Dear editor,

We thank the referees for providing comments that helped to improve the manuscript. We addressed their comments and applied changes where necessary. Text is updated and clarified, figures are improved and an overview of the numerical experiments is presented in a new table. Additionally, supplementary material is provided (as an electronic supplement) for the interpretation of the graphs that show the differences in horizontal distribution at 700 hPa.
In this document we combine the individual responses to the referees, which contain the original comments, and the marked-up manuscript generated by latexdiff.

With kind regards,

Huug Ouwersloot

Response to Referee #1

We thank Referee #1 for his/her comments that help to sharpen the manuscript and are glad that he/she appreciates the importance of an optimized convective tracer transport module in EMAC. Below we respond to these comments point by point and include the modifications that will be applied to the revised manuscript. Original comments are displayed in italic font.

As a general comment, Referee #1 wonders whether the modifications have a similar significant effect for tracer transport in the "real world" as is shown for academic tracers that decay exponentially with various lifetimes, mentioning that radon would be a good compound for such a quantification. Furthermore, he/she suggests to analyze how the quantified deviations in tracer transport change for different season.

First, we would like to emphasize that radon is an inert exponential decaying tracer. As such, the only difference with the employed academic tracers is the specific lifetime (3.8 days) and the emission distribution (only over soil). For a general overview, we deliberately prescribed atmospheric tracers that are not chemically produced or depleted within the atmosphere and that are not characterized by heterogeneous emissions so that the investigated effects would not become diluted by additional processes. This is consistent with similar previous comparison studies, e.g. Lawrence and Rasch (2005). In our manuscript we present a first-order evaluation of the induced differences due to the altered convective transport representation, based on lifetime. The final impact for individual atmospheric compounds under specific conditions will of course depend on many different factors, including chemistry and emission patterns, but can be investigated using the updated EMAC code in follow-up studies.

For the sake of this reply, we reran the ORG and I100 numerical experiments including ^{222}Rn. The final RMSD, calculated in the same way as described in the manuscript, is 31.306 %, which is consistent with the analysis in the manuscript. Additionally, we chose to present differences in the yearly averaged data, since these are already very significant. In line with general statistics principles, the root-mean-square deviation is on average higher when determined using data that is averaged over shorter periods. This effect would be strongest if the RMSD would be determined over instantaneous data, even if averaged over a year afterwards. However, as shown in Table 1 this effect is also apparent if the RMSD is determined per season. In general, the RMSD per season is higher than the RMSD determined over the year, but the order remains the same. Only

Table 1: Weighted root mean square deviations [%] between numerical experiments ORG and I100.

#Period	1000 s	1 hour	6 hours	1 day	2 days	^{222}Rn	25 days	50 days
DJF	8.292	12.213	30.791	44.778	42.886	42.369	11.931	7.074
MAM	8.423	12.420	31.497	46.178	44.359	37.410	11.975	7.002
JJA	8.615	12.760	32.493	48.066	46.719	31.095	12.912	7.525
SON	8.314	12.285	31.355	46.258	44.601	33.122	12.270	7.208
YEAR	8.068	11.858	29.935	43.326	41.319	31.306	11.007	6.433

for radon a significantly stronger RMSD can be noticed for (mainly) the DJF season, related to its emission pattern. By showing that the applied changes in the convective transport representation in EMAC are significant for yearly averaged concentrations, we automatically demonstrate that these changes are significant for shorter averaging periods as well.

Major comments

It is still not clear how the sub times length is used in the model. I am not sure if I understand it correctly which can be caulated from equation (8) in Page 3122. Then the intermediate time steps will be the global time step in sub time stepes with length delta (t_sub). But the main problem is that the sub time steps will be different at each level or each location. Does the model call the CVTRANS submodel at every time step (12 minutes) steps?

The reviewer is right that Eq. (8) on page 3122, together with the given that the amount of sub time steps has to be an integer, determines the length of the intermediate time step. This is determined per column. Within each call to the CVTRANS submodel (in our case with a time step of 12 minutes), the convective transport is calculated for each horizontal position using the locally required amount of sub time steps. This will be clarified in the text by adding "For every horizontal location the convective transport in the column is calculated independently in CVTRANS using the locally required amount of sub steps." at the end of Sect. 2.2.1.

It is mentioned that the "no nudging is applied to meteorological data during the simulation" in Line 7 Page 3125. Therefore, the results are from free running CCM simulations. However, I think it would be better to use the nudged model because you will have the same convective mass fluxes from the CONVECT scheme since the meteorological conditions are identical. That is more meaningful when you compare the results using different f_maxfrac.

The reviewer is right that this would be important if f_maxfrac would impact the meteorological conditions. However, in EMAC the CVTRANS submodel only determines the convective transport of tracers other than water. The convective transport of water is linked to the convection scheme and is therefore directly calculated by the CONVECT submodel. Since the prescribed atmospheric tracers do not interact with radiation and do not affect cloud formation, meteorological conditions are not altered between the numerical experiments. We will clarify this by including "for tracers other than water" in line 10 on page 3120.

Can you explain why there are high mixing ratio the 1day lifetime tracers in Fig1 (a) and Figure 2(a) from the standard model simulation (ORG)? It would be better to check the convective mass fluxes and/or PBL boundary layer mixing. Why the relative mixing ratio is still high in the polar region in Figure 2b? It would be better to plot Figure 2a as a log scale in the mixing ratio, otherwise, it is hard to say why the relative difference in other plots are important.

As mentioned in the original manuscript, the timescale of convective transport is of the same order of magnitude as this lifetime. Therefore, mixing ratios are relatively high in the boundary layer.
These figures provide a general insight in the (altered) distribution of atmospheric compounds, related to the applied convective transport representation, that an analysis of boundary-layer properties would not provide.
The relative mixing ratio difference in Fig. 2b is that high over the polar region, because the original mixing ratio (Fig. 2a) is that low. A small absolute difference therefore results in a strong relative difference. As such, Fig. 2a helps to interpret Fig. 2b. Absolute differences are strongest in the lower troposphere. However, by itself an absolute difference is without meaning. For example, if given a difference of 10 ppm in the observation of a chemical species, one would always need to know the base concentration to assess its relevance. Likewise, when comparing EMAC with observations or other models these percentages are important. This is also why previous studies (e.g., Lawrence and Rasch, 2005; Tost et al., 2010) presented induced differences in the same manner.
While locally these relative differences are very important, indeed they can distort the picture of the impact on the global distribution of atmospheric compounds. In the original manuscript this is explained explicitly with the use of Figs. 1a and 2a. For an objective quantification of the change in the tracer global distribution, the RMSD calculation is introduced.

I do not quite understand the Figure 5 and "instantaneous differences can be more significant, e.g., of the order of 10% in the lowest kilometer of the atmosphere" and Figure 5. Since the only change between "altered concentrations at updraft base" and "Analytic expression at cloud base" is to apply a factor (f_trans) below 2500m or below PBL height. So I thought the big changes should at that levels. But there are large changes even at 10 or 15 km.

The factor, f_{trans}, is not applied everywhere below PBL height or 2500 m, but rather solely at the base of de updraft plume, k_b, if it is located below the top of the PBL (or between PBL top and 2500 m). However, the concentrations in the air that enters the plume from below are altered. Since this is the main inflow for the plume, at all levels the properties of the plume are changed. Thus all layers are affected.

This work seems to be important for the strong convection cases, therefore, the results should highlight some strong convection cases, rather than using the 1 year averaged presented here.

Indeed, the applied changes result in the most significant differences for strong convection cases. However, as explained while answering the general comment, by presenting the significant differences in 1 year averaged data we show that the impact is not just limited to such cases. Of course, a quantification of the individual induced differences for all possible time periods, locations, different chemical species and conditions is impossible. Therefore, we limit ourselves to this demonstration of the significance of the applied alterations.

Minor comments

The quality of all Figures are not good.

If the reviewer could elaborate, we could apply changes. If the problem is (only) related to the light colour of the labels and the presence of raster lines within the contour plots, we would like to clarify that these are probably due to conversion issues from high quality figures. We will take care to improve the figures quality in the final manuscript as well. Please inform us if the reviewer dislikes the figures for other reasons.

Page 3122 Line 1, rewrite as "in the grid cells part affected by plumes".

We will rewrite it to "The temporal evolution of the mixing ratios in the grid cells parts that are affected by the plumes is expressed by".

Page 3126 equation (14), change it to "RMSD"

We thank the reviewer for pointing out our spelling error.

References

Lawrence, M. G. and Rasch, P. J.: Tracer transport in deep convective updrafts: plume ensemble versus bulk formulations, J. Atmos. Sci., 62, 28802894, doi:10.1175/JAS3505.1, 2005.

Tost, H., Lawrence, M. G., Brühl, C., Jöckel, P., The GABRIEL Team, and The SCOUT-O3- DARWIN/ACTIVE Team: Uncertainties in atmospheric chemistry modelling due to convection parameterisations and subsequent scavenging, Atmos. Chem. Phys., 10, 19311951, doi:10.5194/acp-10-1931-2010, 2010

Response to Referee #2

We thank Referee #2 for his/her comments that contribute to clarify the manuscript. Furthermore, we are pleased that he/she appreciates the necessity of the presented improvements for realistic convective transport of atmospheric tracers. In general, the major comment of Referee #2 is the use of the word "significant" where no statistical significance is determined. This will be remedied in the revised manuscript. Below we respond to the comments point by point and include the modifications that will be applied to the revised manuscript. Original comments are displayed in italic font.

The use of a single experiment of one years length for each configuration makes it quite difficult to gauge the significance of any differences. The manuscript uses the vocabulary "significant" throughout the manuscript with no foundation. I would recommend either running small ensembles, longer experiments, or as a minimum removing the word "significant" from the manuscript and substituting the vocabulary about definitive differences with more relative terminology (ie., the mixing ratio in the xxx experiment is 10% larger than in the xxx experiment).
and
General: Please remove the use of the word "significant" when discussing differences among experiments. Please use the value of the RMS relative to the mean mixing ratio, ie., 10% difference.

We agree with the reviewer that the use of the word "significant" is misleading, since it is not used in the statistical sense. Indeed, we don't use it to quantify whether induced changes are unlikely to be caused by chance (alone), but rather to say whether induced changes have an impact that affects numerical studies. To prevent misunderstanding, we will rephrase throughout the document and make use of synonyms that do not refer to statistical significance. As per Referee #2's suggestion, changes will be expressed in relative deviations everywhere.

The use of one of the sub-stepping experiments as the standard for other experiments seems unwarranted. At best an experiment with small time steps seems like a potential "ground truth". Without a better "standard for truth" the vocabulary about improvements and degradations has no basis. Please either use a short time step run as the standard, or amend the vocabulary about differences to remove the value assessments.

Linked to the previous comment, we will amend the vocabulary.
Furthermore, for the sake of clarification, it should be noted that all changes are actually significant (i.e. not the result of chance), based on two observations: first, (random) fluctuations in other components than convective transport of tracers do not influence the comparison between numerical simulations, since the convective transport of the inert tracers does not affect the atmospheric dynamics, leading to binary identical results where the atmospheric tracers are not concerned. (Note that convective transport of moisture is treated by the CONVECT module, as will be clarified in the revised manuscript.) Second, as presented in the response to Referee #1, the weighted Root Mean Square Deviations (RMSD) are similar for different seasons, showing that the deviations are not a matter of chance.
Since the deviations are shown to converge for smaller values of f_{maxfrac} and recirculation effects are captured better when using more intermediate time steps, we are confident that I001 is a solid base experiment, which is closest near the absolute truth and closer to that than to e.g. experiment I005. However, we do acknowledge that I001 is not the absolute truth itself and will rather represent it as "best representation" in the revised document. Moreover, Table 2 will be updated to also present the influence of the adapted updraft plume base and the convective cloud cover on experiment I001.

It is not clear whether CVTRANS is used for transport of chemical species only, passive tracers only, or for the transport of moisture and heat as well. it reads as though CVTRANS is NOT use to transport moisture (and cloud condensate). if that is the case, please discuss/justify.

The interpretation of the reviewer is right. In EMAC the CVTRANS submodel only determines the convective transport of tracers other than water. The convective transport of water is linked to the convection scheme and is therefore directly calculated by the CONVECT submodel. We will clarify this by including "for tracers other than water" in line 10 on page 3120.

In addition - the restriction on the convective in the control experiment is not quite clear - when the CFL criterion is violated, is all transport turned off, or is the transport limited to the amount needed to meet CFL?

In the original code, transport is indeed limited to the amount needed to meet the CFL criterion. This is stated on page 3122, lines 15 - 16: "if F^k_{up} exceeds $\frac{M^k}{\Delta t}$, it is truncated to that value in the CVTRANS calculations to prevent instabilities and negative mixing ratios that may arise".

The description of the "analytical expression" is also not clear. Does the control experiment not use this "analytical expression" for the change in mixing ratio below cloud base? So the subsidence does not extend down into the cloud base *in the control experiments?*

As the analytic expression is one of the applied modifications, it is not present in numerical experiment ORG. Subsidence does still extend down into the cloud base, but the effect of recirculation is not accounted for: all air that escapes has the original properties of the grid cell below cloud base and is replaced by subsiding air masses. The analytic expression "accounts for the [in certain cases] significant influence of the updraft plume on the sub-plume mixing ratio evolution within the time step". As explained in Sect. 2.2.2, this is done by applying $\langle C_{\mathrm{env}}^{k_\mathrm{b}} \rangle$ (expressed by Eqs. (10-11)) instead of $C_{\mathrm{env}}^{k_\mathrm{b}}$ in Eq. (5).

Please explain why you reduce the mass flux per unit ares in the CC experiment. One could imagine an option where the conv mass flux per unit area is unchanged and the assumption of total cloud cover would mean an INCREASE in total mass flux in a grid box.

As the mass flux is not determined by the CVTRANS module, it is not adapted by the applied modifications and differences in settings. As stated in Sect. 2.1, the total mass flux is determined by the convection module, CONVECT, which functions independently from CVTRANS. For CVTRANS, the cloud cover needs to be diagnosed to determine over what area the "leaky pipe" representation is concentrated.

the description of the experiments is confusing at best. a table listing the experiments and their names is sorely needed. How long did the experiments run for?

Although the naming convection is straightforward and explained in Sect. 3, we will include a summarizing table that contains the settings and run time of the numerical experiments.

There is no reference for the relevance of the magnitude of the standard deviations. For instance, P. 3127 Line 12 refers to standard deviations of 5% of mixing ratio. Is that large (as the text suggests?) or small, or within natural variability?

Considering that yearly averaged data is evaluated, a difference of 5 % is large. Of course, the importance of the deviation depends further on the application and as such has a subjective component. When e.g. two numerical models are compared with identical initial and boundary conditions, a 5 % difference will be more reason for concern than the same difference between numerical model results and observations, for which the uncertainty in initial and boundary conditions, as well as the uncertainty in observations, should be considered.
Furthermore, we would like to reiterate that in our numerical experiments the changes in CVTRANS only affect the distribution of atmospheric tracers, since the inert tracers do not interact with the thermodynamics and dynamics. As a

result, the dynamics are binary identical between the different numerical experiments. Therefore, all differences are solely attributed to the applied modifications. The modifications further lead to clear patterns that are e.g. consistent for different values for f_{maxfrac}. Additionally, we want to mention here again that when evaluating individual (shorter) periods, similar values for the RMSD are found (as presented in the response to Referee #1). This all indicates that the induced differences are systematic. Furthermore, the systematic nature of the changes is supported by the given that the presented resulting patterns do correspond with the expected shifts in tracer distribution.
Whether the systematic difference of 5 % is within the random natural variability is a reasonable question, but does not diminish the applicability of our modifications. When e.g. weather patterns are different, the induced differences could be stronger than the difference between the original and revised numerical representations. However, when averaged over a longer period, those random differences will disappear while these systematic differences remain.
For the quantification of the differences it is important to realize that convective transport of moisture is treated by the CONVECT module and is therefore not affected in this study. As indicated earlier in this response, this will be clarified in the revised manuscript.

A single experiment with each configuration of 2-years duration (where we see only the results of the averages for one of the years) is not sufficient to measure differences. Longer (or more) experiments would strengthen any argument about differences.

We disagree that for tracers with a maximum lifetime of 50 days a year of data after a year of spinup would be insufficient to measure differences. It even exceeds common practice like averaging over a month (Lawrence and Rasch, 2005) or 4 months (Tost et al., 2010). Again, the robustness of the differences is supported by the RMSD evaluation for different seasons.

Discussion of figure 1 - what is the surface value? i.e.., the figure shows values near 5-10 or less in the ORG experiment and another 30 in the 100I experiment. difficult to assess without knowing surface mixing ratio. is vertical transport in the ORG experiment almost eliminated? What is the behavior of the transport in this experiment with a smaller time step?

We chose to only present the figures that contain most information, but agree that relevant information for the interpretation of these figures is missing. To provide readers the opportunity to analyze the figures in further detail while keeping the manuscript concise, additional figures will be included in an electronic supplement. For each global difference plot (Figs. 1b and 6b), the reader will have access to the mixing ratios for both experiments, both at the surface and at a height of 700 hPa, as well as the mixing ratio difference, both absolute and relative to the original values at that height.

Not clear that both figures 1 and 2 are needed to show that the difference between an experiment with and an experiment without much convective transport of constituents is to find more tracer aloft. perhaps figure 2 suffices.

Both figures give different information. While Fig. 1 serves to illustrate the global patterns and indicates geographical areas where strongest differences are found, Fig. 2 shows the distribution with height.

Page 3129 lines 1-5 - by what criterion do you assess the ORG transport to be overestimated and the 100I experiment to be overestimated? If you have no basis for these terms please use relative terminology.

The underestimation of convective transport in the ORG numerical simulation directly follows from the procedure in which mass fluxes are capped to fulfill the CFL criterion. Furthermore, it is supported by comparing it with the results from numerical experiment I001, which is the best representation and close to the "ground truth". Likewise, the overestimation of convective transport in numerical experiment I100 is to be expected since convection can transport majority of the air in grid cells away within one step without accounting for replenishing air being partly used for this outward transport as well. It boils down to a differential equation that is numerically solved with coarse time steps. As a result, the air that is removed is less influenced by subsiding air. Since the subsiding air is characterized by lower mixing ratios for exponentially decaying tracers that are emitted near the Earth's surface, convective transport is overestimated. Again, this is confirmed by comparing this numerical experiment to numerical experiment I001.

The material in this section illustrates the issue with not having any sort of objective criterion about which transport is correct. Please add some discussion in either the introduction or in the section describing the model of the performance of the control (ORG) simulation with realistic tracers as compared to observations.

It is clear that numerical experiment I001 represents the "real transport" best. In this case convective tracer transport is resolved with the finest time steps (only allowing maximum 1 % of a grid cell to flow out of the control volume within one time step). As such, constrained by the representation of the mass fluxes in the CONVECT subroutine, this is the most accurate representation of convective transport of atmospheric tracers.
We will emphasize the use of I001 as best representation to quantify the RMSDs in the revised document.

the discussion about small (and probably not statistically significant) differences between two experiments should be removed. if the differences cannot be shown to stand above noise then there are no differences.

As stated before in this reply, there is no noise in the comparison between numerical experiments, since the dynamics are binary identical. Furthermore, there are differences present that are expected based on reasoning and are represented using Large Eddy Simulation Studies. The differences might be small, but the effect is systematic. Considering the recent literature and the fact that it is part of the presented model development, we will retain this section.

line 3 on page 3133 says that the differences are "very significant". please remove this as it has not been shown. Differences of 4% would probably we within the noise, and 27% may or may not be. The description of the results of these experiments can be removed.

The removal of the word "significant" will be included in the aforementioned rephrasing throughout the document. We disagree that the systematic change is unimportant due to noise. Furthermore, we stress that the resulting patterns, as shown in the figures, are consistent with expectations based on theory and indicate that deviations are not randomly distributed.

Figures 2,3 - please add some values to the vertical axis other than 1000 and 100. In addition, because the color bar chosen makes it difficult to see the zero line, please add a zero contour.

We will add the zero contour line and add additional information on the pressure axis.

figure 4 - the text in the legend is garbles in the pdf file.

We will clarify the use of I### by adding "Numerical experiments" in front.

Panel 'a' of figures 2,3,5,6 can be removed. it is the difference that is being discussed in the manuscript.

It is true that the differences shown by the figures are discussed in the manuscript, but that does not warrant removing the figures. We would like to emphasize that the differences shown by the figures are explicitly not equal to the quantification by the RMSD and assist to provide insight into the (changes in) distribution of atmospheric tracers. They indicate where convective transport is active and where it is enhanced or diminished. Furthermore, they reinforce that deviations are not random, but result in systematic patterns, which is shown to be important in this reply as well. As such, these figures support the manuscript.

References

Lawrence, M. G. and Rasch, P. J.: Tracer transport in deep convective updrafts: plume ensemble versus bulk formulations, J. Atmos. Sci., 62, 28802894, doi:10.1175/JAS3505.1, 2005.

Tost, H., Lawrence, M. G., Brühl, C., Jöckel, P., The GABRIEL Team, and The SCOUT-O3- DARWIN/ACTIVE Team: Uncertainties in atmospheric chemistry modelling due to convection parameterisations and subsequent scavenging, Atmos. Chem. Phys., 10, 19311951, doi:10.5194/acp-10-1931-2010, 2010

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Revision of the convective transport module CVTRANS 2.4 in the EMAC atmospheric chemistry–climate model

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Abstract. The convective transport module, CVTRANS, of the ECHAM/MESSy Atmospheric Chemistry (EMAC) model has been revised to better represent the physical flows and incorporate recent findings on the properties of the convective plumes. The modifications involve (i) applying intermediate time stepping based on a settable criterion, (ii) using an analytic expression to account for the intra time step mixing ratio evolution below cloud base, and (iii) implementing a novel expression for the mixing ratios of atmospheric compounds at the base of an updraft. Even when averaged over a year, the predicted mixing ratios of atmospheric compounds are ~~significantly affected~~ affected considerably by the intermediate time stepping. For example, for an exponentially decaying atmospheric tracer with a lifetime of 1 day, the zonal averages can locally differ by more than a factor of 6 and the induced root mean square deviation from the original code is, weighted by the air mass, higher than 40 % of the average mixing ratio. The other modifications result in smaller differences. However, since they do not require additional computational time, their application is also recommended.

1 Introduction

A key process in global modeling of atmospheric chemistry and climate is the vertical exchange of air (Lelieveld and Crutzen, 1994). Convective vertical motions redistribute energy, moisture and reactive trace species between different vertical layers within the troposphere. For clear sky conditions, this transport between e.g. the Earth's surface and the top of the troposphere acts on timescales of the order of weeks. However, moist convective transport associated with cumuliform clouds reduces it to time periods of hours (Lawrence and Rasch, 2005; Tost et al., 2010). Especially short-lived atmospheric compounds are ~~significantly~~ strongly affected. Although important, the convective clouds cannot be explicitly resolved in general circulation models and need to be parameterized (e.g., Arakawa, 2004; Kim et al., 2012). Useful tools to derive and check these parameterizations are large-eddy simulation (LES) models that operate in smaller domains with a higher resolution (e.g., Bechtold et al., 1995; Siebesma and Cuijpers, 1995; Ouwersloot et al., 2013).

Here, we revise the parameterization in the convective transport scheme (CVTRANS, Tost et al., 2010) of the ECHAM/MESSy Atmospheric Chemistry (EMAC) model (Jöckel et al., 2006). This module is based on the bulk formulation for convective plumes introduced by Yanai et al. (1973) and treated and validated by Lawrence and Rasch (2005). While the original implementation already performs satisfactorily for weak to moderate convective transport, for strong convective transport the calculated mass transfer in one time step can exceed the total air mass of the plume at that location. When this happens, the updraft mass flux at an interface level is limited to transport exactly the total mass of the plume at the grid level below. This causes a misrepresentation of the actual physical flows and replenishes the air of entire grid cells in one time step, resulting in a too coarse calculation and unrealistic trace gas venting. By introducing intermediate time stepping in the module we remedy and quantify this issue. Additionally, an analytic expression is added to further account for intra time step changes of the air properties below the cloud base. Finally, it was found in a recent LES study (Ouwersloot et al., 2013) that cloud-induced large-scale atmospheric structures in the subcloud layer can affect the properties of the air that enters the convective plumes from below. The improvement to the convective transport parameterization proposed in this study is applied here as well. In addition to assessing the effects of the aforementioned revisions, we evaluate the impact of a different convective cloud cover representation on convective transport.

In Sect. 2 we describe the model and applied modifications. The setup to study the induced changes is presented in Sect. 3. These differences are then quantified and discussed in Sect. 4.

2 Model

2.1 Original representation of convection

In this study we apply and improve version 2.50 of the MESSy framework (Jöckel et al., 2005, 2010), which is an interface structure that connects a base model to various submodels. Although our modifications are applicable to different base models as well, we validate the results using the ECHAM/MESSy Atmospheric Chemistry (EMAC) model, first described by Jöckel et al. (2006). This system combines MESSy with version 5.3.02 of the European Centre Hamburg general circulation model (ECHAM5, Roeckner et al., 2006).

The moist convective transport for tracers other than water is calculated by the CVTRANS submodel (Tost et al., 2010), which represents the bulk formulation for convective plumes described by Lawrence and Rasch (2005). A single plume, also referred to as "leaky pipe", is considered for the updrafts and downdrafts separately. These plumes can laterally entrain and detrain at every level, resulting in a vertical mass flux that varies with height. The fluxes themselves, in $\mathrm{kg\,m^{-2}\,s^{-1}}$, are not calculated in CVTRANS, but are gathered from the CONVECT submodel (Tost et al., 2006).

In the algorithm, the properties of the air that detrains from the plumes are determined according to[1]

$$C^k_{\text{up, det.}} = \frac{\left(D^k_{\text{up}} - f_{\mathrm{d}} E^k_{\text{up}}\right) C^{k+1}_{\text{up}} + f_{\mathrm{d}} E^k_{\text{up}} C^k_{\text{env.}}}{D^k_{\text{up}}}, \tag{1}$$

$$C^k_{\text{down, det.}} = C^k_{\text{down}}, \tag{2}$$

where k is the height index, decreasing with altitude. The subscripts up, down and env. indicate properties of respectively the updraft, the downdraft and the ambient air in the cloud environment. If additionally the subscript det. is used, the variable represents the property of air that is detrained from the plume in that grid cell. C is the mixing ratio in $\mathrm{mol\,mol^{-1}}$, and D and E are respectively the rates of detrainment from and entrainment into the convective plume, with unit $\mathrm{kg\,m^{-2}\,s^{-1}}$. Part of the air that is entrained in the updraft is detrained again in the same grid cell (Lawrence and Rasch, 2005). The fraction of entrained air in a layer that is detrained again in the same layer is denoted by f_{d}. Although this fraction is dependent on multiple factors, including grid resolution, it is generally set to a value of 0.5. If necessary, f_{d} is adapted to ensure that the detrained mass flux that originates from the entrained air, $f_{\mathrm{d}} E^k_{\text{up}}$, never exceeds the total detrained mass flux, D^k_{up}, and that $f_{\mathrm{d}} E^k_{\text{up}}$ is high enough so that the total amount of detrained air from the plume, D^k_{up}, does not exceed $F^{k+1}_{\text{up}} + f_{\mathrm{d}} E^k_{\text{up}}$. F^k is the mass flux, in $\mathrm{kg\,m^{-2}\,s^{-1}}$, at the top interface of grid level k.

The mixing ratios in the plumes, which are also needed for Eqs. (1) and (2), are instantaneously calculated as

$$C^k_{\text{up}} = \frac{F^{k+1}_{\text{up}} C^{k+1}_{\text{up}} - D^k_{\text{up}} C^k_{\text{up, det.}} + E^k_{\text{up}} C^k_{\text{env.}}}{F^k_{\text{up}}}, \tag{3}$$

$$C^{k+1}_{\text{down}} = \frac{F^k_{\text{down}} C^k_{\text{down}} - D^k_{\text{down}} C^k_{\text{down, det.}} + E^k_{\text{down}} C^k_{\text{env.}}}{F^{k+1}_{\text{down}}}. \tag{4}$$

The mixing ratio in the updraft plume is initialized at the lowest level where the mass flux exceeds 0, indicated by index k_{b}. In the original CVTRANS code

$$C^{k_{\mathrm{b}}}_{\text{up}} = C^{k_{\mathrm{b}}}_{\text{env.}}. \tag{5}$$

The temporal evolution of the mixing ratios in the grid cells parts that are affected by the plumes ~~affected part of the grid cells~~ is expressed by

$$C^k_{\text{env.}}(t+\Delta t) = \frac{M^k_{\text{orig}}}{M^k} C^k_{\text{env.}}(t) + \frac{\Delta t}{M^k} \times \left(\left(F^k_{\text{up}} - F^k_{\text{down}}\right) C^{k-1}_{\text{env.}} + D^k_{\text{up}} C^k_{\text{up, det.}} + D^k_{\text{down}} C^k_{\text{down, det.}} \tag{6}$$

where Δt is the time step and M_{orig} is the mass per unit area of air, in $\mathrm{kg\,m^{-2}}$, whose mixing ratio is not altered due to the plumes in one time step. This is calculated as

$$M^k_{\text{orig}} = M^k - \Delta t \left(\left(F^k_{\text{up}} - F^k_{\text{down}}\right) + D^k_{\text{up}} + D^k_{\text{down}}\right). \tag{7}$$

M without subscript is the total mass per unit area of air in which plumes occur in the grid cell, calculated as the total air mass per unit area in that grid cell times a certain cover. This cover can be selected as 1 or as the more representative convective cloud cover, calculated in the CONVECT module.

2.2 Modifications to CVTRANS

2.2.1 Intermediate time steps

If the vertical mass fluxes are very strong, M^k_{orig} tends to 0 and the discretization does no longer suffice. Moreover, if F^k_{up} exceeds $\frac{M^k}{\Delta t}$, it is truncated to that value in the CVTRANS calculations to prevent instabilities and negative mixing ratios that may arise. However, as a result the physical flow is no longer properly represented. To remedy these issues we introduce intermediate time stepping, where we divide the global time step in sub time steps with length Δt_{sub}. The

[1] Note that (only) the mass fluxes and mixing ratios in the up- and downdraft plumes are specified at the top interface of the indexed grid cell.

amount of sub time steps per global time step is determined per vertical column to ensure that at every level, k,

$$F_{\mathrm{up}}^{k}\Delta t_{\mathrm{sub}} < f_{\mathrm{maxfrac}}\min(M^{k}, M^{k-1}). \tag{8}$$

Here, f_{maxfrac} is an a priori chosen fraction of M that is allowed to leave the grid cell through the upward plume per sub time step. This fraction is set in the updated CVTRANS namelist. For every horizontal location the convective transport in the column is calculated independently in CVTRANS using the locally required amount of sub steps.

2.2.2 Analytic expression at cloud base

Near the convective cloud base, we can account for recirculation effects within a single time step in a computationally less inexpensive manner by applying an analytic solution for the sub-cloud mixing ratio evolution. At cloud base level k_{b}, $C_{\mathrm{env}}^{k_{\mathrm{b}}}$ evolves in time according to

$$\frac{\partial}{\partial t}M^{k_{\mathrm{b}}}C_{\mathrm{env}}^{k_{\mathrm{b}}} = \underbrace{-F_{\mathrm{up}}^{k_{\mathrm{b}}}C_{\mathrm{env}}^{k_{\mathrm{b}}}}_{\text{upward plume}} + \underbrace{F_{\mathrm{up}}^{k_{\mathrm{b}}}C_{\mathrm{env}}^{k_{\mathrm{b}}-1}}_{\text{compensating subsidence}}, \tag{9}$$

since air leaves the grid cell with properties of the environmental air and is replenished by compensating subsidence with properties of the environmental air in the overlying grid cell. During the time step the mass and mass fluxes do not change, resulting in

$$\langle C_{\mathrm{env}}^{k_{\mathrm{b}}}\rangle = C_{\mathrm{env},0}^{k_{\mathrm{b}}-1} + \left(C_{\mathrm{env},0}^{k_{\mathrm{b}}} - C_{\mathrm{env},0}^{k_{\mathrm{b}}-1}\right)\frac{1-\mathrm{e}^{-f_{\mathrm{frac}}}}{f_{\mathrm{frac}}}, \tag{10}$$

$$f_{\mathrm{frac}} = \frac{F_{\mathrm{up}}^{k_{\mathrm{b}}}\Delta t_{\mathrm{sub}}}{M^{k_{\mathrm{b}}}}, \tag{11}$$

where $\langle\ \rangle$ indicates a temporal average over the sub time step and subscript 0 refers to the value at the start of the sub time step. Using $\langle C_{\mathrm{env}}^{k_{\mathrm{b}}}\rangle$ instead of $C_{\mathrm{env.}}^{k_{\mathrm{b}}}$ in Eq. (5) does not yield ~~significantly~~ substantially different results if $\frac{F_{\mathrm{up}}^{k_{\mathrm{b}}}\Delta t_{\mathrm{sub}}}{M^{k_{\mathrm{b}}}} \ll 1$. Otherwise, this revised representation accounts for the ~~significant~~ major influence of the updraft plume on the sub-plume mixing ratio evolution within the time step and for the resulting reduced impact of vertical mixing ratio gradients around the plume base.

2.2.3 Altered concentrations at updraft base

As a third modification, we include a recently published parameterization for the vertical transport of chemical reactants at the convective cloud base (Ouwersloot et al., 2013). Related to induced large-scale circulations in the convective boundary layer below the convective plumes, it was found that the mixing ratios of atmospheric chemical species at the base of the updraft plume, $C_{\mathrm{up}}^{k_{\mathrm{b}}}$, differ even more from $C_{\mathrm{env}}^{k_{\mathrm{b}}-1}$ than $C_{\mathrm{env}}^{k_{\mathrm{b}}}$. Considering $C_{\mathrm{env}}^{k_{\mathrm{b}}}$ to be representative for the mixing ratio in the sub-cloud layer, their Eq. (13) is applied by replacing our Eq. (5) by

$$C_{\mathrm{up}}^{k_{\mathrm{b}}} = C_{\mathrm{env}}^{k_{\mathrm{b}}} + (f_{\mathrm{trans}}-1)\left(C_{\mathrm{env}}^{k_{\mathrm{b}}} - C_{\mathrm{env}}^{k_{\mathrm{b}}-1}\right), \tag{12}$$

where f_{trans} is a namelist setting with a standard value of 1.23 (Ouwersloot et al., 2013). When both this parameterization and the analytic solution below the cloud base are applied, Eq. (5) is again replaced by Eq. (10), while Eq. (11) is updated to

$$f_{\mathrm{frac}} = \frac{f_{\mathrm{trans}}F_{\mathrm{up}}^{k_{\mathrm{b}}}\Delta t_{\mathrm{sub}}}{M^{k_{\mathrm{b}}}}. \tag{13}$$

These updated mixing ratios are only applied if the updraft plume is affected by convective boundary-layer dynamics. This is considered to be the case if the bottom of the plume is located below the boundary-layer height that is diagnosed by the TROPOP module or below a height limit that can be set in the CVTRANS namelist. In this study it is kept to the standard setting of $2500\,\mathrm{m}$.

3 Simulation setup

We performed numerical simulations with EMAC to quantify the impact of the various code modifications. In these simulations, the MESSy submodels that are listed in Table 1 have been enabled. Unless specified differently, standard settings are used. For illustration purposes, the convective transport is tested for the standard convection parameterization in EMAC, which is based on Tiedtke (1989) and Nordeng (1994). The simulations are all performed at the T63 horizontal resolution (192×96 grid) with 31 vertical hybrid pressure levels and a time step of $12\,\mathrm{min}$. The simulation period spans the years 2000 and 2001, of which the former year is considered spinup time. The initial state is prescribed by ECMWF operational analysis data. To check the undisturbed effects of the applied modifications, no nudging is applied to meteorological data during the simulation.

Convective transport is evaluated using passive tracers with exponential decay and a constant spatially uniform emission pattern. The lifetimes of these tracers, τ, are $1000\,\mathrm{s}$, 1, 6 h, 1, 2, 25 and 50 days, and were chosen to represent various atmospheric compounds that are affected by convective transport. By prescribing passive, exponentially decaying tracers we prevent feedbacks between chemical species and meteorology and can focus on the relation between the modified convective transport and the lifetime of the tracers. Since processes in EMAC are mass conserving and these tracers are not chemically active, the total mass of a tracer at a given time is the same for each numerical experiment.

Multiple numerical experiments have been performed. Experiments whose name start with "ORG" do not use the intermediate time stepping, but if an experiment name starts with an "I", it does employ the intermediate time stepping and it is followed by a 3-digit number that is equal to $100\times f_{\mathrm{maxfrac}}$. The most precise experiment, I001, thus sets f_{maxfrac} to 0.01.

Note that in our analyses, *I001* is considered to represent convective tracer transport best and is used as the reference simulation to quantify deviations. If the numerical experiment is followed by an "A", the analytic expression for the temporal evolution of mixing ratios below the convective cloud base is applied as well. In general, the adapted convective transport near cloud base is not applied and we use the convective cloud cover as calculated in CONVECT to determine the fractions of the grid cells that are affected by the updraft and downdraft plumes. However, numerical experiments UPDP and CC, both based on numerical experiment I050A, are exceptions to this. In UPDP the adapted convective transport parameterization at the updraft plume base is enabled. In CC the convective transport is calculated using a convective cloud cover of 1, representing the extreme case where convective plumes span entire grid cells. Note that the resulting mass transport per affected unit area is weaker and therefore applying intermediate time steps ~~is less significant.~~ has less impact. To complete the quantification of differences, additionally numerical experiments UPDP$^+$ and CC$^+$ are conducted, which are similar to UPDP and CC, but based on experiment I001 instead of I050A. An overview of the different numerical experiments is presented in Table 2.

While evaluating induced differences, only data averaged over 2001 is considered. Hence, we do not consider short term fluctuations, but rather focus on long term shifts related to the different convective transport representations. For quantification, the root mean square deviation (RMSD) over the numerical grid is used, weighted by the air mass, M, in each grid cell. For two different simulations, denoted by indicators A and B, the RMSD of a mixing ratio, c, is defined as

$$\text{~~RSMD~~}\,\text{RMSD}_{\text{A,B}}(c) = \sqrt{\frac{\sum_i \overline{M_i}\left(\overline{c_{\text{A},i}} - \overline{c_{\text{B},i}}\right)^2}{\sum_i \overline{M_i}}}, \quad (14)$$

where indicator i iterates over the individual grid cells and an overbar denotes a temporal average over 2001. To put into perspective, the RMSD is always expressed as a percentage of the air-mass weighted mixing ratio, $\sum_i(\overline{M_i c_i})/\sum_i \overline{M_i}$. Note that the air-mass weighted mixing ratio is the same for all numerical experiments, since we evaluate chemically inert species with constant emissions.

4 Results

In Sect. 4.1 the effect of intermediate time steps on the atmospheric compounds is shown. The effect of using the analytic expression, for the temporal mean mixing ratio during a time step below the updraft plume, is discussed in Sect. 4.2. Subsequently, the optimal settings for intermediate time steps and the analytic expression are determined in Sect. 4.3 for the current numerical setup. The changes induced by considering the updated parameterization for mixing ratios at the updraft plume base and a different convective cloud cover are treated in Sects. 4.4 and 4.5, respectively.

The weighted root mean square deviations between different numerical experiments are listed in Table 3.

4.1 Intermediate time steps

As can be seen from Table 3, the strongest deviations are found for a lifetime of 1 or 2 days. This is related to the timescale of convective transport being of the same order of magnitude. Atmospheric compounds with longer lifetimes are generally well mixed with height and their distribution is therefore less affected by convective transport. Shorter lived species are mainly concentrated near the sources at the Earth's surface, resulting in low mixing ratios and, consequently, low absolute deviations where convective transport is active. However, even for short ($\tau = 1000\,\text{s}$) or long ($\tau = 50\,\text{d}$) lifetimes, the root mean square deviations of the 2001 averaged mixing ratio are over 5 % of the respective weighted mean mixing ratios.

In Fig. 1, the 2001 averaged mixing ratio for the atmospheric compound with a lifetime of 1 day is depicted at the $700\,\text{hPa}$ level. This level is generally located in the lower free troposphere, above the sub-cloud layer or clear-sky atmospheric boundary layer, except for areas at high elevation where the surface pressure is low. Since the atmospheric compound is emitted at the Earth's surface and decays much faster than the timescale of vertical exchange for clear sky conditions, its mixing ratio is low in the free troposphere compared to the atmospheric boundary layer, except for locations where convective transport is active. From Fig. 1a it can be seen that indeed relatively high mixing ratios are found in regions that are either characterized by a high elevation, thus evaluating boundary-layer air, or by more active convection, like the Intertropical Convergence Zone, the South Pacific Convergence Zone and the westerly storm tracks.

In the ORG numerical experiment, convective transport is capped when the upward mass flux would transport more air in one time step than present in the underlying grid cell. This nonphysical capping of the flow can be removed when intermediate time steps are enabled. As shown by Fig. 1b, this results in enhanced vertical transport and thus higher free tropospheric mixing ratios, particularly in the areas with strong convection. Supporting images are presented in Fig. 1 of the Supplement. In the boundary layer, as illustrated by the areas with high elevation, the mixing ratios become slightly lower due to the enhanced vertical transport. The increase in mixing ratios in the free troposphere are of the same order as the mixing ratios in the ORG numerical experiment and the final mixing ratios in I001 can be up to a factor 5 higher (not shown). This high factor is mainly due to the low mixing ratios in ORG at those locations, which yields large relative differences for small absolute mixing ratio differences. Therefore, the air-mass weighted root mean square deviation of the 2001 averaged mixing ratios is used for the quantification, which is equal to 43 % of the ~~mean~~ air-mass weighted mixing ratio for the tracer with a lifetime of 1 day.

The ~~significant~~ substantial change in the representation of convective transport with intermediate time steps is also clear from Fig. 2, with changes over 500 % in the yearly and zonally averaged mixing ratios compared to ORG numerical experiment. Although these high relative differences typically occur in regions with relatively low mixing ratios, they can be compared to similar figures for the effects of different convection parameterizations (e.g., Fig. 2 in Tost et al., 2010) and of the use of an ensemble plume model instead of a bulk plume model (e.g., Fig. 4 in Lawrence and Rasch, 2005). Even though mixing ratios were averaged over shorter periods in those studies, much lower relative changes were found with maximum differences between 20 and 100 %. That the ~~significant~~ consequential variations in representing convective transport applied by Lawrence and Rasch (2005) and Tost et al. (2010) yield smaller differences in the distributions of trace species emphasizes the importance of applying the intermediate time steps.

Note from Table 3 that coarser intermediate time steps, e.g., I100, yield similar differences compared to ORG as I001, and that the deviations between I001 and I100 are more than 10 times smaller. This shows that the ~~most significant~~ strongest effect results from the convective transport by the updraft plume no longer being capped, since in I100 entire grid cells can still be depleted of air in individual sub time steps. Since within each intermediate time step I100 does not account for the recirculation of air and the mass of the entire grid cell can be removed, the effectiveness of convective transport is actually overestimated, while it was underestimated in ORG. This is why the RMSD values between I100 and ORG are slightly higher than those between I001 and ORG. To better account for this recirculation, lower values for f_{maxfrac} can be chosen and the analytic expression for the temporal mean mixing ratio below the convective cloud base can be employed.

4.2 Analytic expression

By applying the analytic expression for the (sub) time step average mixing ratio below cloud base of Eq. (10), we can account for the subsiding motions that compensate for mass loss below the cloud base due to the updraft plumes within this (sub) time step. Through this process, air is replenished and the mixing ratio at the updraft plume base is not only determined by the environmental mixing ratio below plume base, but also by the environmental mixing ratio in the first layer aloft. This effect is stronger with higher updraft mass fluxes. As a result, it will no longer occur that the entire air mass in the grid cell below the plume base is replaced by environmental air from the grid cell above the plume base.

Since part of the air at the updraft plume base now originates from the environment above cloud base, the effect of vertical mixing by convective transport is reduced. This results in stronger vertical gradients with higher mixing ratios near the surface and higher mixing ratios in the upper troposphere, as confirmed by Fig. 3. Because vertical transport is underestimated in ORG, due to the capping of the mass fluxes of the updraft plumes, the RMSD between ORGA and I001 is actually higher than between ORG and I001. However, for all numerical experiments with intermediate time stepping, where mass fluxes are not capped, the RMSD compared to I001 reduces when the analytic expression is employed. This effect is especially ~~significant~~ influential for shorter lived species, roughly halving the RMSD compared to the reference case for $\tau = 1000\,\mathrm{s}$.

As most clearly illustrated by the RMSD between ORG and ORGA in Table 3, the analytic expression increases in significance when the lifetime of the tracer is shorter. We hypothesize that this is related to the vertical distribution of the exponentially decaying tracers. For shorter lifetimes, a ~~more significant~~ greater part of these tracers is located in the lower troposphere, where the effect of the represented recirculation around cloud base is strongest.

4.3 Performance

While the dynamics are best represented by using intermediate time stepping with a low f_{maxfrac} in combination with the analytic expression of Eq. (10), these settings can be computationally expensive. Therefore, an optimal setting should be chosen that limits the amount of required computational time, but results in low RMSD values compared to the reference simulation, I001. For illustration, these values are shown as a function of computational time in Fig. 4 for the tracers with lifetimes of 1000 s and 1 day. For this we take the computational time that each respective numerical experiment needed to finish the 2 year simulation with the settings listed in Sect. 3.

The RMSD is roughly proportional to the value of f_{maxfrac}, while the extra required computational time with respect to ORG scales inversely to f_{maxfrac}. In this setup we select $f_{\mathrm{maxfrac}} = 0.50$ as most desirable for further analyses, since the error is halved compared to I100 with only a limited increase in computational time. When other computationally expensive modules (e.g., chemical reactions) are enabled, the increase in computational expense for the CVTRANS module becomes even less ~~significant~~ consequential for the total simulation completion time and lower f_{maxfrac} values can be chosen.

Applying the analytic expression does not change the computational time ~~significantly~~substantially, but always improves the results when intermediate time stepping is applied. This improvement reduces the RMSD only by a small amount ($\sim 10\,\%$) for longer lived tracers, but rather ~~significantly~~ considerably for shorter lived species (e.g., $\sim 50\,\%$ for $\tau = 1000\,\mathrm{s}$).

As we find that setting f_{maxfrac} to 0.50 and applying the analytic expression results in the optimal tradeoff between required computational time and resulting RMSD, I050A will be used as base numerical experiment and reference to study the effects of the adapted mixing ratio parameterization at the base of the updraft plume (Sect. 4.4) and of using a different convective cloud cover (Sect. 4.5).

4.4 Adapted updraft plume base

Here we apply the improved representation for mixing ratios in the base of the updraft plume that was presented by Ouwersloot et al. (2013). In Fig. 5, the resulting deviations in zonally and yearly averaged mixing ratios are shown for atmospheric tracers with a lifetime of 1000 s and 1 day. In general, stronger relative deviations in these mixing ratios are found for the tracers with a lower atmospheric lifetime. However, the strongest of these relative differences are located in areas with low mixing ratios, so that their impact on the total root mean square deviation is low. Although the strongest impact on this metric is also found for tracers with the lowest lifetime, for all atmospheric tracers the RMSD is less than 0.6 % of the air-mass weighted mixing ratio. The reason that faster decaying tracers are affected more ~~significantly~~ strongly is the same as for applying the analytic expression for (sub) time step average mixing ratios below cloud base (Sect. 4.2). Both processes affect the efficiency of convective transport near the base of the updraft plume.

The low deviations are most likely related to the limited vertical mixing ratio gradients around cloud base. Except for a τ of 1000 s or 1 h, the RMSD related to applying the improved representation at the updraft plume base is always less than the RMSD between the most accurate numerical experiment, I001, and the selected base numerical experiment for the intercomparison, I050A. Also for these shorter lifetimes the RMSD values between I050A and UPDP are lower than the effect of using very coarse intermediate time steps, quantified by the RMSD between I001 and I100. From this perspective the improvement is not very ~~significant~~important. However, this small improvement comes without enhanced computational cost. Furthermore, this metric was evaluated globally using data that was averaged over 2001. Local, instantaneous differences can be more ~~significant~~noteworthy, e.g., of the order of $10\,\%$ in the lowest kilometer of the atmosphere. Therefore, we still recommend to apply this updated calculation.

4.5 Convective cloud cover

As indicated in Sect. 3, in the previously treated numerical experiments the convective transport is concentrated in a fraction of the grid cells, determined by the convective cloud cover. The current calculation of convective cloud cover in EMAC is rudimentary, assuming that

$$c_{\text{conv}}^k = \frac{F_{\text{up}}^k}{\rho_{\text{air}}^k v_{\text{upd}}}, \tag{15}$$

where c_{conv} is the convective cloud cover, ρ_{air} is the density of air in $\mathrm{kg\,m^{-3}}$, and v_{upd} is the updraft velocity that is assumed to be constant at $1\,\mathrm{m\,s^{-1}}$. Alternatively, in CVTRANS the convective transport can be distributed over the entire grid cells, which is identical to assuming a convective cloud cover of 1. Considering that both settings are possible and that the current calculation of convective cloud cover could be updated, it is worthwhile to investigate what the impact is of this chosen convective cloud cover. To investigate this, numerical experiment CC is performed, which is identical to I050A except for distributing the convective transport over the entire grid cells.

Due to the larger area, the plumes transport a smaller fraction of the affected air mass and there are less recirculation effects. Therefore, the vertical transport from the lower cloud layers to the upper cloud layers becomes more effective and especially higher mixing ratios are found in the upper troposphere, as shown in Fig. 6a. In areas of strong convection, this leads to decreased mixing ratios in the lower altitude regions where convective transport is active. This effect is visible from the averaged mixing ratios at a pressure of $700\,\mathrm{hPa}$ in Fig. 6b. Supporting images are presented in Fig. 2 of the Supplement. Similar to applying intermediate time stepping, the strongest effects are found for atmospheric tracers with intermediate lifetimes. The reasons are similar, since the transport is affected in the entire plume and the effective vertical transport is enhanced. The shift in the tracer lifetime that corresponds with the most ~~significant~~ pronounced change, towards a τ between 6 h and 1 day, is caused by the ~~significantly~~ strongly affected lower part of the convective plumes. For this assumed convective cloud cover of 1, enabling intermediate time steps yields smaller differences (RMSD $< 1\,\%$) due to the weaker local mass transport.

In total, the effect of using a different convective cloud cover definition is ~~very significant~~substantial, with RMSD values ranging from 4 % (for $\tau = 50\,\mathrm{d}$) to 27 % of the air-mass weighted mixing ratio. This shows that it is important to apply a valid representation of the convective cloud cover when evaluating convective transport.

5 Conclusions and outlook

We presented various modifications to the CVTRANS module in the EMAC model to update and revise the representation of convective transport of atmospheric compounds. The new, optional functionality consists of (i) intermediate time stepping when updraft mass fluxes are too strong compared to the air mass in individual grid cells, (ii) an analytic expression that accounts for the intra (sub) time step evolution of air properties below the base of the convective plume, and (iii) a recently published parameterization for the mixing ratios of atmospheric compounds at the updraft base.

It was demonstrated that applying the intermediate time stepping results in a ~~significant~~ substantial difference in atmospheric mixing ratios, even when averaged over 2001. The most important effect turned out to be that physical flows no longer need to be capped due to numerical limits. For high values of f_{maxfrac}, the effects of air recirculation due to the compensating subsiding motions in the cloud environment are underestimated. However, this error is much smaller than that originally introduced by the capping of the physical flows and can be diminished by applying a lower f_{maxfrac}. Additionally, applying the analytic expression accounts for the recirculation around the base of the updraft plume and reduces this error. The updated mixing ratios at the updraft base enhance the efficiency of the convective transport, but the induced deviations are of the same order as applying the analytic expression. The magnitudes of all induced differences depend on the lifetime of the evaluated atmospheric compound, related to the associated vertical distribution of the tracer and to the regions that are mainly affected by the applied modification. The intermediate time stepping proved most ~~significant~~ influential for lifetimes of the order of a day, while the other two modifications become more ~~significant~~ influential with shorter lifetimes.

Even though the analytic expression and updated plume base mixing ratios are not as important as intermediate time stepping and only result in root mean square deviations in the temporally averaged mixing ratios of less than 1 % of the air-mass weighted mixing ratios, these improvements come without extra computational cost. Furthermore, these metrics were determined for averaged mixing ratios over 2001, while local, instantaneous mixing ratios will likely differ more ~~significantly~~strongly. This will be of importance when comparing model data directly with time-dependent observations. For future numerical experiments we therefore recommend to enable all three modifications. Only when intermediate time stepping is disabled, the analytic expression should not be applied to prevent a further underestimation of the convective transport. The optimal setting of f_{maxfrac} depends on the selected submodels in EMAC. If more computationally expensive submodels are enabled, a lower f_{maxfrac} will result in decreased deviations without a ~~significant~~ noteworthy increase in computational time. In the evaluated numerical experiment a value of 0.5 was chosen.

As a future development of the convective transport, the current "leaky pipe" representation could be further investigated. In the current implementation, at every individual time step an independent realization of the convective up- and downdrafts is calculated. This could be updated to a plume that evolves in time, similar to the environmental air. Furthermore, it would be worthwhile to further quantify, and subsequently apply, the correct value for f_{d} for the various applied numerical grids. Finally, it has been shown that the convective cloud cover representation ~~significantly~~ substantially affects the distribution of atmospheric compounds. Based on Cuijpers and Bechtold (1995), more representative estimates of this convective cloud cover have been proposed (e.g., Neggers et al., 2006). However, as discussed by Sikma and Ouwersloot (2015), these have to be further adapted. To accurately represent convective transport, it will be important to include these updated parameterizations.

Code availability

The Modular Earth Submodel System (MESSy) is continuously further developed and applied by a consortium of institutions. The usage of MESSy and access to the source code is licenced to all affiliates of institutions that are members of the MESSy Consortium. Institutions can be a member of the MESSy Consortium by signing the Memorandum of Understanding. More information can be found on the MESSy Consortium Website (http://www.messy-interface.org).

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Table 1. Optional MESSy submodels that are enabled for the numerical experiments.

Submodel	Executed process	Reference
CLOUD	Original ECHAM5 cloud formation	Roeckner et al. (2006)
CONVECT	Convection	Tost et al. (2006)
CVTRANS	Convective tracer transport	Tost et al. (2010) and text
OFFEMIS	Prescribed emissions of trace gases	Kerkweg et al. (2006)
PTRAC	Prognostic tracers	Jöckel et al. (2008)
TNUDGE	Pseudo-emissions of tracers	Kerkweg et al. (2006)
TREXP	Exponentially decaying tracers	Jöckel et al. (2010)
TROPOP	Tropopause and boundary-layer diagnostics	Jöckel et al. (2006)
VISO	Diagnostics at isosurfaces	Jöckel et al. (2010)

Table 2. Description of the different numerical experiments. Listed are the differences in settings between the simulations and required computational time, in CPU h. If f_{maxfrac} is set to –, intermediate time steps are not enabled. The columns “Analytic” and “Updraft” denote respectively whether the analytic expression and the updated concentrations at the updraft base are applied. The applied cloud cover is either diagnosed in the CONVECT module or set to 1.

Name	f_{maxfrac}	Analytic	Updraft	Cloud cover	Time [CPU h]
ORG	–	No	No	Diagnosed	349
I100	1.00	No	No	Diagnosed	386
I050	0.50	No	No	Diagnosed	416
I025	0.25	No	No	Diagnosed	514
I015	0.15	No	No	Diagnosed	608
I010	0.10	No	No	Diagnosed	748
I005	0.05	No	No	Diagnosed	1,175
I001	0.01	No	No	Diagnosed	4,544
ORGA	–	Yes	No	Diagnosed	349
I100A	1.00	Yes	No	Diagnosed	383
I050A	0.50	Yes	No	Diagnosed	421
I010A	0.10	Yes	No	Diagnosed	763
I001A	0.01	Yes	No	Diagnosed	4,864
UPDP	0.50	Yes	Yes	Diagnosed	420
UPDP^{+}	0.01	No	Yes	Diagnosed	4,360
CC	0.50	Yes	No	1	339
CC^{+}	0.01	No	No	1	435

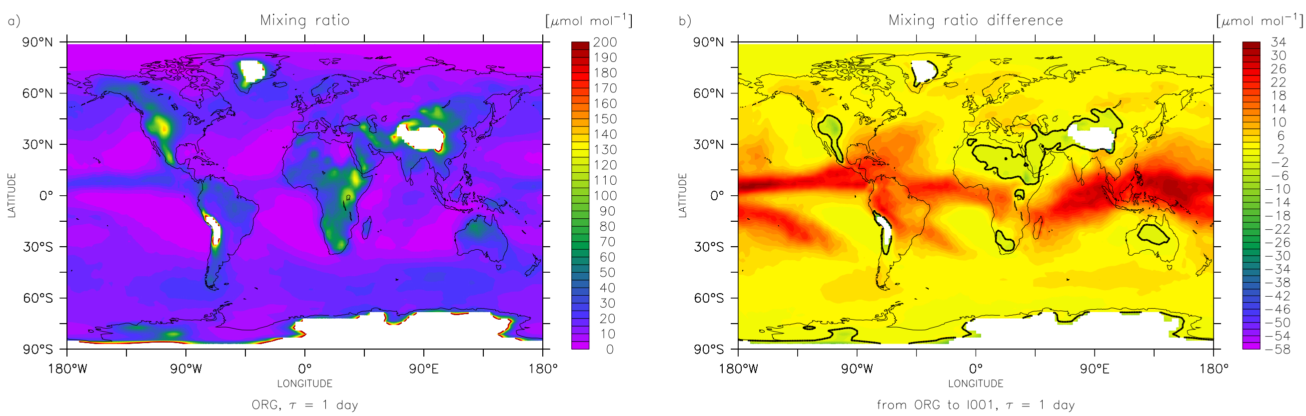

Figure 1. Horizontal distribution of the decaying scalar with a lifetime of 1 day, averaged over 2001 at 700 hPa. Shown are **(a)** the distribution for the ORG numerical experiment and **(b)** the mixing ratio difference for I001 compared to ORG.

Table 3. Weighted root mean square deviations between two numerical experiments. Results, expressed as percentages of the respective air-mass weighted mixing ratios, are listed for the seven tracers.

Comparison		RMSD [%] for tracers with a lifetime of:						
Exp. 1	Exp. 2	1000 s	1 h	6 h	1 day	2 days	25 days	50 days
ORG	ORGA	0.108	0.087	0.079	0.104	0.174	0.198	0.130
ORG	I001	7.462	11.022	28.156	41.170	39.442	10.536	6.145
ORG	I100	8.068	11.859	29.945	43.354	41.342	11.006	6.431
I001	ORGA	7.543	11.080	28.203	41.206	39.467	10.566	6.170
I001	I001A	0.005	0.005	0.004	0.003	0.002	0.001	0.001
I001	I005	0.026	0.038	0.084	0.101	0.088	0.022	0.013
I001	I010A	0.028	0.057	0.161	0.208	0.183	0.044	0.027
I001	I010	0.059	0.085	0.188	0.227	0.197	0.050	0.030
I001	I015	0.092	0.133	0.291	0.351	0.306	0.077	0.047
I001	I025	0.158	0.227	0.498	0.599	0.520	0.131	0.079
I001	I050A	0.160	0.326	0.883	1.119	0.982	0.237	0.142
I001	I050	0.325	0.468	1.013	1.210	1.050	0.263	0.159
I001	I100A	0.339	0.668	1.725	2.142	1.872	0.453	0.273
I001	I100	0.652	0.936	1.973	2.318	2.004	0.505	0.308
I050A	UPDP	0.583	0.523	0.378	0.246	0.174	0.029	0.016
I001	UPDP^{+}	0.581	0.522	0.379	0.249	0.177	0.029	0.016
I050A	CC	9.085	14.322	27.233	26.891	23.022	7.091	4.222
I001	CC^{+}	8.890	13.891	26.861	26.894	23.084	7.111	4.238

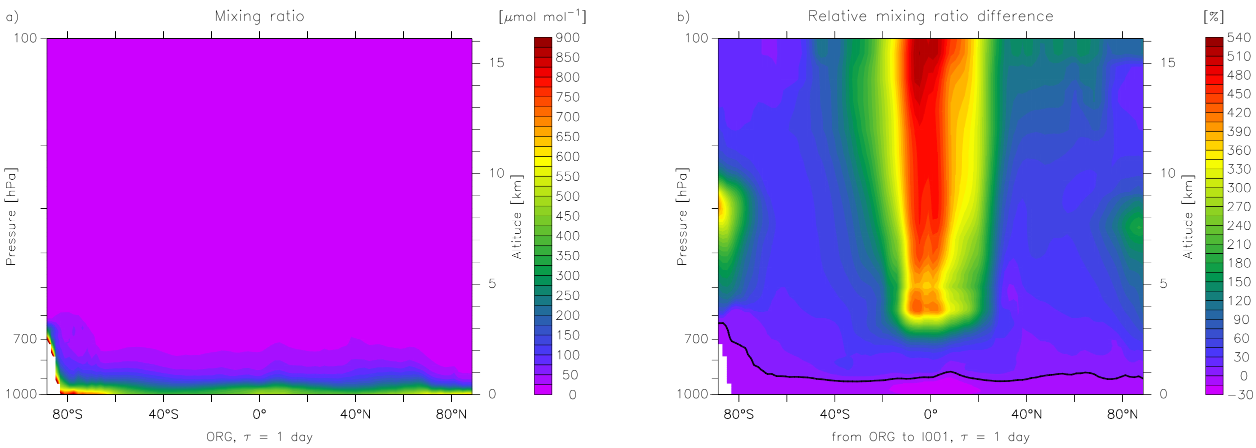

Figure 2. Decaying scalar with a lifetime of 1 day, averaged zonally and over 2001. Shown are **(a)** the distribution for the ORG numerical experiment and **(b)** the relative mixing ratio difference for I001 compared to ORG.

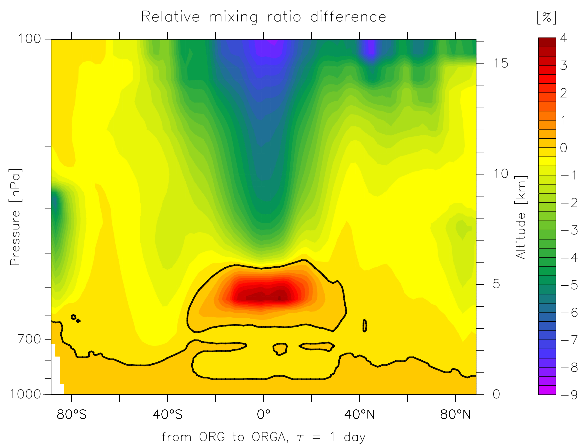

Figure 3. Relative difference in zonally and 2001 averaged mixing ratio for ORGA compared to ORG. Results are shown for the tracer with a lifetime of 1 day.

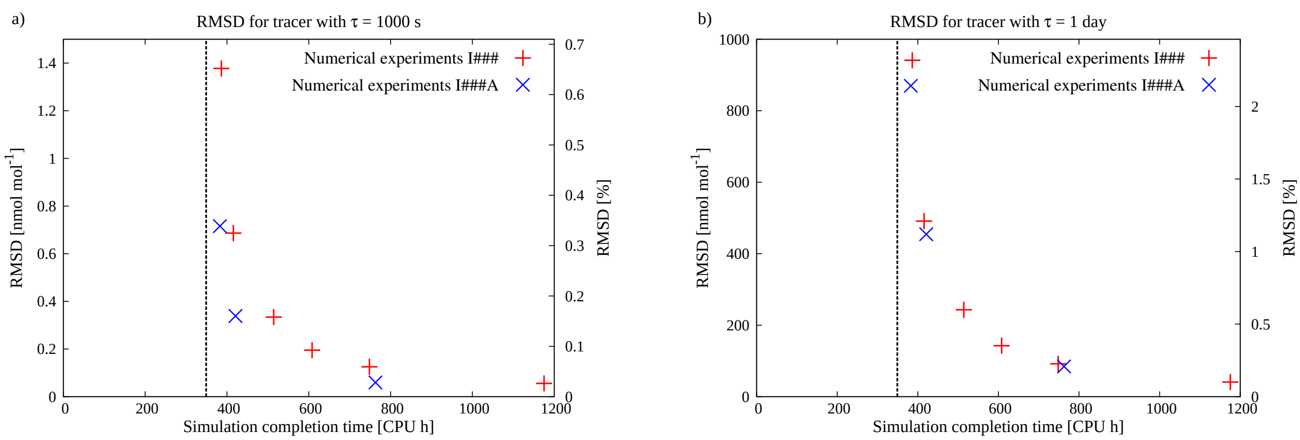

Figure 4. Root mean square deviations of the 2001 averaged mixing ratios compared to reference case I001 for decaying scalars with a lifetime of **(a)** 1000 s and **(b)** 1 day. On the vertical axes, the RMSD is expressed in both absolute numbers and as percentages of the air-mass weighted mixing ratios. On the horizontal axis, the computational time used by the numerical experiments is depicted. The red pluses, from left to right, represent the numerical experiments I100, I050, I025, I015, I010 and I005. The blue crosses represent the numerical experiments I100A, I050A and I010A. The dotted line expresses the computational time used by ORG.

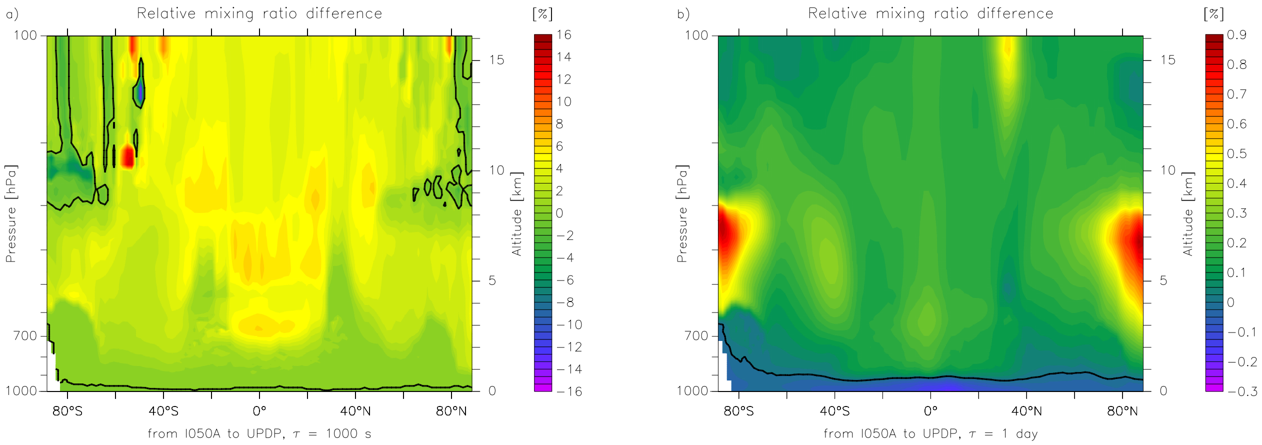

Figure 5. Relative difference in zonally and 2001 averaged mixing ratio for UPDP compared to I050A. Results are shown for the tracer with a lifetime of **(a)** 1000 s and **(b)** 1 day.

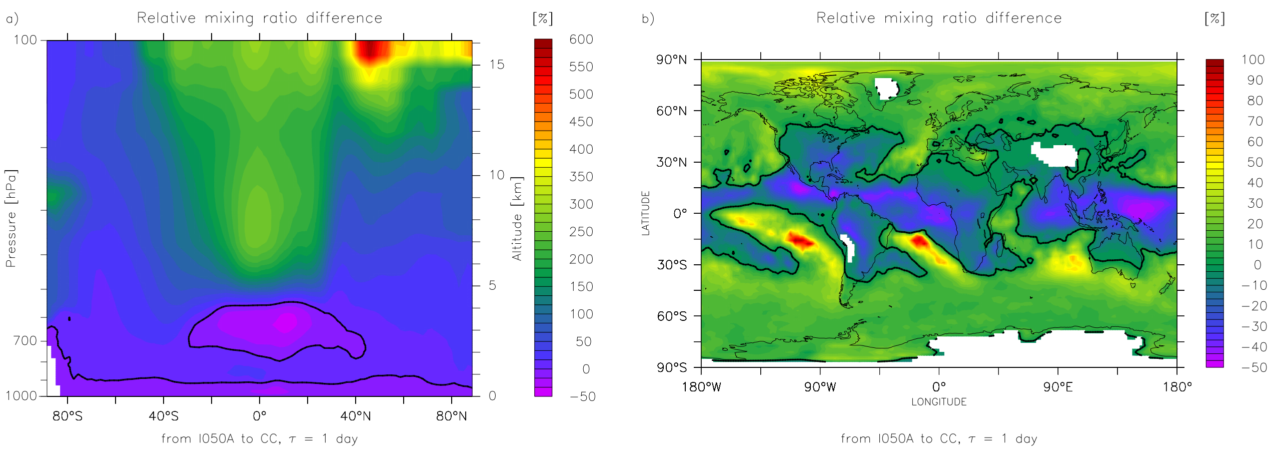

Figure 6. Relative difference in the 2001 averaged mixing ratio of the atmospheric tracer with a lifetime of 1 day for CC compared to I050A. Results are shown for **(a)** the zonally averaged data and **(b)** the difference at the 700 hPa level.