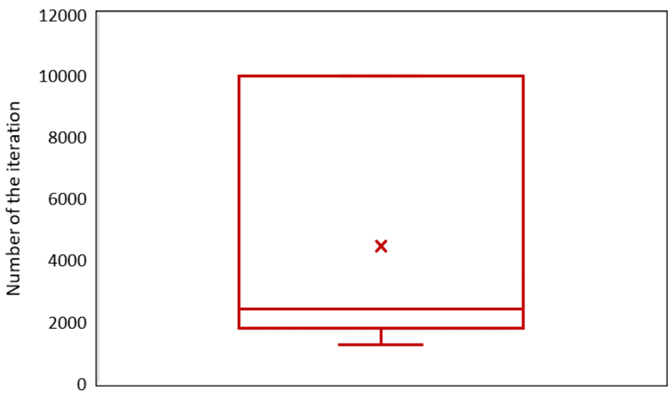

Figure. The distribution of iteration number of 1600 simulations.

Revisions in Manuscript:

(1) Materials and Methods. Line 226-227.

In summary, the average iteration steps of total 1600 cases were 4,443.

(2) Materials and Methods. Line 260-261.

The average mesh number in total 80 street canyon models is 1,367,965.

(3) Materials and Methods. Line 206-207.

Distances between urban canopy layers (UCL) boundaries and the domain top, domain inlet and domain outlet were set as 5*H*, 5*H*, and 20*H*, respectively.

Question 11

What is the spatial resolution of CMAQ /WRF?

Response:

Thanks for your question. The WRF-CMAQ system draws on a 4-nested run with a horizontal resolution at 1.33 km of the innermost domain. This introduction was added into the manuscript.

Revisions in Manuscript:

(1) Materials and Methods. Line 165-166.

The spatial resolution of the innermost domain in both WRF and CMAQ model was 1.33 km×1.33 km.

Question 12

Add ref. for the observation data in Fig. 5. Figure captions should generally be improved to facilitate the reading?

Response:

Thanks for your advice. We have added the references in Figure 5 to facilitate the reading.

Revisions in Manuscript:

(1) Figures.

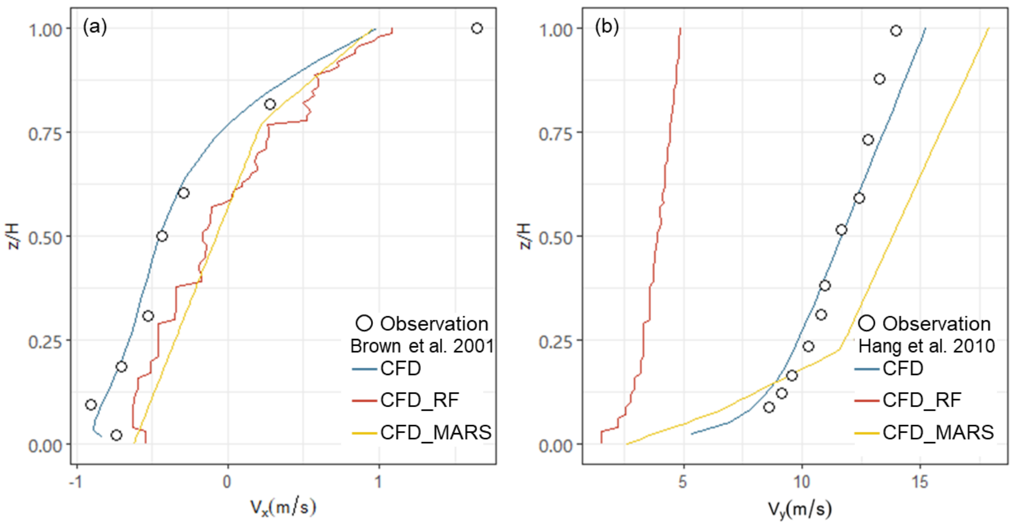

Figure 5: Performances of machine learning on velocity profile in wind tunnel experiments. The street canyon was perpendicular (a) or parallel (b) to the wind direction at the roof level in different experiments. The detailed description of each experiment was introduced in

Section 2.2.3.

Question 13

Clarify the innovation aspect in the introduction.

Response:

Thanks for your advice. The innovation of this study is that we developed a hybrid model to combine the advantages of the dispersion model and CTMs, where a cost-effective way using ML was proposed to simulate the street-level wind environment. We have already introduced advantages and limitation of different models, including CFD, the dispersion model and CTMs. In addition, the review of multi-scale air quality model was also introduced. In the revised introduction section, we have clarified the aim and innovation aspect more explicitly in the Introduction.

Revisions in Manuscript:

(1) Introduction. Line 98-99.

The objective of the present work is to investigate the street-level NO_2 concentrations and quantify the contribution of vehicle emissions considering the influence of the refined wind flow in complex urban environment.

(2) Introduction. Line 102-104.

We developed a Machine Learning-based Street Canyon Flow (MLSCF) parameterization scheme to estimate the wind filed in a cost-effective way, which was based on integrating two machine learning methods using big wind profile data from 1600 CFD simulations.

Question 14

Section S1 is incomplete. How are Z mix , convective velocity scale w * , surface friction velocity u * , and Monin-Obhukov length recalculated?

Response:

Thanks for your question. The mixing height Z_{mix}, convective velocity scale w^*, surface friction velocity u^*, and Monin-Obhukov length L_{MO} were recalculated based on AERMOD method (Cimorelli et al., 2005; Epa, 2019).

Revisions in Supplement:

(1) Section S1. Urban heat island scheme.

And then the mixing height Z_{mix}, convective velocity scale w^*, surface friction velocity u^*, and Monin-Obhukov length L_{MO} were recalculated based on AERMOD method (Cimorelli et al., 2005; Epa, 2019).

Question 15

What are the specific input data used in RLINE?

Response:

Thanks for your question. The input data of RLINE including road information, receptor information, meteorological parameters from WRF model, background concentrations from non-vehicle sources provided by CMAQ-ISAM model, and real-time on-road emission, which are contents of the square box in Figure 1.

Question 16

How the facbg is further used in the photochemical scheme? Is [NO2]b = facbg*[NO2]cmaq ? If yes, are O3 and NO also scaled with facbg?

Response:

Thanks for your question. In the scenario CMAQ-RLINE, the vertical mixing scheme is not included, so the fac_{bg} is not calculated. In the scenario CMAQ-RLINE_URBAN and CMAQ-RLINE_URBAN_nc, the fac_{bg} is calculated in the vertical mixing scheme and further used in the photochemical scheme, so the NO_2, NO, and O_3 are scaled with fac_{bg} to derive $[NO_2]_b$, $[NO]_b$, and $[O_3]_b$. We added this

(1) Section S3. NOx photochemical parameter scheme.

If the vertical mixing scheme is used in the hybrid model, $[NO]_b$, $[NO_2]$, and $[O_3]_b$ are derived by multiplying background concentrations from CMAQ-ISAM model with fac_{bg}.

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