

EGUSPHERE-2022-1125 | Development and technical paper

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Passive Tracer Modelling at Super-Resolution with WRF-ARW to Assess Mass-Balance Schemes

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Author Responses to Referee Comments

Color Code

RC, Referee Comments in Black

AC, Author Comments in Blue

Response to Anonymous Referee #1

Comment on egusphere-2022-1125

Anonymous Referee #1

Referee comment on "Passive Tracer Modelling at Super-Resolution with WRF-ARW to Assess Mass-Balance Schemes" by Sepehr Fathi et al., EGUsphere, <https://doi.org/10.5194/egusphere-2022-1125-RC1>, 2023

RC1_01: This work features high-resolution numerical simulations with the model WRF-ARW using realistic meteorological boundary conditions and employing a multistep nesting approach. A tracer transport module is used to simulate the dispersion of various emission sources at the finest LES scale. Ground-based and airborne observations are used to evaluate meteorological parameters, which generally showed satisfactory performance, though some questions regarding the wind-speed evaluation remain. Finally, the mass-balance scheme was applied on 4-D model output to infer source emission rates and to evaluate local and global mass conservation of the tracer transport scheme. This part of the study can still be better elaborated as suggested by the comments given below. The structure of the manuscript, the quality of the figures, and the presentation of the data and results can be further improved.

AC1_01: We thank you for your valid and thorough comments. We made several revisions in response to your comments which helped improve our manuscript. Specific responses to each comment are provided below.

Major comments

RC1_02: The authors evaluate the performance of the WRF tracer transport scheme regarding mass conservation and the positivity of transported concentrations. I think since this is one of the most relevant results of this study, a more detailed description of the transport schemes in the paper is necessary. What is the differential equation to be solved? How are the advection and diffusion terms discretized in space and time? What kind of flux redistribution is applied for positivity? The authors state that the turbulent diffusion step is mainly responsible for the observed negative mass creation. This seems not very plausible unless it is shown by example. Did the authors test the transport scheme with diffusion turned off? The transport scheme is supposed to be conservative (based on the flux- divergence formulation). How is it then possible that a vertically changing grid spacing results in a violation of mass conservation? This needs further clarification.

AC1_02: Thank you for raising these valid and important points. Additional discussions were added throughout (especially to Section 2) to expand on descriptions for transport schemes, differential equations, advection and diffusion, positive definiteness, negative mass creation and mass conservation. Regarding the diffusion scheme, we included the following in the revised manuscript section 2.2: "Various formulations are available in ARW solver for explicit spatial diffusion (turbulent mixing) including a sixth order spatial filter proposed by Xue (2000). The implementation of this scheme in ARW is described in Knievel et al. (2007). The sixth order turbulent diffusion scheme is also prone to creating negative mass due to negative up-gradient diffusion. Monotonicity can be enforced in the model (user specified option) by setting negative diffusive fluxes to zero, however it does not conserve scalar mass (Shamrock et al., 2008). Hence, in our simulations we used the sixth order diffusion scheme without the monotonic option." Also, the new Figure S10 was added to show the comparison of the monotonic and non-monotonic diffusion options in WRF. We chose the non-monotonic option due to the fact that the monotonic diffusion, while positive, is not necessarily conservative. The following text was added to first paragraph of Section 3.4 "As discussed in Section 2.2, in our simulations we used a positive-definite transport scheme combined with a sixth order diffusion scheme. Negative up-gradient diffusion flux near sharp concentration gradients resulted in partial creation of erroneous mass within the modelling domain. Positive flux and monotonicity can be enforced in the model by setting negative fluxes to zero, however this is not mass conserved (see Figure S10). Therefore, we configured our simulation using the diffusion scheme without the monotonic option.

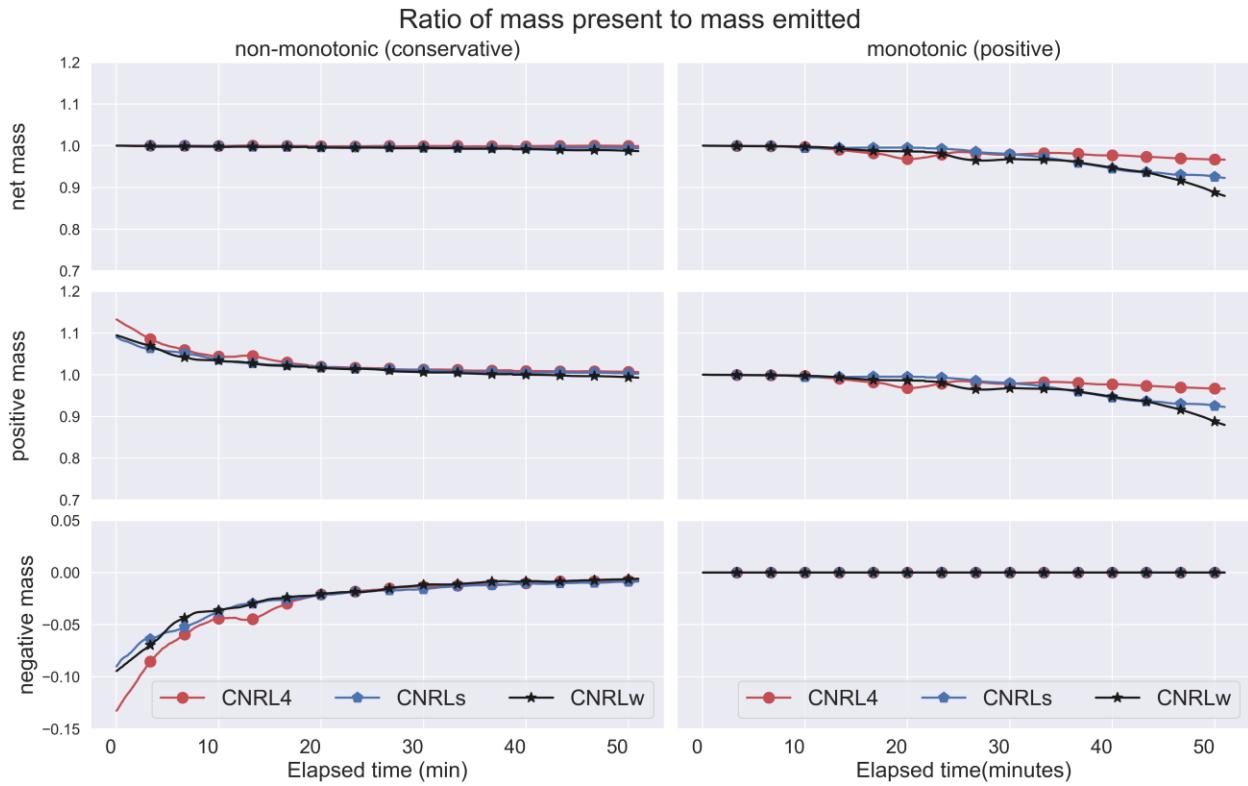


Figure S10. Comparison of WRF-ARW default non-monotonic diffusion scheme (left column) with the monotonic-positive diffusion scheme (right column), as the ratio of mass present in the modelling domain to mass emitted.

RC1_03: The implementation details of the mass-balance technique are still only poorly described. The authors should give some details on how the advective and diffusive fluxes ($F_{C,H}$, $F_{C,H,T}$, $F_{C,V}$, $F_{C,V,T}$) at the flux-box boundaries are computed in discrete form. How are the scalar values, which are defined at mass points, interpolated/reconstructed at the cell faces, where the velocity components are defined? Does the offline computation of the fluxes based on model output match the flux computation of the WRF advection/diffusion scheme?

AC1_03: Table S1 was added to the supplement for discrete integral expressions of terms used in the mass-balance equation. The following text was included in Table S1 caption “Model wind fields were linearly interpolated onto mass grid-points for the discrete integral calculations.” Further, the following text was added to the last paragraph of Section 2 “See Table S1 for discrete integral expressions of different terms in the mass-balance equation (Eq.6). Note that for flux calculations in this work, model wind fields were linearly interpolated onto the mass grid-points (where concentration fields are defined).”

Table S1. Discrete integral expressions of Eqs. (3), (4), (5), (B1) and (B2) to be substituted in Eq. (6). Constants Δx , Δy and Δs are equal to model grid resolution in the horizontal, 50 m. t is the time index; i , j and k are the 3D-space indices and s is the path index around the control volume (box). Model wind fields were linearly interpolated onto mass grid-points for the discrete integral calculations. Throughout, the second-order central finite-difference scheme was used to numerically solve the time derivatives ($\Delta/\Delta t$) with the residual error of order $O(\Delta t^2)$, where Δt is equal to the 1 sec model output time-step.

Term	Discrete Numerical Integration
S_C^t	$= \Delta x \Delta y \sum_{i,j,k}^{n_x, n_y, n_z} \frac{\Delta \chi_{C,ijk}^t}{\Delta t} \Delta z_k$
$F_{C,H}^t$	$= \Delta s \sum_{s,k}^{n_s, n_z} \chi_{C,sk}^t U_{\perp,sk}^t \Delta z_k$
$F_{C,HT}^t$	$= -K_h \Delta s \sum_{s,k}^{n_s, n_z} \frac{\Delta \chi_{C,ijk}^t}{\Delta x_{\perp}} \Delta z_k$
$F_{C,V}^t$	$= \Delta x \Delta y \sum_{i,j}^{n_x, n_y} \chi_{C,ij}^{t,top} W_{ij}^{t,top}$
$F_{C,VT}^t$	$= -K_v \Delta x \Delta y \sum_{i,j}^{n_x, n_y} \frac{\Delta \chi_{C,ijk}^t}{\Delta z_{\perp}}$

RC1_04: The horizontal grid-refinement ratio of 1:5 in the nesting process is quite large (typically 1:2 or 1:3 is used). Are there any specific reasons for using such a large grid-refinement ratio? Are there any tests available from which nesting errors could be estimated? How large are the vertical grid refinement ratios near the ground? Δz for d03 and d04 are missing in the paper.

AC1_04: The WRF user guide recommends horizontal nesting ratios of up to 1:5, which is what we used as a compromise between computational cost of our simulations and achieving the desired resolution of 50m in the finest domain from the 31km resolution input reanalysis fields. The following text was added to section 2.2: "With regards to nesting in the horizontal, Shamrock et al. (2008) recommended the use of odd nesting ratios such as 1:3 and 1:5 (as opposed to even ratios like 1:2), due to the staggered structure of the Arakawa C-grid used in WRF-ARW modelling framework. Mohan and Sati (2016) investigated the impact of different nesting ratios in WRF and found no statistically significant difference in simulated results with ratios 1:3, 1:5, and 1:7, suggesting that larger ratios can be used to reduce the computational cost in nested simulations. However, larger ratios (e.g., 1:9) can result in increased interpolation errors and are not recommended. In this work, as a compromise between numerical accuracy and computational cost, we used a 1:5 nesting ratio". Also, vertical grid refinement ratios were added to Table 3 "d04: d03 grid refined (~1:3) below 2500 m agl, d05: d04 grid refined (~1:7) below 540 m agl".

RC1_05: Regarding the wind speed evaluation with WBEA observations: The sensitivity of wind speed to model resolution was not satisfactorily explained. It is not convincing that the nesting error would result in a systematic increase in wind speed at each nesting step. Such a conclusion certainly cannot be drawn from Daniels et al. (2016). This brings me to the question of whether the vertical interpolation of model data to the measurement height of 10m was based on a proper logarithmic law? A comparison of vertical profiles of wind speed between domains d03, d04, and d05 would be helpful to further investigate this large apparent sensitivity.

For model output from domain d05, the first two model layers were at 6m agl and 18m agl, and so the 10m agl wind was determined by interpolating between these two levels. Model output data from domains d03 and d04 included diagnostic variables for U and V at 10m agl. See the newly added Figure S2 where wind profiles from domains d03, d04, d05 are compared. Further, points 2 and 3 in section 3 (old section 3.1 / new section 3.2) were revised as follows:

"2. The wind speeds in the NARR reanalysis data (at 31 km resolution) used as input for our simulations, were higher than WBEA observed values by 2-3 m/s for the region and the periods of interest. Consequently, the bias in NARR winds was carried through model nested simulations. If replicating the observed atmosphere is an objective of the modelling, it is recommended that input data (e.g., NARR reanalysis) to be adjusted to observations first.

3. Dynamical down-scaling of NARR reanalysis data from 31.25 km resolution to 50 m resolution with five nested domains and vertical grid refining is another source of uncertainty. In concurrent grid nesting as used in this work, output from parent domain is interpolated to provide initial and boundary conditions for each respective nested domain. Horizontal, vertical and temporal interpolation errors are therefore compounded with each nesting. This can result in biased wind fields as in Daniels et al. (2016), which is consistent with our results where d04 wind speeds were higher than d03 by about 1 m/s, and d05 winds were higher than d04 by about 1-2 m/s (see Table 4 for d04 vs. d05). While there may be a relationship between nesting a wind speed error, these results do not directly demonstrate a change in wind speed due to nesting."

RC1_06: Figure 5: Did the authors really show the full vertical extent of model data from the first model layer above ground? If so, it is strange that the wind speed in the model does not decrease towards the ground. The WBEA data shows consistently lower wind speeds than the aircraft data, which obviously

reflects the logarithmic wind law within the surface layer. Your model results give no hint of that.

AC1_06: Note that the profiles depicted in Fig. 5 are averaged profiles over the horizontal extent of domain d05 and over the simulation time. Bars show the respective standard deviations (spatial + temporal). Further, Fig. 5 was revised to show data as a function of height above ground level (agl), and to include aircraft data for the box flight portion of the sampling, which reduces (but does not eliminate) the increase at the surface. Figure S2 is added, where wind profiles (not averaged spatially or temporally) from domains d03, d04, d05 are depicted. These profiles show decreased wind speeds towards ground for all three domains. The following text was added to last paragraph of section 3.2: "Model data were averaged horizontally over domain d05 and the simulation time (Fig. 5), for comparison to aircraft data that were collected during 1-2 hours flight time over the oil sands region. Note that the near surface increase in wind speeds in Fig. 5 is the result of averaging over varying (complex) topography (see Figure S2 for instantaneous profiles at the location of the main CNRL stack). "

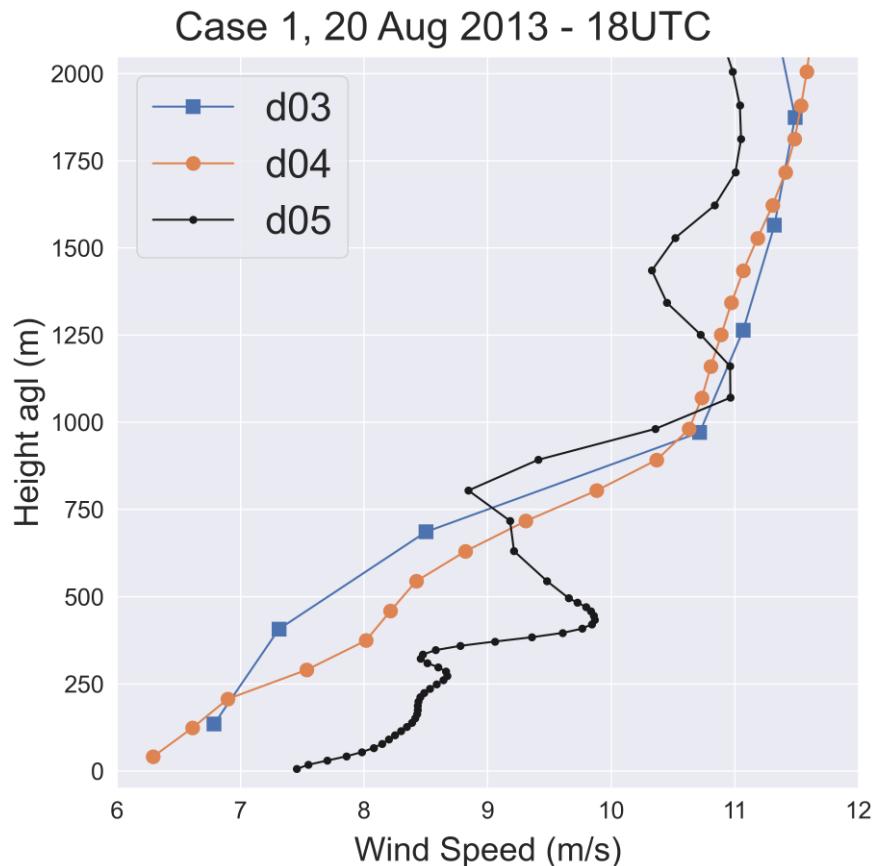


Figure S2. Wind vertical profiles from domains d03, d04 and d05 compared at the location of the main CNRL stack for case 1 on 20 Aug 2013 at 18 UTC.

RC1_07: Figure 7 alone provides a very weak basis for the discussion of the vertical mixing characteristics of the plumes. Some features the authors describe (like the effect of the Athabasca river basin) may be just attributable to random turbulent fluctuations. I suggest providing at least an additional plot for temporal mean turbulent statistics, like the average vertical turbulent flux of tracer mass or turbulent stresses.

AC1_07: Further discussion on the role of turbulent mixing was added to the end of Section 3.3.

RC1_08: The structure of the manuscript needs to be improved:

Section 2.2: I suggest separating the model description from the technical setup more clearly. The paragraphs do not seem to follow any clear logic. I would suggest the following paragraphs:

A concise description of the WRF model

The tracer module should be described in more detail (governing equation + spatial discretization), as it is the main focus of the study.

Introduction of the simulation domains d0-d5 with the static information (horizontal + vertical resolution, horizontal extent, coverage) along with the nesting technique
Simulation settings of domains d0-d5 + driving data of coarsest domain d0
Implementation of the point and area emission sources in d05

AC1_08: Section 2.2 was revised accordingly. The following text was added to the first paragraph "The Advanced Research WRF (ARW) solver features a suite of fully-compressible Euler-nonhydrostatic equations for solving prognostic variables including velocity components in Cartesian coordinates (u , v , w), and scalars such as water-vapour mixing ratio and tracer concentration. The 3rd order Runge-Kutta scheme (RK3) is used for time integration in ARW (Wicker and Skamarock, 2002). The spatial discretization in WRF-ARW uses a Arakawa C-grid staggering with thermodynamics/scalar variables (e.g., moisture, tracer) defined on grid cell centres (mass points), and velocity components defined normal to respective faces of model grid cells (one-half grid length from mass points). 2nd to 6th order spatial discretization and RK3 time-integration scheme are available in ARW to solve for advection of momentum, scalars, and geopotential in flux form (the governing equations). The RK3 transport/advection (combined with flux divergence) in WRF-ARW is conservative, however it does not guarantee positive definiteness on its own. Negative mass creation is offset by positive mass such that tracer/scalar mass is conserved over the modelling domain (Skamarock et al., 2008). Negative mass can be set to zero, but this will result in erroneous

increase of tracer mass within the modelling domain. By choosing a positive-definite scalar advection option in WRF-ARW, as we did in our simulations, a flux re-normalization is applied to the transport step to remove the nonphysical effects such as creation of the negative mass (Skamarock and Weisman, 2009). To summarize, if the outgoing fluxes (removing mass from the control volume) in the final step of RK3 predict a negative updated scalar/tracer mixing ratio, the outgoing fluxes are re-normalized to be equivalent to mass within the volume. For more details see Section 3.2.3 in (Skamarock et al., 2008). Various formulations are available in ARW solver for explicit spatial diffusion (turbulent mixing) including a sixth order spatial filter proposed by (Xue, 2000). The implementation of this scheme in ARW is described in Knievel et al. (2007). The sixth order turbulent diffusion scheme is also prone to creating negative mass due to negative up-gradient diffusion. Monotonicity can be enforced in the model (user specified option) by setting negative diffusive fluxes to zero, however it does not conserve scalar mass (Skamarock et al., 2008). Hence, in our simulations we used the sixth order diffusion scheme without the monotonic option.”

RC1_09: Section 3.1: The authors should first provide a complete and purely descriptive comparison of model data (domain d05) with WEBA and aircraft observations before they draw any further conclusions regarding model performance. The content from line 310 until the end of the section describes in fact only model sensitivity and does not provide a model evaluation at the location of the oil-sand facility. From line 321 onwards the authors just mostly repeat the content of Table 4, which is quite confusing to read. I would suggest dedicating this paragraph to model sensitivity, labeling it as such, and presenting the data in a more structured way.

AC1_09: Revisions were made accordingly with the discussions on model sensitivity gathered in a new “Section 3.1: Model Sensitivity” and, the Section 3.2 dedicated to model evaluation against observational data.

RC1_10: Section 3.3: It is started here again with a model description. The authors should move this first paragraph to Section 2.2, where the tracer module is introduced.

AC1_10: Revised accordingly, relevant text was moved to Section 2.2.

RC1_11: Many figures need revision:

The subplots of multipanel figures should be labeled in alphabetic order and referenced as such in the caption. The caption should only contain precise and concise descriptive information and no evaluative comments. The caption of Fig. S2 is incomplete and contains an evaluative comment. What

exactly is “level tracer count sum” in Figure 7, S4, and S5? The authors should only use terms that are clearly defined.

AC1_11: Fig. S2 (S3 in the revised manuscript) caption was revised to “Model output meteorological fields from the two fine resolution domains d04 and d05 were evaluated against domain d03 output for the location of CNRL facility in terms of root mean square error (rmse) and mean bias (me). Time series are shown for wind speed at 10 m agl (a, b), temperature at 2 m agl (c), relative humidity at 2 m agl (d), and seal level pressure (e).” Fig 7, S4, and S5 captions were revised “Data shown is the tracer amount summed in the horizontal level and normalized to the maximum value for each source.” Color labels for these figures were changed to “Total Mass in Horizontal”.

RC1_12: The colorbars of Figures 11 and S1 are still missing. The colorbars of Figures 7, S3, S4, S5, S6, and S7 can be improved (logarithmic scaling of ticks and larger tick labels).

It is difficult to see the wind barbs in Figures S3, S6, and S7, and the thin contour lines (I assume this is terrain height?) further interfere and do not provide further useful information.

AC1_12: Text was added to Fig 11 caption “Colour darkness is proportional to log of column total tracer mass.” Figures 7, S3, S4, S5, S6, and S7 were revised accordingly. Colorbar was added for Fig 11.

RC1_13: The labeling of the time axis in Figures 4 and S2 needs to be revised (what is the “20” in front of the time stamp?). Please also include bias values in each subplot of Figure S2, like done for rsme. For a better comparison of data in Figure 3, I suggest using the same percentage axis (e.g., 0, 10, 20, ..., 60) in the wind-rose plots.

AC1_13: Figures 3, 4 and S2 were revised accordingly.

RC1_14: The tick labels of the x- and y-axis need to be increased in Figures C1-C3. What simulation domain is presented in Figures C1-C3, and is the depicted data horizontally averaged?

AC1_14: Data shown in Figures C1-C3 are from domain d05. The depicted data is horizontally averaged over domain d05 and averaged over time. Figures were revised accordingly. The following text was added to figure captions “The profiles were averaged horizontally over domain d05 and over the simulation time. Bars show standard deviations.”

RC1 Minor comments

Line 29: missing comma before “which”

Revised

Line 51: “were successful”

Revised

Line 65: Please provide also an estimate for the sampling frequency besides the flying speed. How one gets $dx \leq 100m$ and $dt \leq 1s$?

Revised, text added “e.g., onboard instrument $\geq 1Hz$...”

Lines 85-86: “from the Joint Canada-Alberta Implementation Plan on Oil Sands Monitoring airborne campaign (JOSM 2013).”

Revised

Line 114: “are considered”.

Revised

Line 123: “large area rectangular surface source” is a bit strange. It should be clear to the reader that it is a surface source. Maybe “large rectangular area source” is better? Please check also other instances in the manuscript, e.g., “multi-section line surface source” (line 124).

Revised to “large rectangular area (surface) source” and “multi-segment line (surface) source”

Table 2: Please provide an extra column for “Size” for the numbers ~ 20 km, ~ 50 km 2 , etc. Done, the “Spatial extent” column was added.

Caption of Figure 1: Is Hwy an abbreviation for highway? Yes, revised to “highway”

Line 142: This is not a complete sentence. Suggested correction: “...simultaneously. The process where the coarse “parent” domain’s output is interpolated to provide initial and lateral boundary conditions for the fine “child” domain is referred to as one-way nesting.” Revised

Line 149: “and this is” Done

Line 153: Please either consistently use “JOSM 2013” or “2013 JOSM” throughout the manuscript. Done

Caption of Table3: What exactly are “Coarse” and “Fine” for the vertical grid? Please provide a clear explanation with numbers here or in the main text. According to the main text, “Fine” is not exactly the same for d04 and d05? What is Z_{top} ? Please use precise language and introduce every variable properly.

The column “vertical grid description” was added to Table 3. Table 3 caption’s last sentence was revised to “With model top layer at 15.623 km (15.350 km agl) and pressure level of 10 kPa for all domains”.

Line 165: “in the figure Figure 2b.”

Line 167: “complex flow conditions” Revised

Line 169: Please provide a reference with section numbers for “In the following sections”. Done

Lines 170-175: This paragraph deals again with vertical model resolution (already introduced before line 160) and contains repeated information (see line 158).

The repeated information was removed and the rest of the discussion in the paragraph was moved to lines 159-162 “Note that the vertical resolution of about 12 m for the bottom 500 m agl (above ground level) is sufficient for investigating and evaluating different methods for extrapolating sampled data below the lowest flight level...”.

Line 183: Is this really part of the subgrid-scale parameterization or just numerical diffusion to remove spurious small-scale noise of the advection scheme? What exactly is the default option?

Revised to “In order to simulate small-scale atmospheric dynamical processes, the finest two model domains (d04 and d05) were configured with the following dispersion scheme, and Large Eddy Simulation (LES) sub-grid parameterization options available in the WRF model...”

Line 185: What exactly are these modifications? I checked Blaylock et al. (2017) and could not find any WRF modifications related to tracer transport.

Text was revised to “To simulate the emission of passive-tracers, the WRF dynamical-solver source code was modified following an approach similar to Blaylock’s (as described in Blaylock 2017) used in Blaylock et al. (2017).”

Reference: Blaylock, B. K.: Tracer Plumes in WRF (last accessed: March 8, 2023), https://home.chpc.utah.edu/~u0553130/Brian_Blaylock/tracer.html, 2017.

Line 205: Please provide the section number here (“...are discussed in Section xx”). **Done**

Line 308: “were more severe is larger” **Revised**

Line 308: “We discuss later” Where exactly? **Revised** “(Section 3.4)”

Line 311: “due to the fact that” **Revised**

Line 311: “(see above)” Where exactly this is shown? **Revised to** “(see discussions at the beginning of Section 3.1 and also see Figure 3)”

Line 339: “below” Where exactly (Section xx)? **Revised** “discussed in Section 3.3”

Line 361: What is an “emission flight”? **Revised to** “box flight (see Section 2.1)”

Line 361: “in relevant publications” Which publications? Only Fathi et al. (2021)? **Revised to** “was rejected for emission rate calculations due to low and variable wind speeds as reported in Fathi et al. (2021)”

Line 391: If I am not wrong, mass conservation is determined by the spatial discretization (flux-divergence formulation) and is not directly related to the Runge-Kutta scheme, which is just a time integration scheme.

The Runge-Kutta scheme is the transport scheme used in our WRF simulations which ensures conserved transport of tracer amounts the model transport step as described in Shamrock et al., 2008, which is cited in the sentence which follows.

Line 397: “The turbulent diffusion step in the model is also prone to creating negative mass, but to a lesser degree.” Can the authors please provide a reference for this? Standard second-order diffusion does not create negative mass (see e.g., Fig. 2a in Xue (2000): High-Order Monotonic Numerical Diffusion and Smoothing).

We used the sixth-order diffusion scheme without the monotonic option as this is not conservative, which as you can see in Fig. 2c in Xue (2000) can create negative values. Relevant discussions were added in Section 2 first paragraph.

Lines 463 and 473: use singular “Table 6” **Done** (new Table 7).

Line 465: "with model input emission rates (MIE)" Revised

Line 481: Why negligible estimated emission rates? The estimated emission rates for case 2 were within 5% of MIE (except case CNRL0).

Revised to ", which resulted in negligible estimated emission rates based on flux calculations alone (i.e., not accounting for storage)".

Lines 485-490: Based on the results, I would be cautious to draw such a conclusion. Higher resolution does not always mean more accurate wind fields (see case 1, where d03 seems to be more accurate than d05). Where can I find the observation of (FC,H < 20%)?

Text was revised to "While both modelling setups replicated the same meteorological (advection) conditions, the relatively coarser resolution of GEM-MACH simulations resulted in larger computational (grid) diffusion and consequently larger downwind dispersion of tracer amounts (and larger predicted horizontal mass flux). This in part demonstrates the benefits of employing super-resolution over high-resolution modelling. The WRF super-resolution simulations in this work were successful in closely replicating the observed weak advection conditions and GEM-MACH predicted FC,H<20% for the same period (Fathi et al., 2021), but at a higher spatio-temporal resolution. "

Line 502: "as indicated in Fig. 11" Revised

Line 524: Where are these modifications described in the manuscript? Is this related to the hard coding of emissions?

Yes, they are, see the revised text in lines 201-203 of the revised manuscript: "To simulate the emission of passive-tracers, the WRF dynamical-solver source code was modified following an approach similar to Blaylock's (as described in Blaylock 2017) used in Blaylock et al. (2017)."

Reference: Blaylock, B. K.: Tracer Plumes in WRF (last accessed: March 8, 2023), https://home.chpc.utah.edu/~u0553130/Brian_Blaylock/tracer.html, 2017.

Lines 536-538: This is quite speculative unless the authors provide more details on the numerical schemes.

The corresponding text in the Conclusion section was revised to "Our results suggest that the unbalanced creation of erroneous mass at sharp concentration gradients, such as at the vicinity of point sources, is intensified on an irregular grid (an artifact of model dispersion). However, more investigations with longer simulation times (beyond the scope of this

paper) are required to further investigate such effects. Small negative diffusive fluxes and the use of the positive-definite re-normalization scheme in our modelling setup prevented nonphysical effects (e.g., negative mass creation) for 10 out 11 emission sources (assigned on a regular grid). "

Lines 543-544: What happens if the tracer plume is vertically advected into layers with an irregular grid spacing? Then there is the same problem with losing mass.

That's correct, and we have discussed it in the last paragraph of Section 3 "Estimates were also partially affected by the changing vertical grid spacing for upper model layers, for tracer amounts mixing to higher altitudes (> 500 m). This is similar to mass loss for CNRL0 emissions, but to a much lesser extent."

Lines 552-553: See the previous comment.

Response to Anonymous Referee #2

Comment on egusphere-2022-1125

Anonymous Referee #2

Referee comment on "Passive Tracer Modelling at Super-Resolution with WRF-ARW to Assess Mass-Balance Schemes" by Sepehr Fathi et al., EGUsphere, <https://doi.org/10.5194/egusphere-2022-1125-RC2>, 2023

"Passive Tracer Modelling at Super-Resolution with WRF-ARW to Assess Mass-Balance Schemes" by Sepehr Fathi, Mark Gordon, and Yongsheng Chen

Recommendation: Major revisions

General comments:

RC2_01: This manuscript introduced a turbulence-resolving (or super-resolution) passive tracer modeling system and assessed its performance in terms of 1) meteorological parameters in the atmospheric boundary layer (ABL), 2) characteristics of small-scale passive tracer structures in the ABL, and 3) conservation of passive tracers. The super-resolution tracer modeling system was developed based on a one-way nesting capability of the WRF model. Specifically, a gradual downscaling from reanalysis scale (31.25 km) to an LES scale (50 m) was implemented in horizontal, and grid-refining in vertical was applied for the two innermost sub-kilometer grid-spacing domains. Meteorological evaluations were performed for three cases in comparison to station and aircraft observations of surface pressure, temperature, humidity, and wind. The first major concern I have is about the methodology used in meteorological evaluations, especially the inconsistency of the reference data (base case), i.e., the use of d03 results for evaluation of d04 results vs the use of d04 results for evaluation of d05 results etc. The characteristics of plume dispersion were then investigated focusing on differences caused by emission scenarios — e.g., emission source height, and emission type (point, line, and surface) — and by meteorological conditions — i.e., three different weather cases. My second major comment is that this manuscript lacks discussions on role of the ABL turbulent mixing in the plume characteristics, even though the results presented in the manuscript indicate that the ABL turbulence plays a significant role in determining the tracer dispersion that appears differently according to the emission source height and meteorological conditions.

AC2_01: We thank you for your constructive and detailed comments. We implemented your suggestions in revising our manuscript. Revisions in response to each comment are provided below.

Major comments:

RC2_02: 1. Revisions are needed in the methodology used in meteorological evaluations.

1.1. Wind speed, which is the most critical meteorological variable in accurate prediction of tracer dispersion modeling, shows large biases in comparison to observations. The authors suggested possible reasons of the large bias, including the NARR reanalysis data that have positive biases. To take account of the impacts of this reanalysis error carried over to the simulations, the authors used coarser resolution simulations to evaluate nested-domain simulations, instead of observations. I agree to the impact of reanalysis errors on the nested domains, but I think evaluation results in comparison to both observations and coarser-domain results need to be presented together, together with tables summarizing bias and RMSE scores, in the main text.

AC2_02: Thank you for your suggestion. A new table was added (the new Table 5) comparing domain d05 meteorological fields to WBEA observations.

Table 5. Meteorological evaluation of domain d05 simulations against WBEA observational data at the geographical location of Bertha Ganter–Fort McKay (AMS01) station. Model performance is shown in terms of root mean square (rms) error and mean bias. Positive/negative values indicate over/under-estimates by d05 relative to WBEA-AMS01 observations.

		2-m RH(%)	2-m Temperature (°C)	10-m Wind Speed (m/s)	10-m Wind Direction (deg.)
Case 1	WBEA mean	44.52	22.97	2.85	244.96
	rms error	2.76	5.10	5.63	19.11
	mean bias	1.40	-5.08	5.60	11.26
Case 2	WBEA mean	83.90	19.61	2.08	93.5
	rms error	24.55	2.59	0.99	20.00
	mean bias	-24.54	-2.58	0.99	18.73
Case 3	WBEA mean	56.14	24.07	4.07	239.83
	rms error	5.81	2.29	3.37	169.70
	mean bias	-1.56	-1.97	3.36	26.17

RC2_03: 1.2. This study used percentage error as an evaluation metric. Most meteorological variables, except for wind speed, have large absolute values (e.g., pressure, RH, temperature, and wind direction), therefore using the

percentage error as an evaluation metric could mislead about the performance of the modeling results. I suggest adding a table that summarizes bias and RMSE scores of the meteorological variables in comparison to observations, similar to Table 4.

AC2_03: Text was revised in Section 3 to present model evaluation in variable units instead of percentage error. Also, a new table was added (Table 5, see the previous comment).

RC2_04: 1.3. There are a number of places that plots and main texts are inconsistent. Wind-rose diagrams in Figure 3 show that winds are from north-east and east, while the main text mentions that the wind directions are from west and west south west (Line 265, Page 11).

AC2_04: Note that in the first version of the manuscript in Fig 3, winds were depicted as blown towards, rather than blown from. Hence the information in the Figure and the text are consistent: winds are from west and west southwest. In the revised version of the manuscript, Fig. 3 is revised to show winds as blown from.

RC2_05: 2. This manuscript lacks discussions on the role of turbulent mixing in determining plume characteristics, while the results presented in the manuscript indicate it is critical to understand the differences of the plume characteristics by emission source height and also between cases.

2.1. Plume characteristics from the emission scenario CNRL0 indicate the different role of turbulent mixing across the atmospheric boundary layer (ABL) top: i.e., within the ABL where turbulent mixing plays a dominant role in vertical structure of the ABL, including tracer concentration, vs. above the ABL where turbulent motions are suppressed by negative buoyance of the stably stratified inversion layer overlying the ABL.

In Case 1, the plume dispersion resulting from the emission scenario CNRL0 shows very different behaviors (e.g., Figure 7) from other stack scenarios. The source height of the CNRL0 scenario is located at 483 m, which is around the ABL top where the vertical mixing by turbulence ceases due to the capping temperature inversion. The ABL height can be inferred from the potential temperature profile in Figure C1, which shows a stably stratified layer with small spatial variability (standard deviation) around 500 m. The tracers emitted from other sources are quickly (within a few minutes) mixed in vertical within the ABL from the surface to the ABL top, leading to a similar vertical structure at ~ 10 km downstream regardless of the source height (Figure 7). On the other hand, the vertical dispersion of tracers in the CNRL0 scenario is confined to a smaller vertical domain, due to the relatively weaker turbulence mixing above the ABL top than within the ABL.

2.2. Differences in plume characteristics between Case 2 vs. other two cases can also be explained by the role of turbulence mixing. The meteorological profiles shown in Figure C2 indicate stronger turbulence activities in Case 2 than in other two cases, with the ABL top at around 1300~1500 m. In Case 2, I guess the plume dispersion of the CNRL0 would be very similar to other CNRL scenarios (though not shown nor mentioned in the manuscript), because all sources are located within the ABL in this case. Based on the meteorological profiles of Case 3 presented in Figure C3, I think Case 1 and Case 3 would show very similar results; the ABL top is located around 500 m in both cases, resulting in only the CNRL0 emission source being above the ABL top. More in-depth comparison of the plume characteristics between Case 1 and Case 2 could be made, based on the different role of turbulence mixing between the two scenarios. The manuscript did not provide any of these important points.

AC2_05: Thank you for your suggested discussion. Figures C1, C2, C3 were revised, a new figure for case 2 was added to the supplement, and the following text was added to the end of Section 3.3 "Average inversion heights Z_i (inferred from potential temperature profiles) for the three cases are marked with dashed lines in Figs. C01, C02, and C03. Z_i for cases 1 and 3 was between 300-400 m agl, placing the tracer sources (all except CNRL0) within the atmospheric boundary layer (ABL) where turbulent mixing plays a dominant role in modifying the vertical structure of the atmosphere including tracer concentrations. As a result tracer amounts released from these sources (at different heights) were mixed quickly in the vertical extent of the ABL within the 10 km downwind distance resulting in similar uniform vertical profiles (Fig. 7). For cases 1 and 3 the CNRL0 release height at 483 m agl was above Z_i , where turbulent mixing is suppressed by negatively buoyant atmosphere in the stably stratified inversion layer. Which confined the dispersion of CNRL0 tracer amounts within a smaller vertical extent and detached from the ground surface up to 10 km downwind distance (see Fig. 7). For case 2, Z_i was between 1400-1500 m agl, placing all source including CNRL0 well within the ABL and resulting in similar vertical mixing for tracers released at different heights from ground surface up to 483 m agl (see Figure S9)."

Case 2 : 2013 Aug 26 - 19:43:00

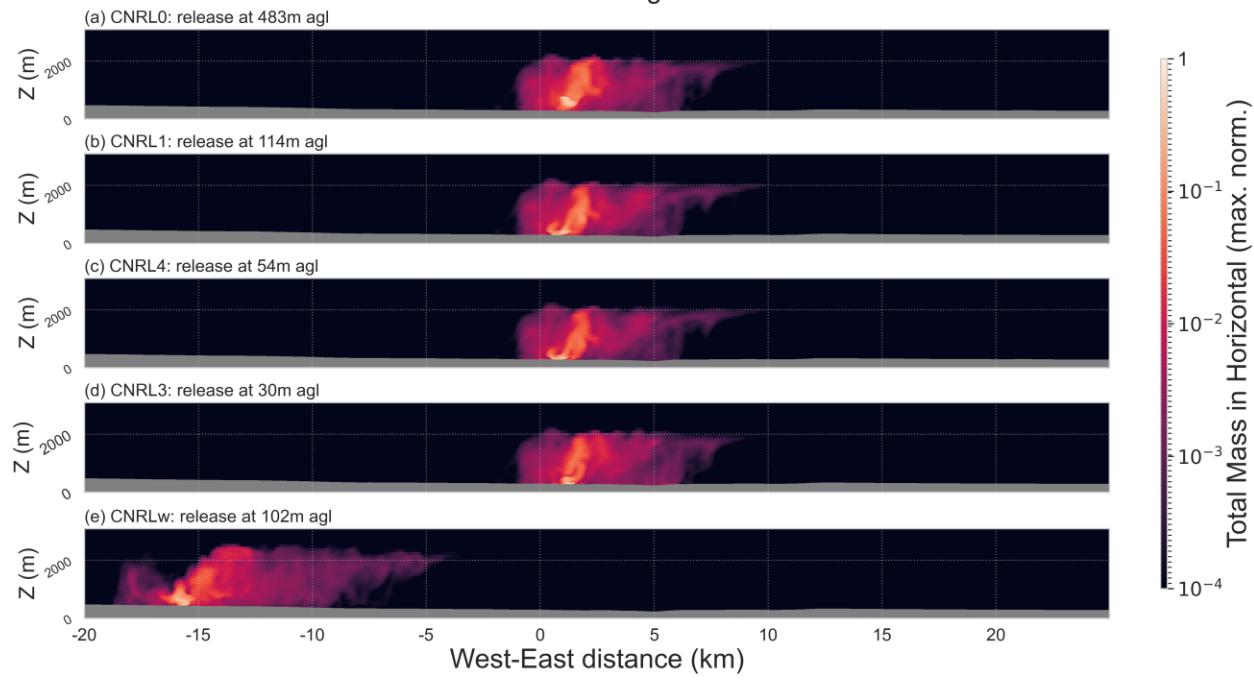


Figure S9. Domain d05 west-east vertical cross-section for case 2 on 26 August 2013. Vertical cross-section of tracer plumes from stack/point emission sources are shown with release heights indicated for each source. Data shown is the tracer amount summed in the horizontal level and normalized to the maximum value for each source. The origin for south-north distance in km is at domain centre.