Response to Reviews for the Manuscript "The Boundary Layer Dispersion and Footprint Model: A fast numerical solver of the Eulerian steady-state advection-diffusion equation"

Response to Reviewer #2

We sincerely appreciate the referee's thorough review of our manuscript and the valuable comments and suggestions provided. The feedback has been instrumental in enhancing the quality of our research. We have carefully considered each of the remarks and will make comprehensive revisions to the manuscript based on the content of the study. Next, we will provide a detailed point-by-point response to all comments, citing the reviewer statements in black font, while our answers are given in blue font.

Major Comments

The manuscript explains the underlying differential equation and the simplifying assumptions. A more precise and detailed description of the numerical method and computational results would greatly benefit the manuscript:

1. Line 148: The manuscript mentions the linear shooting method to solve the boundary value problems. The authors should explain the method and justify its use in this context.

   We thank the referee for this comment. We will add a paragraph addressing the explanation and justification of the shooting method: "The main idea of the method is to reduce the solution of the BVP to solving two IVPs with arbitrary but linearly independent initial values and reconstruct the BVP solution by a linear combination of the two IVP solutions, allowing for deployment of standard numerical IVP solvers."

2. Lines 157–162, Appendix A: The presentation of the numerical method is currently too brief. The manuscript provides limited context as to why this method was

chosen and what advantages it offers over alternative numerical approaches. In addition, the authors claim in the main text that the method is consistent, stable, and robust; is there evidence supporting this claim? In the Appendix, is the scheme (A1)–(A4) taken from Hochbruck and Ostermann (2010), and have the authors modified it using the approximations (A5)–(A6)? If so, could they provide readers with a rough estimate of the computational time saved by not evaluating the sine and cosine terms?

We appreciate the reviewer's comment. The advantage of the exponential integrator method in comparison to other numerical methods is that it gives exact solutions to linear ODEs with constant coefficients. We will emphasize this fact in a revised version of the manuscript. To provide a more sound investigation of the numerical scheme, we will perform numerical convergence tests and prove exponential error decay, supporting our initial claim of consistency, stability, and robustness. Furthermore, we will improve BLDFM by a more precise treatment of the vertical boundary condition and introducing stretched vertical coordinates to further speed up the algorithm. To evaluate the impact of approximating the sine and cosine terms emerging in the Exponential Integrator Method, we run the same experiment as described in Section 5 but without the Taylor approximation of the sine and cosine terms. Instead of 9 sec, the solver now needed 35 sec. The time difference is substantial.

3. Section 3: Do the authors implement the Dirac delta distribution mentioned in section 3 in their numerical solver? If so, how is this achieved in practice?

   We thank the referee for the insightful question. In fact, the Dirac delta function has a simple representation in Fourier space: it is the constant one. This property is used and implemented in BLDFM. It offers the additional advantage that the integral is also precisely one, which is important for mass conservation.

4. Do the authors evaluate the convolutions in Eqs. (26) and (27) in their numerical implementation? If so, how is this done in practice? They might also consider including a short remark about potential parallelization.

   We appreciate this question. In the numerical implementation, the Green's function is shifted in Fourier space to the tower location, which amounts to a simple multiplication by a phase. After applying the inverse Fourier transform, the convolution simplifies numerically to a sum over all spatial indices in real space, which is mentioned in the manuscript. BLDFM is indeed parallelized. Please refer to our response to point 6.

5. Section 5: The authors write: "In order to corroborate convergence, other resolutions and different parameter settings were tested as well. The relative error decreases with higher resolution (not shown here)." However, these results should be presented–e.g., in a table or a figure–to allow the reader to assess the convergence behavior quantitatively. Additionally, the BLDFM solver consists of several

components, including a Fourier transform, a linear shooting method, 1 and an exponential integrator. The statement that ”the relative error decreases with higher resolution” is too general. The authors should discuss how each component contributes to the overall numerical error.

We are thankful for this comment. In a revised version of the manuscript, we will present additional plots that will show the error convergence for different resolutions. Since BLDFM consists of several numerical methods, mainly the Fourier Method for the horizontal integration and the Exponential Integrator Method for the vertical integration, different test cases will be designed to challenge each component individually. The Fourier method has, theoretically, an exponential error decay; the Taylor approximated exponential integrator should be polynomial of order three. Using the analytical solution as a test case should mostly challenge the Fourier method. Since the vertical profiles are constant, the (not approximated) exponential integrator should be exact. A test case specifically challenging the exponential integrator can be constructed with variable vertical profiles when using a high-resolution simulation as reference. The decay rates will also be measured and reported.

6. Section 5: The authors should also discuss which parts of the code are amenable to parallelization in order to achieve faster solutions, as this is an important aspect of performance for practical applications.

   We are grateful for this remark. BLDFM is indeed parallelized. In fact, the vertical integration by the exponential integrator method can be executed independently for each wave number tuple, which makes parallelization straightforward. An explanatory sentence will be added to the manuscript.

7. Line 248: The authors state: “This difference may be explained by the distinct model choices.” It would be helpful to briefly discuss whether numerical errors in BLDFM could contribute to these differences. Ensuring that the observed discrepancies are indeed due to model assumptions rather than numerical artifacts would strengthen the interpretation of the results. The same consideration applies to the unstable case.

   We appreciate this comment. This section will be rewritten completely in order to make the differences between BLDFM and the Korman & Meixner model much more distinct. We plan to implement a modified version of BLDFM, which also obeys the slender plume assumption, to make the comparison to the FKM model more explicit and direct. To rule out any numerical artifacts, we also plan to perform numerical convergence analyses.

Minor Comments

1. The authors perform a detailed analytical study of the system. It would be helpful to briefly highlight this contribution in the abstract or introduction, as it provides valuable guidance for the numerical implementation.

We thank the referee for this comment. However, we do not agree with the reviewer: the analytical solution to the atmospheric transport equation is well known in the literature, which is also cited in the manuscript. Furthermore, the analytical study is mentioned in both the abstract and introduction and does not need further emphasis in our opinion.

2. Lines 43, 47: To give the reader a better sense of the scales involved, it would be helpful to provide typical ranges for the atmospheric microscale in the planetary boundary layer and for the mesoscale.

   We will reformulate the paragraph in question to make it more precise and give typical numbers for the atmospheric scales.

3. Lines 45-47: The authors state that advection predominantly occurs on the microscale, while the temporal evolution of wind patterns occurs on the mesoscale. Could the authors clarify whether they refer here specifically to eddy-scale fluctuations rather than mean-flow advection? This would help avoid potential confusion about the scales at which advection acts.

   Indeed, the term advection is misleading, as it divides into the mean flow and the turbulent component in the Reynolds average. To make the matter clearer, we will emphasize that we consider the Reynolds-averaged equations and add the term 'mean-flow advection' where necessary.

4. Line 66: Could the authors comment on whether steep gradients in the scalar field occur in their typical application scenarios, and if so, how the Fourier-based solver deals with them? Since spectral methods may exhibit oscillations near sharp features when resolution is limited, a brief discussion of this aspect would help readers better understand the robustness of the approach.

   We appreciate this observation. The Fourier method is indeed prone to artificial oscillations at sharp gradients. The extreme case of this Gibbs ringing is when we use the unit point source of infinitesimal diameter to define the footprints. However, in typical use cases, this phenomenon does not pose any issue because the turbulent mixing mathematically represented by the harmonic operator in the form of the Laplacian rapidly smooths out any small-scale oscillations as it is proportional to the wavenumber squared. The benefits of the Fourier method–very fast and conservative–easily outweigh this minor inconvenience.

5. Line 96: It would be helpful if the authors could briefly comment on how idealized the assumption of periodic (or vanishing) lateral boundary conditions is. Additionally, do the authors have any thoughts on how this approach could be extended to non-periodic boundary conditions? How would that change the efficiency of the computation of the numerical solution?

   We thank the reviewer for this observation. Since BLDFM uses the Fourier method, the boundaries are periodic by construction. In order to represent non-periodic domains, a halo of zero flux is used around the domain of interest, effectively increasing the computation domain. This halo must be sufficiently big such that tracer material that leaves the domain of interest at some edge must not enter at the opposing edge. This treatment of the boundaries makes the algorithm slightly computationally more expensive, but still provides very fast calculations due to the usage of the Fast Fourier Transform. We will add an explanatory paragraph to the manuscript.

6. Lines 114ff, Equations (9) - (12): For the unbounded domain $z \in [z_M, \infty)$, the authors discard the growing exponential term in the solution. This can be interpreted as a physically motivated choice to ensure that the solution remains bounded for large z. It might help to clarify this point and distinguish it from the classical maximum principle, which is formulated for bounded domains. Clarifying this point could help readers better understand the reasoning behind the boundary treatment. In addition, could the authors briefly comment on whether a nonzero coefficient B would be physically meaningful or whether it would necessarily lead to unbounded growth?

   We are grateful for bringing this issue to our attention. The formulation in the manuscript is somewhat imprecise. To be more thorough, actually the weak version of the maximum principle needs to be applied. This will be corrected in the manuscript.

7. Equation (22): The manuscript provides the formula for α without explanation. A brief note on how it was computed and how it follows from the linear combination of the two IVP solutions would improve clarity.

   We appreciate the comment. We will add an explanatory sentence: "Notice that the initial values were chosen–without loss of generality–to yield compact expressions for the coefficients of the linear combination, which are computed by accounting for the boundary values at z_T."

8. Section 3: It might help the reader if the authors explicitly stated that the Green's function depends on the particular problem.

   We agree with the referee and will improve the manuscript accordingly by calling it the Green's function of atmospheric dispersion.

9. Equations (26), (27): The authors might remind the reader that Q_0 is related to the boundary condition or provide a reference to the corresponding equation.

   The reference to equation (2) will be added to the manuscript together with an explicit mention of the variable Q_0.

10. Section 6: The authors mention that FKM uses simplified assumptions, but it is not clear to the reader which specific equation BLDFM is being compared to. The manuscript would benefit from explicitly stating the governing equations and assumptions of the FKM model to clarify the basis of the comparison.

We thank the reviewer for bringing this lack of explanation to our attention. This paragraph in question will be rewritten substantially. As mentioned earlier, we plan to implement a modified version of BLDFM that also obeys the slender plume assumption to make the comparison to the FKM model more explicit and direct.

11. Line 270: "BLDFM's performance has been tested against a special analytical solution." Please clarify that this assessment refers to numerical accuracy and not computational runtime or efficiency.

    We will rephrase this sentence, making the results of the assessment more clear.