Reply to the comments of Dr. Simon Unterstrasser on article gmd-2023-26

Toshiki Matsushima, Seiya Nishizawa, Shin-ichiro Shima

Thank you for taking the time to read through our manuscript and provide us with positive and helpful comments. Below are our point-by-point responses to your comments.

1.) From Fig. 6, I understand, that the SD spatial distribution is affected by the interpolation scheme, but what is the effect of it on the cloud as a whole. You could, e.g., add a panel to Fig. 7 showing the differences between CVI-1 and CVI-2. Other model adaptations should be described similarly to better understand the physical implications of your improvements.

You may even add an additional figure with time series of selected total cloud properties to make the comparison between the different model version more quantitative.

Response:

Thank you for your important question. During our research, we attempted to find how much the numerical accuracy of the CVI scheme affects the whole cloud system. In the experiments described in the manuscript, we could not find a clear difference in terms of LWC and the origins of the initial positions of droplets before the submission. To address your question, we investigated how the numerical accuracy of the CVI affects the time evolution of the tracer fields and how it might affect the clouds. In this letter, we would like to share the results with you.

We performed additional experiments to investigate the impact of the numerical accuracy of the CVI scheme on the time evolution of the tracer fields. These were modifications of the warm bubble experiments described in our manuscript. The domain size for these experiments is $300\,\mathrm{m} \times 8{,}000\,\mathrm{m} \times 5{,}000\,\mathrm{m}$ for x, y, and z directions. The spatial resolution is $100\,\mathrm{m} \times 500\,\mathrm{m} \times 500\,\mathrm{m}$. We introduced a prescribed two-dimensional Benard-convection-like flow in which the cell positions oscillate periodically. The density and the mass stream function are represented as follows:

$$\rho_0 = 1\,[\mathrm{kg \cdot m^{-3}}], \tag{1}$$

$$\psi(y,z,t) = \frac{50{,}000}{\pi} \sin\left(\frac{\pi z}{5{,}000\,\mathrm{m}}\right) \left[\sin\left(\frac{2\pi y}{8{,}000\,\mathrm{m}}\right) + \epsilon \cos\left(\frac{2\pi y}{8{,}000\,\mathrm{m}}\right) \cos\left(\frac{2\pi t}{1{,}800\,\mathrm{s}}\right)\right] [\mathrm{kg \cdot m^{-1} s^{-1}}], \tag{2}$$

$$\rho_0 v(y,z,t) = -\frac{\partial \psi}{\partial z}\,[\mathrm{m \cdot s^{-1}}], \tag{3}$$

$$\rho_0 w(y,z,t) = \frac{\partial \psi}{\partial y}\,[\mathrm{m \cdot s^{-1}}]. \tag{4}$$

Here, $\epsilon = 0.5$. Even for such a simple 2D flow, the time evolution of particles can be chaotic because the flow is unsteady (Malhotra et al. 1998). The momentum fields and the mass stream function at the initial time ($t = 0\,\mathrm{min}$) are shown in Fig. 1. The vorticity of the flow is given by

$$\zeta = -\left[\left(\frac{\pi}{5{,}000\,\mathrm{m}}\right)^2 + \left(\frac{2\pi}{8{,}000\,\mathrm{m}}\right)^2\right] \psi(y,z,t). \tag{5}$$

As described in our manuscript, the CVI-1 cannot incorporate the effect of shear and vortical flow within a cell to the SD movement, but CVI-2 can. Thus, the prescribed flow serves as a case in which the effects of the numerical accuracy in the CVI are likely to be verified.

First, we investigate the time evolutions of the particle distributions. An average of 3,200 particles per cell (128 for $100\,\mathrm{m}^3$ volume) was initially distributed in 3D space quasi-uniformly (Sobol sequences). The time integrations of particle positions using the CVI-1, CVI-2, and analytical expression of velocities were performed for 21,600 s by $\Delta t = 1.0\,\mathrm{s}$. The time evolutions of particle distributions are shown in Fig. 2. When the CVI-1 is used, a staircase-like pattern appears, and the particles mix

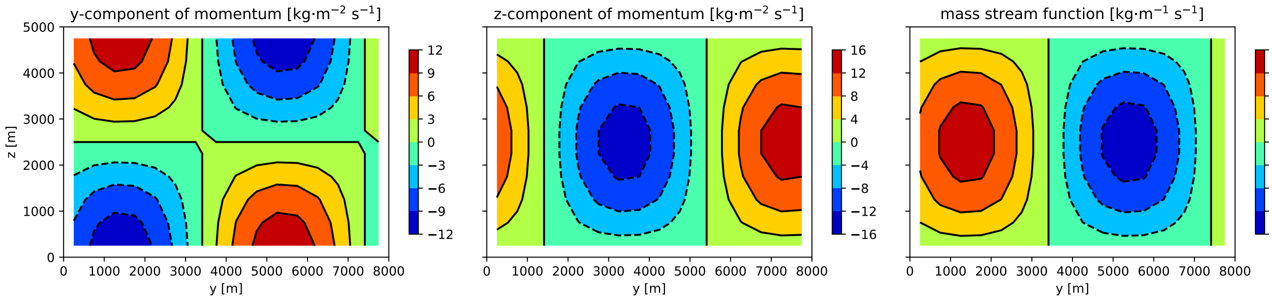

Figure 1. The momentum fields and the mass stream function at the initial time.

well, especially at the central positions of the vorticities centered around $y = 1{,}500\,\mathrm{m}$ and $y = 5{,}500\,\mathrm{m}$. In contrast, such patterns are not present in CVI-2 and ANL; Instead, small and thin filaments are depicted in CVI-2 and ANL. In our original manuscript, we could not compare the particle distributions obtained by CVI-1 and CVI-2 to the reference solution. However, our latest results confirm that switching from CVI-1 to CVI-2 improves particle distributions, aligning them more closely with the reference solution.

Now, we address how the numerical accuracy of particle distributions affects that of the tracer distributions (i.e., the statistics over the grid fields). In our calculations, we can track each particle's ID (or initial position of particles), enabling us to monitor the time evolutions of tracer fields for arbitrary initial tracer fields without the need to recalculate the time evolutions of the particle distributions. The initial conditions of the tracer field ϕ are defined as follows.

$$\phi(y,z,t=0) = \sin\left(\frac{\pi k z}{5{,}000\,\mathrm{m}}\right)\left[\sin\left(\frac{2\pi l y}{8{,}000\,\mathrm{m}}\right) + \epsilon\cos\left(\frac{2\pi l y}{8{,}000\,\mathrm{m}}\right)\right] + \sqrt{1+\epsilon^2} \tag{6}$$

We construct the initial tracer fields by scaling and shifting the stream function described in Eq. (2) to ensure $\phi \geq 0$. Additionally, we introduce wavenumber parameters (k,l) to control the spatial scale of the initial distributions. Instead of sampling particles to ensure consistency between the particle number density and tracer concentration, we sample numerous particles quasi-uniformly across the computational domain. We then assign a multiplicity to each particle, allowing us to manage tracer distribution time evolutions more efficiently. We examine the time evolution of the tracer fields for the initial distributions with the wavenumbers $(k,l) = (1,1), (4,3)$, and $(8,5)$. The error is quantified as the L^2 norm of the difference between the tracer fields obtained using CVI-1 or CVI-2 and analytical velocities. These time evolutions of the errors are shown in Fig. 3. Note that the time evolutions of the tracer fields can be found in the appendix of this letter. In all cases, the errors when using CVI-2 are reduced compared to CVI-1, especially during the time $t < 180\,\mathrm{min}$. The numerical accuracy of the CVI scheme has a more significant impact on the errors as the wavenumbers increase. The errors grow over time when $(k,l) = (1,1)$, and the differences between CVI-1 and CVI-2 become statistically indistinguishable. However, CVI-2 still manages to reduce the errors even during extended simulated time, and the statistical differences between CVI-1 and CVI-2 remain apparent when $(k,l) = (8,5)$.

These results provide insights into the effect of the numerical accuracy of the CVI scheme on cloud simulations.

- The particle distributions and transient time evolutions of the tracer fields are significantly improved in alignment with the reference solution when using the CVI-2 scheme instead of CVI-1.
- The impact of the CVI's numerical accuracy on errors is minimal for large-scale initial distributions. Since small-scale fluctuations of the DSD cannot be represented at the spatial resolutions often used in LES, it might be challenging to verify the CVI-2 scheme's impact on whole-cloud structures.
- In contrast, the effect of the CVI scheme's numerical accuracy is evident for small-scale tracer distributions. Although particle-based advection avoids numerical diffusion for each particle's information due to its algorithms, the CVI-1's effect might manifest as macroscopic and spurious numerical diffusion.
- If this occurs in meter-to-submeter scale cloud simulations, we might detect a statistical difference in the LWC between CVI-1 and CVI-2, as the LWC fluctuates due to small-scale turbulence mixing. This detection is analogous to how we discern the numerical accuracy of advection schemes through differences in effective resolution.
- The statistical difference in small-scale tracer fields might indirectly affect large-scale cloud fields through interactions between the eddies and microphysics.

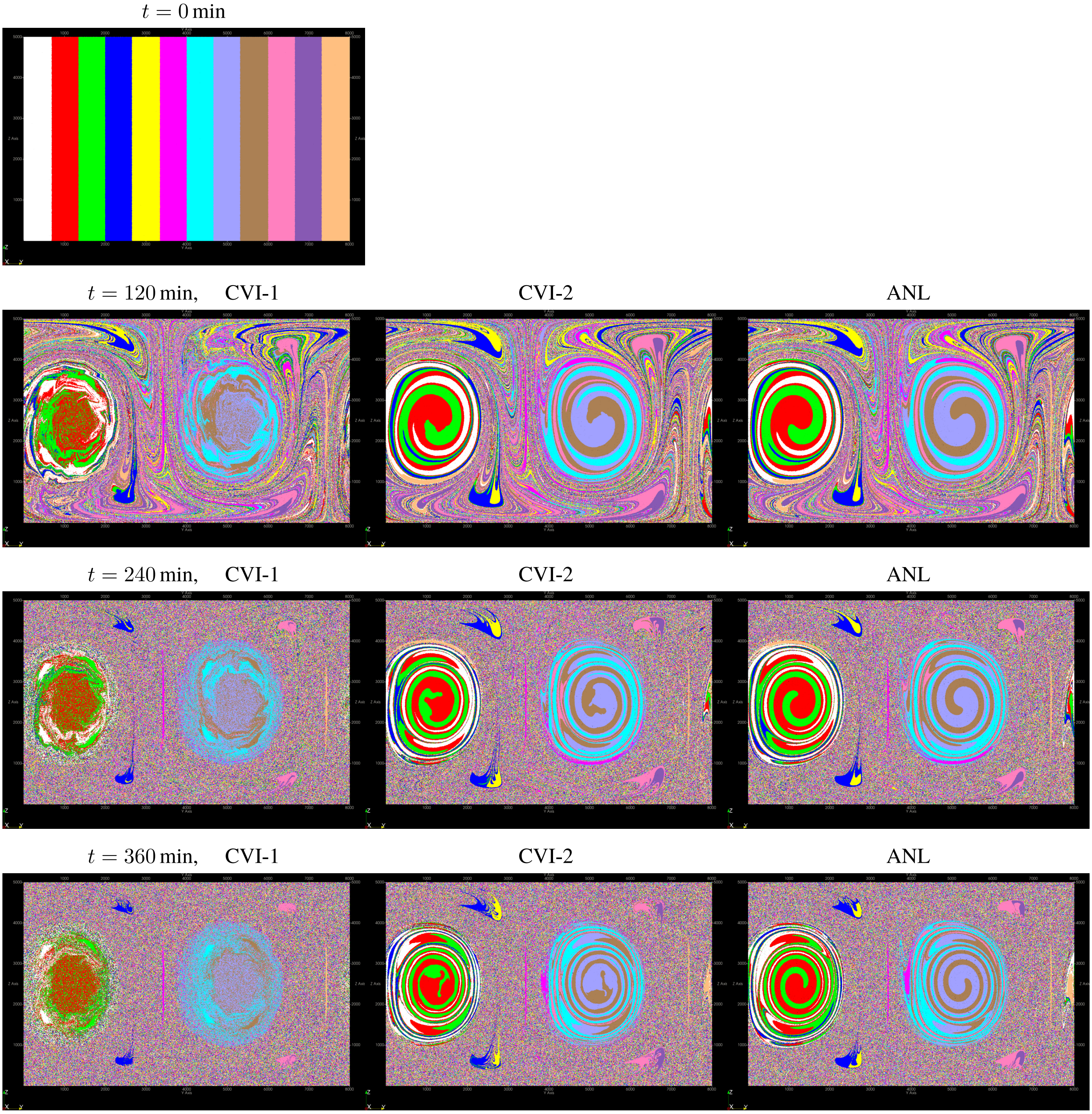

Figure 2. Distributions of particle positions colored by the initial y coordinate (Y) when CVI-1, CVI-2, and analytical velocities are used for particle movement.

In the revised manuscript, we will briefly outline the implications of our findings. We could expand our methodology to investigate further the impact of the CVI's numerical accuracy on clouds, using the warm bubble experiment as a basis. For instance, the CVI's numerical accuracy would be enhanced beyond 2nd-order spatial accuracy if we calculate the vector potential of the momentums using the spectral method. This would involve interpolating velocity at the particle position through the vector potential's interpolation, using the expansion of the basis function. Then we could compare the tracer distributions (moments of the DSD) obtained using CVI-1 and CVI-2 with a reference solution obtained using a spectral CVI. Unfortunately, implementing such a method in our model is not straightforward. Therefore, we intend to leave it to future work to provide a complete answer to your question. Additionally, we have decided to exclude the above discussion from the main body of the revised paper, as it is not directly related to the impacts on clouds. However, we will still provide this information in the supplemental material.

The differences in the time evolutions of the LWC when using different model versions and CVIs are provided in the Data set available at `https://doi.org/10.5281/zenodo.8103378`. In this Data set, the figures and data are public to readers.

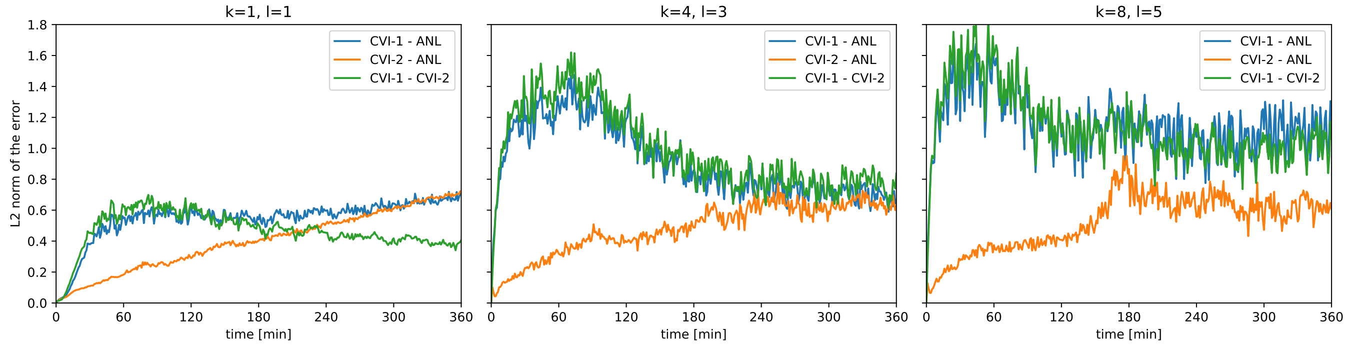

Figure 3. The time evolutions of the errors between the tracer fields obtained using CVI-1 or CVI-2 and analytical velocities for each initial tracer distribution with the wavenumbers $(k, l) = (1, 1), (4, 3)$, and $(8, 5)$.

However, we have omitted these figures from the revised manuscript. The rationale for this decision is that the differences in clouds due to the numerical changes are trivially small. The slight differences detected are primarily attributable to sampling errors or the inherent chaos of the systems. We believe that such results do not offer meaningful insights for meter-to-submeter scale cloud simulations. Additionally, considering the already substantial length of the paper, we have deemed the priority of including these results in the manuscript to be low.

2.) Moreover, I understand that including SGS velocity needs a lot of memory (in the LCM of Sölch & Kärcher, SGS turbulence on SD movement is included. But clearly, those simulations do not run on such extremely large grids). But the open question is, if the inclusion of SGS velocity wouldn' t be more important than switching from CVI-1 to CVI-2. How can you demonstrate that such sophisticated methods like CVI-2 are really necessary compared to neglecting GSG turbulence? Wouldn't SGS turbulence lead to more SD mixing and potentially affect your cloud evolution?

Response:

In the original manuscript, we mentioned why we have not adopted the SGS velocity into our model. However, we have modified the description based on feedback from the anonymous referee 2. We plan to implement the SGS velocity in the future.

Whether the impact of the numerical accuracy of the CVI or SGS velocity on clouds is more significant may depend on the spatial scale of the cloud simulations. We assume that for meter-to-submeter scale simulations such as this study and Mellado et al. (2018), the numerical accuracy of the advection schemes and the CVI may become relatively larger because the kinetic energy of the SGS turbulence (LES approach) or the viscous diffusion (DNS approach) becomes small. In the revised manuscript, we discuss the above points briefly.

We admit that the impact of CVI-2 may be less than that of the SGS velocity for low-resolution simulations. However, we would like to avoid stating which components are more important on clouds because our study is to improve the overall model performance but not determine the priority of the model development.

3.) You mention and stress that SD density should be similar to air density. This is a rather strong statement, which I believe is only valid under several assumptions and for a particular SD initialization (which may not be clear to readers).

The initial SD density may not be linked to air density, instead the multiplicities could be accordingly scaled. Moreover, one could initialize SDs only in a confined region of the whole domain. Unterstrasser & Sölch (2014) report about SD splitting and merging. In all those cases, SD density and air density are not linked any longer.

I understand that none of the cases is true in your case. Yet, your statements reads a bit like it is universally valid. This should be clarified to avoid any misunderstandings.

Response:

We agree with your comment and thank you for the important reference provided.

One desirable feature of the SD movement scheme is that the changes in the SD number density follow the changes in the air density. If we initialize SD positions in the computational domain so that the SD number density is proportional to the air density, the consistency between the SD number density and air density is maintained throughout time evolution. This is expected to maintain adequate SD number density in convective clouds.

On the other hand, Unterstrasser and Sölch (2014) introduced SD splitting and merging, specifically to optimize collision–coalescence, a scheme that we understand performs a resampling of SDs. We may also consider introducing a resampling (such as used in particle filter) to maintain SD number density, even if SD positions are initialized independently of the air density.

Although these studies adopt different approaches, they share the purpose of maintaining the SD numbers in clouds. In our revised manuscript, we will first mention this purpose and outline the two approaches. We will then focus on the SD movement scheme that automatically adjusts the SD number density to air density, explaining the desired property of velocity interpolation for designing such schemes. Finally, we will discuss the necessity of numerical accuracy for SD movement in meter-to-submeter scale simulations.

In the attached document you can find many more comments on language, plot layout and so on.

Response:

Thank you for your many comments. We have revised the manuscript to conform to your comments as much as possible. Below are our responses for each.

1. Could you choose a less technical term in the abstract?

   We have changed it to throughput of particle calculations per second.
2. This implies that there is one particular state-of-the-art experiment. But I guess every researchers defines state-of-the- art slightly differently. You refer here to the sheer size of the model domain?

   We have changed it to highest resolution simulation performed so far.
3. The current formulation implies that you have developed more than one particle-based scheme. Is this intended? " In particular, herein we focus on the particle-based super-droplet method (SDM) developed by Shima et al. (2009)." ?

   We have revised the sentence accordingly.
4. could you spell out FCT and provide a reference?

   flux corrected transport (FCT) scheme (Zalesak 1979)
5. In my opinion, you could keep the original version as the explanation was very clear.

   Thank you for your comment. We like the discussion on the convergence to DNS as $\xi \to 1$, which was added following feedback from anonymous referee 2. We would like to leave it as it is.
6. Is it some special notation to have subscripts on the left and right hand side of the letter? I do not know it. It looks peculiar so I believe the format has some special meaning.

   It is one of the notations to denote a number of combinations. We changed them to C_2^N.
7. the number or the length of the time steps?

   fixed
8. are

   fixed
9. that are

   fixed
10. does not vanish

    We have deleted it accordingly.
11. I do not understand why.

    To simplify the loop body for the SDs in a block, it is essential that the gridded values in a block are a collection of similar values, because similar operations or calculations may be applied to these values in such cases.
12. location

    We changed it to area.
13. the

    fixed

14. For this case, we can reduce the information per SD by subtracting information of partition by the MPI process and a block from the global position.

    We have added the explanation to the sentence. Note that amount of information for 2 possible states is $\log_2 2 = 1$ bit. Similarly, partitioning (or possible MPI process and a block for particles) introduce the information: the information that arises from the partitioning of the domain

15. The performance of your algorithm depends on your simulated clouds depending on which Case you encounter more frequently? You may state this clearly at the end of this subsection.

    The performance of our algorithms depends on mainly the number of Newton iterations (i.e., the closeness between the initial guess and solution) rather than whether Case 1 or Case 2 is more frequently encountered. We describe this in the revised manuscript.

16. `https://en.wikipedia.org/wiki/Rosenbrock_methods` ??

    fixed

17. described in Eq.

    fixed

18. the bulk methods solves individual droplets? Okay you write statistics, but the connection of bulk and individual is somehow counterintuitive.

    We have changed it to moments of the DSD.

19. groups

    We have changed it to moments of the DSD.

20. that of

    fixed

21. I am not sure if I understand this sentence. I understand that you deliberately included some additional modifications to the new SDM in order to achieve that the physical results remain similar to the old SDM.

    We made a modification from SCALE version 5.4.5 to generate an initial condition of water vapor mass mixing ratio that is similar to that generated by the original SCALE-SDM. This is just a bugfix for the SCALE version 5.4.5.

22. the

    fixed

23. in my understanding, x,y and z have units m. So please replace z by z/m. Or otherwise substract 1000m.

    We have added the units accordingly.

24. same applies

    fixed

25. statistical fluctuation

    The word, statistical fluctuation, is often used in our manuscript. We assume that what is lacking there is an additional explanation of how it is caused, so we have added the cause for the statistical fluctuation: caused by varying number of SDs in space.

26. are shorter

    fixed

27. SDM-new !!

    fixed

28. If it is easily changed you may turn the black background colour into white. Saves a lot of ink.

    When drawing the distributions of many tiny points, they are more clearly recognized for a black background. Please allow us to use a black background for the figure.

29. you may use white color for the smallest bin. I now see in the online version that there are thin white contour line. In my printed version they are not visible. The colours and the contour lines show both the same quantity?

    We have revised the figure to delete the thin white contour lines and to show the LWC higher than 0.001 $g{\cdot}m^{-3}$.

30. I am not sure, if I understand correctly. You do not want to say "number of grid points"!? You really mean "number of grids". Do you define "grid" as the small subset of the local domain that fits into the cache? Sorry, if I have overlooked it.

We have changed them to the number of grid points.

31. please use BULK2MOM as in all other legends :-) Moreover, is it SDM-orig or SDM-new?

    fixed

32. N

    It is the values on the horizontal axis.

33. do you mean grid points?

    fixed

34. high as

    fixed

35. The font size in the figure is small. You may keep the x-axis description only in the bottom row. Similarly, it is enough to have the "z [km]" only at left-most position. As you use the same color bar in each columns you may move it to the top of each panel. These actions would all save space and allows to better increase the font size.

    We have revised the figures accordingly.

36. per grid

    We have added the sentence to describe more clearly: We represent the SD positions in a block by 50 bits using the mapping described in Eq. (6).

37. what does NH mean?

    node-hours

38. of 1h (In the beginning I was not sure what you mean with integration time; other also use the term "simulated time")

    We have changed them to simulated time.

39. Weak scaling performance of 2m

    We have changed the caption of the figure so that it is more proper to describe the figure: Elapsed times corresponding to the dynamics, microphysics, and the other processes for different number of nodes.

40. is included in a required physical process

    is included in the total elapsed time of the process that requires these conversions for calculations

41. this is only true if SD number is spatially uniform in the beginning, isnt it? would it be clearer to say that changes in the SD density should be consistent with changes in air density?

    We have revised them accordingly.

42. $(50\text{m})^3$?

    fixed

43. thats not clear, do you refer to a particular Delta t VALUE?

    reference value of Δt is defined prior to the sentence. So we have added the word larger or smaller to emphasize comparison with the prior sentence.

44. in the printed version the colour are hard to distinguish.

    We have changed the colors and line styles of the lines in the figure.

45. The caption should only list information that is needed to understand the plot. The marked sentences seem to list results.

    We have moved the results to the main body of the revised manuscript.

46. this formulation is quite generic. Could you state what feature of the cited paper you want to include. By the way the Sölch & Kärcher (2010) has a similar concept, as SDs only exist inside clouds.

    We have revised the sentence as follows: The computational performance of our numerical model may be further improved if we store only the activated cloud and rain droplets in memory, following methods such as those described in Sölch and Kärcher (2010) and Grabowski et al. (2018).

47. for those people reading only the conclusion, it would help to define the abbreviations again in this section. But thats up to you.

    We have changed them to include definitions of the abbreviations again.

48. You may leave out some information that is too technical and anyway no one can understand without reading the paper

    We have removed the explanation of Sinkhorn distances. We have also simplified the explanation of our newly developed initialization.

References

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Zalesak, S. T.: Fully multidimensional flux-corrected transport algorithms for fluids, J. Comput. Phys., 31, 335–362, https://doi.org/10.1016/0021-9991(79)90051-2, 1979.

Appendix: time evolutions of the tracer distributions and the L^2 norm errors

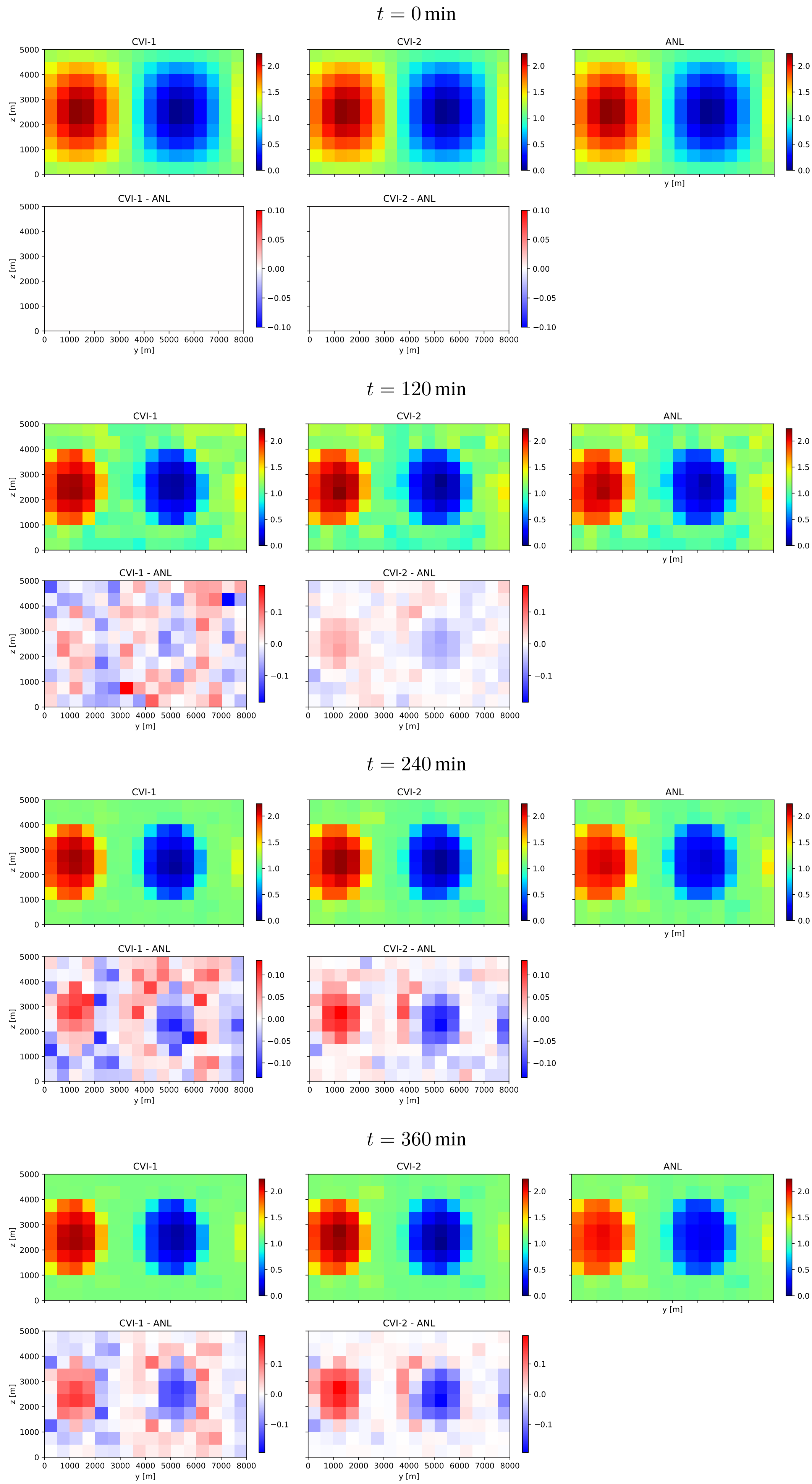

Figure 4. The case for initial tracer distributions with wavenumbers $(k, l) = (1, 1)$

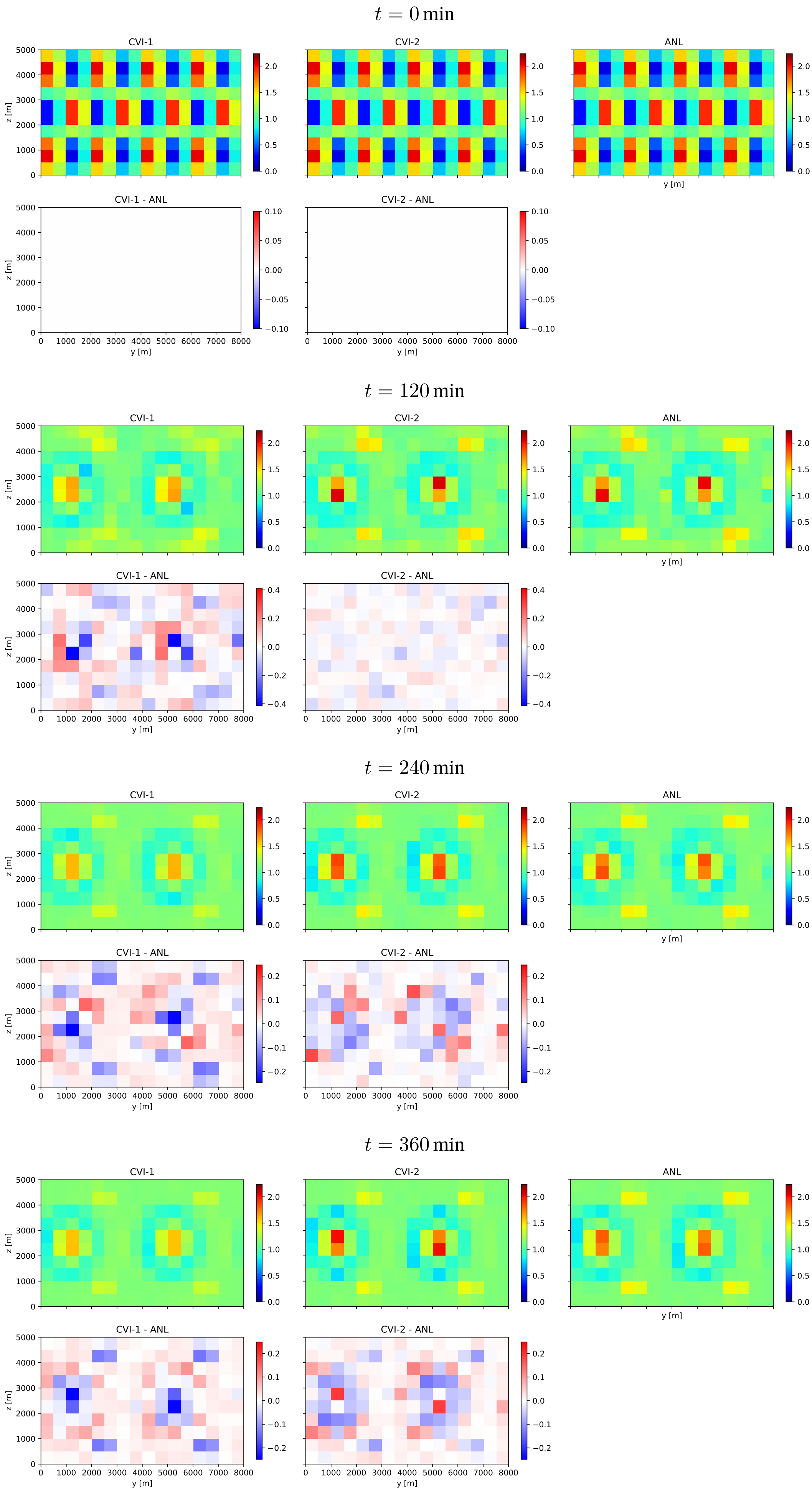

Figure 5. The case for initial tracer distributions with wavenumbers $(k, l) = (4, 3)$

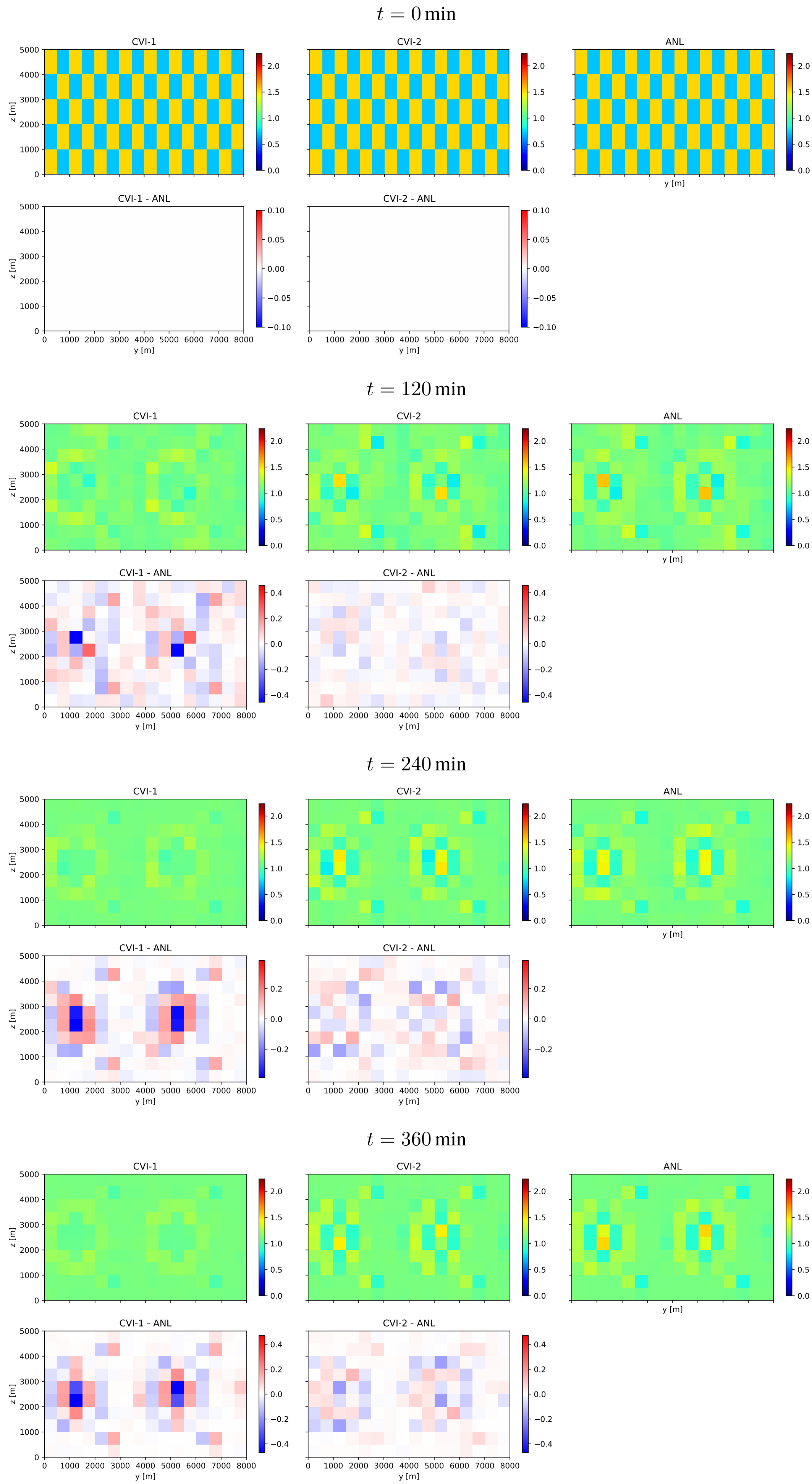

Figure 6. The case for initial tracer distributions with wavenumbers $(k, l) = (8, 5)$

Additional changes made by authors on article gmd-2023-26

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- We have utilized an English editing service for the revision of our manuscript.