Response to Reviewer 2

We thank Reviewer 2 for the thoughtful and detailed comments on our manuscript. Below, we address the two general comments first, followed by the specific line-by-line comments.

Reviewers general comment 1:
My main issues with the paper are first that I think the choice of rate coefficient for microbial oxidation could be discussed further. According to appendix E, half-lives found in the literature vary from 5 days to two years, and then to just consider a single rate coefficient which corresponds to a half-life of around 30 days seems a bit simple. I'm not saying you necessarily need to do more simulations, as I think the point of the paper is more to demonstrate a method than to give definite numbers, but I think this could be discussed further.

Response:
We agree with the reviewer on this point and have expanded the discussion in the "Interpretation of the results" section, where we outline the importance and challenges of including microbial oxidation in the modelling framework. In addition, we conducted a set of sensitivity simulations with a range of rate coefficients to examine the impact on the fate of dissolved methane. This allows us to describe, at least in a semi-quantitative manner, the sensitivity of the modelling framework to different microbial oxidation rates.

Reviewers general comment 2:
Second, the paper is quite long, and dedicates a lot of time to describing a partially new method for calculating concentrations. I am not completely convinced by the authors' arguments that this was necessary, and even if it was (necessary), I think much of Section 2.3 could go in the appendix, as it distracts from the main point. (In my opinion, the main point of the paper is that it's a good idea to combine a bubble model with a 3D transport-fate model for dissolved methane. The rest is just details.)

Response:
We respectfully disagree, and we consider Section 2.3 to be one of the main contributions of the manuscript. This section addresses how realistic concentration estimates can be obtained using a Lagrangian particle dispersion model (LPDM). The choice of density estimator is very important in this context because the number of simulated particle trajectories is constrained by computational resources. As is well established, the commonly used histogram estimator performs poorly when particle numbers are limited, while kernel density estimators (KDEs) can provide substantial

improvements in both accuracy and computational efficiency (see e.g., de Haan, 1999; Vitali et al., 2006; Björnham et al., 2015; Sole-Mari et al., 2019; Egelrud, 2021; Barbero et al., 2023; Yang et al., 2025).

Key challenges with KDEs is the adaptation of bandwidths and boundary control. Both are particularly challenging in coastal ocean regions such as Northwestern Norway, where currents are typically highly dynamic and boundaries complex with numerous islands and fjords (the latter is also typically not an issue in atmospheric applications, where most of the currently available research are conducted). To our knowledge, no existing, currently freely available density estimator simultaneously (i) adapts bandwidths locally to ensure proper smoothing and (ii) handles coastal boundaries appropriately for these types of applications. We therefore concluded that developing a suitable kernel density estimator was necessary to realistically model concentrations in our setting, and that this methodological contribution would be valuable to the scientific community.

We consider Section 2.3 important because:
i) it represents a methodological advancement for concentration estimates relying on LPDMs in the ocean;
ii) it highlights limitations of current practices and proposes a solution;
iii) it is crucial for producing realistic concentration estimates while maintaining reasonable computation times, especially for long-duration simulations or computationally constrained scenarios.

We have revised the text and added further references to clarify this rationale (see the tracked-changes manuscript).

Reviewer comment (Line 7):
In what sense was the modelling "successful"? Did you compare against measurements or other estimate, or do you just mean that the model(s) ran successfully and produced reasonable output?

Response:
We removed the word “successful.”

Reviewer comment (Line 22):
"Atmospheric measurements are currently the only approach…" Surely the current study is based on the assumption that also modelling is a possible approach to estimating atmospheric emissions from seep areas?

Response:
We revised the text here and it now reads:

“Estimation of total atmospheric gas emissions from seep areas \citep[e.g.][]{Myhre2016} rely largely on either ship measurements or large-scale atmospheric inversion models. The former of these approaches only give information on the local flux and require some sort of up-scaling, while the latter is unable to estimate dispersed sources and/or weaker point sources precisely due to its rough scale and inability to completely decouple atmospheric sources from sinks \citep{Thompson2014}.”

We also added references relating to these claims further into the introduction, see reply to reviewer 3 or revised manuscript.

Reviewer comment (Line 33):
Alien gases?

Response:
The text is now revised to:
“Gas content in bubbles are constantly changing due to dissolution (gases in the bubble dissolve into the liquid) and exsolution (gases already dissolved in the liquid enter the bubble) driven by partial pressure gradients across the bubble rim.”

Reviewer comment (Line 41):
What is "in situ data"?

Response:
We revised the first two sentences of the paragraph to:
“Our approach integrates a gas phase model with a hydrodynamic model using particle dispersion modelling to enable estimation of the three-dimensional (3D) distribution of gas in the water column and the total (free and diffusive) atmospheric gas release resulting from observed seabed seepage.”

Reviewer comment (Lines 90 and onwards):
Personally, I find the notation with the square brackets a bit odd, though I suppose it is a matter of taste. And why use subscripts for particle number and square brackets for time? How about subscripts for particle and superscript for time? Or two subscripts? (There's lots of nice inspiration to be had from the world of general relativity: https://en.wikipedia.org/wiki/Christoffel_symbols#Definition_in_Euclidean_space)

Response:
We considered several notational conventions. The use of square versus round brackets to distinguish between discrete and continuous arguments follows standard

conventions in digital signal processing (e.g., Haykin & Van Veen, 1999). This approach avoids a proliferation of sub- and superscripts and helps readers distinguish between quantities defined in the discrete (gridded) domain denoted by square brackets, versus continuous (real-world, non-observable) domains denoted by round brackets. Subscripts are used for physical variables (e.g., particle indices, velocities), while brackets indicate position or distance. This distinction was also implemented to contribute to readability. A minor challenge arises in eqs. (11) – (15) though, where we have both a distance and positions, and in eq. (26) we perform a summation over both subscripts and brackets. However, we don't regard these issues as detrimental to the readability, as these are standard notation in signal processing and applied physics.

The suggested use of combined sub- and superscripts could possibly work in our case, but it would become cumbersome when combined with powers of variables (e.g., Eq. (19)). We therefore chose to maintain our present notation.

Reviewer comment (Lines 95–100):
Strictly speaking, this is not a correct description of the equation of motion for particles in OpenDrift. It solves an SDE, not an ODE, and there is no such thing as the diffusive velocity vector in the scheme used in OpenDrift. (If you try to calculate the diffusive velocity, you will find that it goes to infinity as dt ->0). The correct equation can be found in numerous papers, see for example Eq. (2) in Spivakovskaya et al. (2007): https://link.springer.com/article/10.1007/s10236-007-0102-9

Response:
We modified the last sentence before the equation to:
"OpenDrift calculates the trajectory of each particle individually by numerically solving (using a set of stochastic differential equations, see e.g. \cite{Spivakovskaya2007}), the Lagrangian form of the advection–diffusion equation."

We chose to retain the advection–diffusion equation in the manuscript because it is widely recognized and provides an intuitive illustration of what the LPDM does in principle. This equation is also used in the OpenDrift documentation to describe what OpenDrift does.

Reviewer comment (Lines 107–115):
I think these expressions are not quite consistent. On line 107 you say that the mass of particle \zeta, at time n, \Gamma_\zeta[n], is given by the previous mass and some functions. In Eq. (3), you say that \Gamma_\zeta[n] is defined by the release. At this stage, I am also confused about how you represent different release rates for different sites, and how you deal with the vertical variation in dissolution from the bubbles, if all

particles are seeded with the same amount of mass, but presumably that will be described later?

Response:
We agree that this was a bit unclear, and we have now restructured the relevant paragraphs for clarity. The text now reads:
"The initial mass, i.e,. mass at release, of an arbitrary particle ζ is scaled such that the total released particle mass approximates the total number of moles of gas dissolved in the water column (from all modelled seeps combined) during a time interval Δt centred on t_n. In practice, we distribute the integrated sum of modeled (using the gas phase model) injected gas molecules from $t_n-\Delta t/2$ to $t_n+\Delta t/2$ evenly over the seeded particles. Assuming that the seabed flux is stationary within the time interval $t_n\pm\Delta t/2$, the mass of a particle Γ_ζ seeded at time-step n can be obtained by

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\begin{equation}\label{eq:initial_mass}

\Gamma_\zeta[n] = \frac{\Delta t\sum_{p=0}^{P}\Upsilon_p[n]}{S[n]}

\end{equation}

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where $\Upsilon_1[n], \Upsilon_2[n], \ldots, \Upsilon_{P}[n]$ [mol s^{-1}] are total injected dissolved gas from all P modeled seeps. Approximation to the modelled dissolved gas release profiles at each modelled seep is achieved by seeding a different amount of particles at different depths."

Reviewer comment (Line 122):
Who refers to this as "particle death"? Very dramatic term, what's wrong with "particle removal"?

Response:
We agree, and we have replaced "death" with "removal."

Reviewer comment (Line 130):
Isn't there something wrong in Eq. (5)? Surely if \gamma_s is supposed to be based on the distance between particle s and particle \theta, then the position of particle s would be expected to appear on the right-hand side of the equation?

Response:
Correct. The subscript *s* was a remnant from a previous version. It has been corrected to \tau on the left-hand side.

Reviewer comment (Line 148):
If I understand correctly, you said that you found histogram unsuitable, but you are essentially using a histogram in the vertical direction. Why not use 3D KDE?

Response:
A full 3D KDE would indeed be desirable, but implementing a kernel estimator with adaptive bandwidth in 3D is considerably more complex and computationally demanding. For instance:

- we assumed isotropic kernels to simplify implementation and bandwidth estimation. In 3D, kernels would need to be anisotropic due to the very different scales in vertical vs horizontal dispersion. This would also reduce the robustness of the kernel bandwidth estimation, since we would be prohibited from averaging statistical properties (e.g., integral length scales) in all directions.
- boundary handling becomes more complex in 3D (top and bottom of water column in addition to lateral boundaries), increasing computational costs considerably if we keep using the kernel-specific boundary control algorithm presented in our paper.

Given these challenges, we considered our 2D layered approach sufficient for the present application. Moreover, horizontal dispersion completely dominates vertical dispersion, which reduces the noise introduced by using only a horizontal KDE. We acknowledge, however, that a 3D KDE would be a useful future development.

Reviewer comment (Line 150):
Just a comment, but I think KDEpy is pretty efficient. Might be easier (and maybe faster?) than making a new implementation.

Response:
We would like to refer also to our reply to General Comment 2 and the references cited therein.

In fact, we initially used KDEpy during the early stages of the project. While efficient and user-friendly (KDEfft in particular is very fast), KDEpy lacks several key features required for concentration estimates in coastal dispersion modelling:

1. **No local adaptation of kernel bandwidths.**
   Local bandwidth adaptation is crucial; without it, high-gradient regions become

oversmoothed, while low-density regions become noisy. This issue is analogous to using fixed bin sizes in histograms. Adaptive bandwidths solve this problem by adjusting locally, whereas KDEpy does not.

2. **Insufficient boundary control.**
   In KDEpy, boundary correction is typically applied after the density estimate, e.g. by reflection. While acceptable in simple or infinite boundary problems, this fails in realistic coastal domains with islands, inlets, and fjords. Density can incorrectly "leak" over land masses into ocean areas on the other side of the landmass. Our method explicitly avoids this by enforcing boundary conditions at the kernel level, modifying each kernel shape according to the local geometry (Section 2.3.3).

3. **Inefficient variable bandwidth implementations.**
   KDEpy offers TreeKDE and NaiveKDE for varying bandwidths, however, varying bandwidth is not the same as adaptive variable bandwidth. Furthermore, these algorithms are significantly slower than our adaptive KDE implementation due to the grid projection. A simple performance test is available in our public repository: https://github.com/KnutOlaD/akd_estimator and a plot is provided further down in this report.

Reviewer comment (Line 153):
Whether the density estimate is differentiable or not depends on the choice of kernel.

Response:
We agree. The text has been revised to clarify this point.

Reviewer comment (Line 157):
I don't think the variable V is defined.

Response:
We thank the reviewer for noticing this. The variable V has now been defined in the manuscript.

Reviewer comment (Line 162):
I wouldn't worry about the kernel being consistent with diffusive transport. And in any case, if you wanted the kernel to be consistent with diffusion, wouldn't you have to let the bandwidth grow based on the diffusivity? And you also later truncate the kernel.

Response:
We agree, and we have removed the sentence in question to avoid confusion.

Reviewer comment (Lines 199, 202, and elsewhere):
Two different notations: N_{eff} and N_\mathrm{eff}.

Response:
This inconsistency has been corrected. We now consistently use *N*_{eff}.

Reviewer comment (Line 260):
It's probably not important in the grand scheme of things, but redistributing the mass instead of mirroring fail in some simple test-cases. For example for uniform distribution on a bounded 1D domain, it will fail to reproduce a uniform distribution, but rather giving too low density near the boundaries.

Response:
This is correct, and the kernel centre of mass will also be displaced more than ideal. However, because this redistribution is applied individually to every single kernel (approx. 300,000 times per time step in our test case) before summation - not just to the final (full) density estimate - the deviations become negligible in practice. See section 2.3.3.

Reviewer comment (Line 276):
Wouldn't U_a more commonly be the wind at 10 m height?

Response:
Yes. Both the equation and the ERA-Interim wind data correspond to 10 m above sea level. We have clarified this in the manuscript.

Reviewer comment (Lines 292–296):
Do I understand correctly that any particle loses mass based on the sum of the flux \beta over the entire horizontal grid? So even a particle in an area with no wind will lose mass based on the average loss?

Response:
We highly appreciate this observation, as it revealed an error in the text and the equation was also incorrect(!) In the model, particle weights are adjusted according to the flux from the local grid cell where the particle resides (local release = local loss). The equation and text have been corrected accordingly.

Reviewer comment (Line 318):
Polynomial fit to visual observations of what?

Response:
This refers to bubble size distributions. The manuscript has been revised here to clarify.

Reviewer comment (Line 333 and Figure 6):
What type of average was used?

Response:
A simple arithmetic mean of the tabulated values was used. This is now clarified in the text.

Reviewer comment (Line 336):
Just out of curiosity: Does the deposited concentration actually decrease exponentially, or does it just look approximately exponential? Obviously it cannot be a _true_ exponential if it depends on environmental variables like temperature, but even for a theoretical case of a perfectly homogeneous water column, is it actually exponential?

Response:
The solution to the transfer equation (Eq. (7) in Jansson et al., 2015), under the assumption of a single gas species and an otherwise stationary/constant environment would yield an exponential profile. However, when multiple gases, bubble rise velocity distributions, or variable environmental conditions are included, the result deviates from a strict exponential. In practice, an ambient undersaturated water column typically produces a dissolved profile that only exhibits exponential *appearance* from a simple visual inspection. We have revised the text to say "appears exponential" to reflect this more accurately.

Reviewer comment (Line 343):
What are the units of the atmospheric fluxes?

Response:
The units have been added in the manuscript.

Reviewer comment (Line 348):
1,2,3,N, ? Missing some dots? But also, no need to repeat the concept of the indexing, but rather mention how many particles were used.

Response:
We agree. The sequence has been shortened, and the redundant indexing explanation was removed.

Reviewer comment (Lines 352–353):
No need to repeat terrain-following.

Response:
The repetition has been removed.

Reviewer comment (Line 357):
"therefore" … strictly speaking it does not follow logically from the fact that the model is used by the authorities for acute happenings, that it is also the best model when running a modelling study several years later. (Note: I'm not saying that NorKyst isn't the best model, only that it doesn't follow logically from the statement)

Response:
We agree. The sentence has been removed.

Reviewer comment (Line 392):
Missing units on the rate coefficient.

Response:
Units have been added in the revised manuscript

Reviewer comment (Line 393):
How is the "mass modification term" used? And shouldn't it be negative?

Response:
We revised and expanded this paragraph to better explain the implementation in the revised manuscript. The clarification should also now make it clear that the term is negative.

Reviewer comment (Line 405):
Missing closing bracket. Also, I believe mol/L (molar) is a more common unit than mol/m3.

Response:
We acknowledge that mol/L is common, but for consistency we chose to adhere strictly

to SI units, expressed with powers (mol m^{-3}). This decision was motivated by the wide variety of unit conventions across the literature (e.g., seabed fluxes in ml/min, and diffusive fluxes with non-standard units as in Wanninkhof (2014) etc.)

Reviewer comment (Lines 415–427):
I'm curious about the thickness of the vertical layers, and particularly the top layer, in the model used to calculate the flux from dissolved to the atmosphere. If this layer is to thin, the layer might be depleted on a faster timescale than mixing from the lower layers, since that mixing is modelled by particles that live in a different world, with a different timestep. On the other hand, if the layer is too thick, it will allow the escape of methane from too deep in the water column. In a hybdrid model like this, where the escape to the atmosphere and the transport of the particles are modelled by different approaches, this seems to me to be a point worth investigating and discussing.

Response:
We agree that it is appropriate to highlight this issue. The text has been expanded to also discuss the influence of vertical layer thickness. The revised passage now reads:

"Uncertainties in the eddy diffusivity, vertical transport and distribution are also expected to be large. The somewhat arbitrary choice of grid cell thickness can also modify the end result. If the grid cells are too thin, and the temporal resolution is too coarse, there is a risk of depletion of the surface layer between the model output time-steps. On the other hand, if the grid cells are too thick, one would incorporate CH$_4$ from depths where exchange with the atmosphere is unrealistic, thereby violating the assumptions of the atmospheric exchange bulk model. One can evaluate whether the surface thickness is sufficiently thick by comparing typical values for Eq. \ref{eq:atmospheric_loss} with the typical mass of surface layer particles and ensure that $\gamma_\alpha[n]<<\Gamma_\tau[n]$. "

Reviewer comment (Line 423):
Reads like the microbial flux is driven by wind speed.

Response:
We agree that part of the sentence should not be there and has been removed

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Reviewer comment (Lines 424–425):
Do I read correctly that the loss due to particles leaving the domain is of the same order of magnitude as the loss to microbial oxidation? You have used a fairly high biodegradation rate, which is perfectly fair I think, but some studies claim to have found much slower oxidation rates (see for ekample

https://pubs.acs.org/doi/full/10.1021/acs.est.7b02732). How would you use your model to study the case of slower biodegradation, without the loss due to particles leaving the domain being completely dominant?

Response:
Yes, your interpretation is correct. This limitation arises because the model is constrained in both time and space by computational resources and the hydrodynamic domain boundaries. One option is to extrapolate by assuming that all methane molecules will eventually either reach the atmosphere or be consumed microbially, and that the relative partitioning observed within the model domain is representative of the long-term outcome. This assumption required for this approach means estimates will be increasingly less accurate for lower oxidation rates, since in those cases most methane leaves the domain unconsumed.

For exploring such scenarios, a 1D approach might provide a more robust framework for estimating the ultimate fate of methane. We have added a sentence to the conclusion to reflect this point and a reference to relevant work on this aspect (Nordam et al., 2015)

Reviewer comment (Lines 456–457):
I would have thought that also the vertical eddy diffusivity used in the transport model is quite important. You say that the mass transfer coefficient is stated to have an uncertainty of 20%, my guess would be that the vertical eddy diffusivity from the ocean model, and the effect of that on the transport of methane towards the surface, has a (much) larger uncertainty than 20%. Any comments?

Response:
We agree. Quantifying this uncertainty is not straightforward, as it depends on details of the hydrodynamic model and its coupling to the LPDM. Nevertheless, we have highlighted this issue in the discussion part with following sentence:

*"Uncertainties in the vertical eddy diffusivity and hence vertical water column transport are also expected to be large and are amplified by the somewhat arbitrary choice of thickness of the grid cells, which also impacts the concentration in the surface grid cells.***"**

Reviewer comment (Lines 490–502):
I'm not sure I understand how the M2PG1 model works originally, or the implications of choosing a horizontal cell size. How can the original model take ambient concentrations into account for dissolution of methane from the bubbles, and for mass transfer of dissolved methane to the atmosphere, without calculating a concentration? And it also seems to me that the dissolution mostly happens near the sea floor, where the plume is

narrow, while the mass transfer to the atmosphere only happens at the surface, where the plume is wide, so maybe the cell size should vary with depth? Finally, I wonder how sensitive the results are to this choice. Does much of the mass-transfer from the atmosphere happen in the M2PI1 model, or is that only calculated based on the concentration fields from the particles? And to what degree does the ambient concentration in the water column hinder the dissolution of methane from the bubbles?

Response:
Yes, ideally the cell size should vary with depth (which we have expressed in the appendix), but we use the estimated cell size at the mid-point of the water column, at 100 m depth. Furthermore, this is how M2PG1 works in combination with the concentration model:

1. M2PG1 calculates concentration and uses the background concentration as its initial condition. the concentration within the model domain is then modified iteratively by the dissolution processes. It is possible in M2PG1 to have dynamic background/boundary conditions where this can be modelled/measured, however, in the application/test presented in the manuscript, the boundary conditions are kept constant at the initial condition. An on-line coupling between the concentration/LPDM-based model and M2PG1 is desirable in future developments/applications.
2. The choice of model domain size becomes increasingly important when the concentrations are large, i.e., for more intense seeps than what we modelled here. The dissolution rates depend directly on the dissolved concentration in the water. The dissolved concentration depends on (among other things) the chosen domain size following Eq. (7) in Jansson et al., (2019) which motivated the addition of a grid cell size estimator.
3. The mass-transfer from the atmosphere happening in the M2PG1 model is not included since this is fully handled by the flux from the surface layer in the concentration model (the \beta[i,j,n] field).

We refer to Jansson et al., (2019) for further details.

Reviewer comment (Line 533):
Should be "piece-wise constant function".

Response:
We agree, this is corrected in the revised manuscript.

Reviewer comment (Line 536):
I don't understand why the histogram estimator is "highly sensitive" to the position of the origin. I get that the results can look different if you shift the origin, but "highly sensitive"?

Response:
The text has been revised to: *"can be sensitive."*

Reviewer comment (Lines 550 and 561):
What do the different numbers of particles (1900000 and 10^6) refer to?

Response:
These numbers referred to the same case, and this was inconsistent in the submitted manuscript. We have corrected the manuscript and synthetic test case to consistently use and refer to 2000000 particles, which is both accurate and sounds less arbitrary.

Reviewer comment (Line 551):
What does \mathcal{Z}^{100 \times 100} mean? To me it suggests some esotheric 10000 dimensional discrete space. Perhaps you mean i,j \in [1, 2, ... 100]?

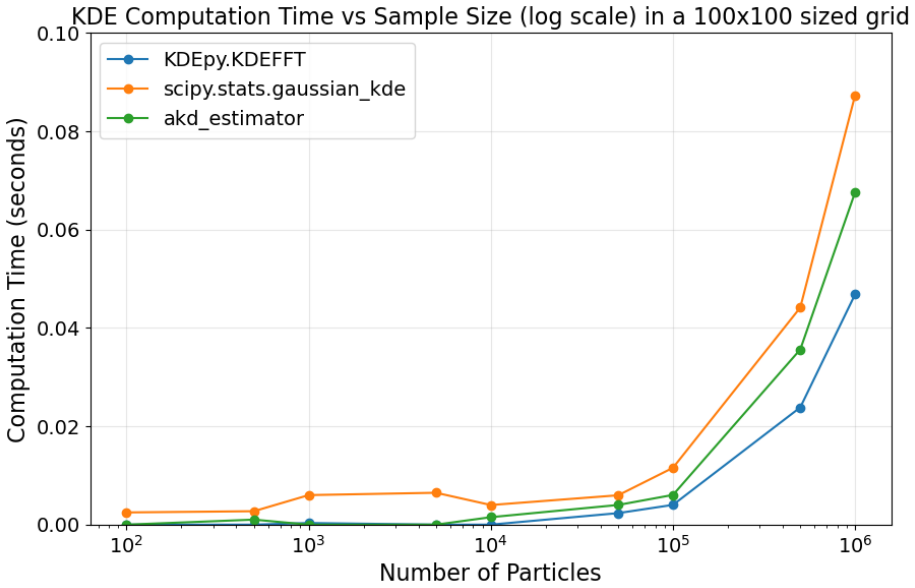
Response:
Yes, that was the intended meaning. The notation has been revised accordingly.

Reviewer comment (Line 553):
Isn't there something odd in Eq. (C1)? The sum is over t, but there is no t in the expression. Also, the units do not match. You mention a timestep later, but it should be included here to obtain displacement from velocity, and the random vector should be scaled by sqrt(dt) to match the units of sqrt(D).

Response:
We agree. The equation has been corrected and clarified. The omission of time and normalization with $\sqrt{\Delta t}$ was an oversight caused by the unity timestep used in testing. The revised version should now be consistent and dimensionally correct.

Reviewer comment (Lines 565–567):
Again, I would suggest including KDEpy (https://kdepy.readthedocs.io/en/latest/) in the comparison. I'm not sure how it will compare, but in my limited experience I've found it quite fast. Also, I'm not sure if Silverman's rule is a very relevant option, I believe it is well known to be less than optimal for multi-modal distributions.

Response:
We acknowledge this suggestion. As noted earlier, we consider that KDEpy does not provide the capabilities (adaptive bandwidth estimation and boundary control) needed for our application. When it comes to performance, we have included simple performance testing in the github repository where it is possible to compare with both the KDEs included in Scipy as well as KDEpy. We now refer to this in the manuscript. Performance-wise the grid projected akd presented in our manuscript is slightly slower than the FFT implementation in KDEpy, which omits bandwidth adaptation and does not allow variable kernel bandwidth (see also figure below for computation time of densities from a 2d gaussian distributed particle cloud).



When it comes to the application of Silverman's rule in our estimator: It is true that Silverman's rule is less than optimal for multi-modal distributions. However, we use Silverman's rule only locally within each adaptation window, for each grid cell centre wherein the assumption of a unimodal distribution is approximately valid (in essence we use Silverman's rule once for each particle containing grid cell to estimate the bandwidths from which we construct the concentration field – which can indeed be multi-modal!).

Reviewer comment (Line 573):
"theoretically ideal". Only a minor detail, but I'm not sure if this would be theoretically ideal (depends on the theory, I guess). In a particle model, where the particles are transported by the diffusivity, this increases the variance of the overall distribution. But the kernel bandwidth also increases the variance of the overall distribution. I seem to rememeber that it is easy to show (at least of all particles have the same kernel and bandwidth) that the variance of the distribution obtain by KDE is the sum of the variance

of the particle positions, and the variance of the kernels. So I wonder if this "theoretically ideal" bandwidth wouldn't in fact double-count the diffusion? You could test it against an analytical solution of the diffusion equation in 1D.

Response:
We removed “theoretically ideal”, however, we are not sure we quite follow the argument about double counting and cannot find any published proof pointing in this direction. Nonetheless, we acknowledge that this is not the right place for delving into proofs of what’s theoretically ideal or not in selecting the kernel bandwidths and have removed “theoretically ideal” from the manuscript.

We also refer to the discussions presented in Björnham, et al., (2015) who allows the bandwidth to grow with the diffusivity in their applied atmospheric model.

Reviewer comment (Line 590):
Some words missing at the end here?

Response:
Correct. The sentence has been corrected.

Reviewer comment (Figure C2):
The histogram example uses very small cells (10000 cells and only 1000 particles), it would probably be closer to the "ground truth" with larger cells.

Response:
Thank you for pointing this out. The caption has been corrected to clarify that the left-hand panel shows the histogram estimate of the test dataset. The “ground truth” was generated using 2,000,000 particles, which should yield a quite smooth distribution for 10000 cells.

Reviewer comment (Line 634):
I suggest a manual proofread as well, there are still a few typos here and there (including on this line).

Response:
A thorough manual proofread has been conducted, and typographical errors have been corrected throughout.

Reviewer comment regarding the advantages of a 3D-model

Just one thing I forgot to mention in the review comments, that you could perhaps also discuss: What are the advantages of 3D modelling compared to 1D modelling? You mention some of the drawbacks (considerable computational effort, loss of mass through particles exiting the domain), so it would be interesting to discuss if it is worth the effort.

Response:

The main advantages of the 3D modelling is now addressed in the conclusion, being i) the ability to incorporate more advanced hydrodynamic processes via established 3d hydrodynamic models ii) the 3D concentration field is necessary in a wide range of other applications/studies of particular processes.

Reviewer comment (Figure 9):
Oh, and one more small point: I think the units on the colorbar in Fig. 9 are wrong, the numbers seem to be in mol/L not mol/m3?

Response:
Regarding the units in Figure 9 we believe that those are correct. We changed the figure caption to hopefully better explain the contents of the figure. We aim to display the anomaly from the background concentrations. The background concentration is $3 \cdot 10^{-6}$ moles/m^{-3}, i.e. 3 nmol/L.

References:

Barbero, D., Ribstein, B., Nibart, M., Carissimo, B., & Tarniewicz, J. (2024). Reduction of simulation times by application of a kernel method in a high-resolution Lagrangian particle dispersion model. Air Quality, Atmosphere & Health, 17, 2105-2117.

Björnham, O., Brännström, N., Grahn, H., Lindgren, P., & Von Schoenberg, P. (2015). Post-processing of results from a particle dispersion model by employing kernel density estimation.

De Haan, P. (1999). On the use of density kernels for concentration estimations within particle and puff dispersion models. Atmospheric Environment, 33(13), 2007-2021.

Egelrud, D. (2021). Kernel density estimators as a tool for atmospheric dispersion models (Publication No. 1592045) [Master dissertation, Umeå University]. Digitala Vetenskapliga Arkivet.

Haykin, S., and Van Veen, B. (1999). Signals and Systems (1st ed.), Wiley.

Jansson, P., Ferré, B., Silyakova, A., Dølven, K., & Omstedt, A. (2019). A new numerical model for understanding free and dissolved gas progression toward the atmosphere in aquatic methane seepage systems. Limnology and Oceanography: Methods, 17 (3).

Sole-Mari, G., Bolster, D., Fernández-Garcia, D., & Sanchez-Vila, X. (2019). Particle density estimation with grid-projected and boundary-corrected adaptive kernels. Advances in Water Resources, 131, 103382.

Vitali, L., Monforti, F., Bellasio, R., Bianconi, R., Sachero, V., Mosca, S., & Zanini, G. (2006). Validation of a Lagrangian dispersion model implementing different kernel methods for density reconstruction. Atmospheric Environment, 40(40), 8020-8033.

Yang, L., Fang, S., Wang, Z., Song, J., Li, X., & Chen, Y. (2025). Optimizing and evaluating multiple kernel density estimators for local-scale atmospheric dispersion modeling at a representative AP1000 nuclear power plant site in China. Nuclear Engineering and Technology, 103880.