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Direct inversion of circulation from tracer measurements – Part 2: Sensitivity studies and model recovery tests

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Abstract. The direct inversion of the 2D continuity equation allows to infer the effective meridional transport of trace gases in the middle stratosphere. This method exploits the information both given by the displacement of patterns in measured trace gas distributions and by the approximate balance between sinks and horizontal as well as vertical advection. Model recovery tests have shown that with the current setup of the algorithm, this method reliably reproduces the circulation patterns in the entire analysis domain from 6 to 66 km altitude. Due to the regularization of the inversion, velocities above about 30 km are more likely under- than overestimated. This is explained by the fact that the measured trace gas distributions at higher altitudes generally contain less information and that the regularization of the inversion pushes results towards zero. Weaker regularization would in some cases allow a more accurate recovery of the velocity fields. However, there is a price to pay in that the risk of convergence failure increases. No instance was found where the algorithm generated artificial patterns not present in the reference fields. Most information on effective velocities above 50 km is included in measurements of CH_4, CO, H_2O, and N_2O, while CFC-11, HCFC-22, and CFC-12 constrain the inversion most efficiently in the middle stratosphere. H_2O is a particularly important tracer in the upper troposphere/lower stratosphere. SF_6 and CCl_4 contain generally less information but still contribute to the reduction of the estimated uncertainties.

1 Introduction

A method to derive meridional circulation fields from two subsequent sets of global zonal mean vertically resolved pressure, temperature and mixing ratios of multiple long-lived trace gases by direct inversion of the continuity equation has been suggested by (von Clarmann and Grabowski, 2016, henceforth abbreviated vCG16). This method is called “Analysis of the Circulation of the Stratosphere Using Spectroscopic Measurements” (ANCISTRUS). The resulting quantities are effective 2D velocities, that is to say, those 2D velocities which best describe the observed temporal changes of air density and constituent mixing ratio distributions by transport. They thus include all effects caused by longitudinal or temporal correlations between mixing ratios and velocities.

Similar as in other applications of inverse modelling, each iteration of the inversion scheme in ANCISTRUS consists of two steps: A prediction step and the inversion itself. In the prediction step, the current guess of the effective velocity field is applied to an initial field of measured atmospheric state variables (air density and mixing ratios of species) to solve the predictive

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version of the continuity equation. Sinks of trace gases are considered as described in von Clarmann et al. (2019) (henceforth vC19). Along with this, the partial derivatives of each atmospheric state variable with respect to each element of the velocity vector are calculated. In the inverse step, the predicted field of the atmospheric state variables is compared with its measured counterpart, and the weighted residual is minimized by inverting the continuity equation. The weights are represented by the inverse covariance matrix, including measurement uncertainties and prediction errors. To keep the inversion stable, a constraint is applied.

The natural application of this method is the analysis of the Brewer-Dobson circulation (Brewer, 1949; Dobson, 1956). ANCISTRUS avoids certain drawbacks of the hitherto common method using the mean age of stratospheric air (Waugh and Hall, 2002) as a diagnostic of the circulation. No age spectra (Andrews et al., 1999; Waugh and Hall, 2002) have to be assumed. Intrusion of mesospheric SF_6-depleted air does not cause artificial "overaging" of the air (Stiller et al., 2012; Reddmann et al., 2001; Ray et al., 2017). And finally, the method does not provide the integrated travel time of an air parcel only but provides time-resolved results.

An application of ANCISTRUS to trace gas mixing ratios measured with the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS, Fischer et al., 2008) results in circulation fields that include the expected features like tropical uplift, polar winter subsidence, elevated stratopauses and so forth (vC19). Furthermore, results proved to be stable in the sense that for each year similar circulation fields were found for any particular time of the year, although the estimates were independent from each other. In this paper, the authors use a variant of the method further developed than that described in the original paper in that sinks of trace gases are considered, and eddy mixing is constrained to zero, resulting in effective velocities which also account for the effect of the latter. Further details are reported in vC19.

Since chemical decomposition has been newly implemented in the most recent ANCISTRUS version, the effect of the consideration of sinks is investigated in Section 2. In order to further increase the confidence the new inversion-based method, in this paper we validate the inverse method by model recovery tests (Section 3). These tests are complemented by an assessment of the dependence of the results on the regularization strength (Section 4). Further, we study the sensitivity of the model to the availability of various trace gas fields (Section 5). In the Conclusions (Section 6) we discuss the power and the limitations of the method as discovered in this work, and make suggestions for further work.

2 Sinks versus transported structures

Intuitively, two candidate mechanisms can explain where ANCISTRUS takes the information from to retrieve the circulation. One mechanism is the interplay between the chemical destruction of trace gases and advection. Without advection, chemical sinks would remove those gases which have their sources at Earth's surface completely from the stratosphere, and the fact that we observe – in the long run, and putting weak long-term trends aside – approximately stationary trace gas distributions can only be explained by horizontal and/or vertical advection. Roughly speaking, with the assumption of a chemically stationary atmosphere in force, i.e., when mixing ratio distributions are assumed not to change with time, at each point of the atmosphere the loss by chemical decomposition is compensated by advection of the related species. That is to say, if a molecule is destroyed,

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another molecule of this species must be brought to this point by transport if the stationarity condition shall be satisfied. This defines a circulation field corresponding to an equilibrium with respect to atmospheric composition. Mixing ratios changing with time can be understood as a perturbation of this equilibrium assumption, but the task could be conceived as finding the equilibrium circulation where transport balances decomposition. Needless to say that this requires the modelling of sinks in the forward model that is used to predict the atmospheric state. In the current version of ANCISTRUS, the sinks of CCl_4, CFC-11, CFC-12, CH_4, CO, HCFC-22, H_2O and N_2O are considered as described in vC19, while, due to its long stratospheric lifetime, SF_6 is considered as inert in the given analysis range. For CO and H_2O also source reactions are considered. Different compared to any approach using the age of stratospheric air as a diagnostic of the circulation, ANCISTRUS is sensitive only to decomposition within the diagnosed latitude and altitude range but not to depeletion above, because it does effectively not work with absolute mixing ratio values but only with differences of values valid for locations within the analysis range. Any depletion of, say, SF_6 on its way through the mesosphere before it subsides again into the stratosphere is thus not relevant.

The other mechanism by which trace gas distributions convey information on the circulation is the transport of structures. If, say, the maximum of the mixing ratio of a certain gas is at a certain point at one day, and 5 degrees further south a month later, this is best explained by a southward velocity of 5 degrees per month. The amplitude of the structures transported is affected by the sinks discussed above.

In real applications, both mechanisms contribute to the full picture. In order to test the sensitivity of ANCISTRUS with respect to each of them, the following tests were performed: As a reference, we use a regular ANCISTRUS result based on zonal mean MIPAS measurements of all 9 trace gases from March to April 2005 (Fig. 1, top panel) and for September to October 2010 (Fig. 2,top panel). The circulation fields roughly match our expectations of a typical middle atmospheric meridional circulation. Northern polar upwelling in March-April 2005 is particularly interesting: this is explained by the displacement of the polar vortex off the pole, which means that at the pole strongly subsided vortex air is replaced by less subsided air, resulting in a local (Eulerian) upwelling in a 2D perspective. Further, we see mesospheric/upper stratospheric subsidence in local autumn, and branches of the Brewer-Dobson circulation. Within the framework of this study, we are not so much interested in the explanation of the atmospheric features but in the sensitivity of the inversion with respect to changes in the setup. The middle panels shows the respective ANCISTRUS run without the consideration of chemical sinks. The structures and circulation patterns described before are still present, but the velocities have changed in a quantitative sense. An additional feature or equatorward transport at about 55 km altitude, 30°S has emerged in March April 2005. As expected, the relevance of sinks is largest at higher altitudes, and, broadly speaking, the relevance of sinks is moderate in a sense that minor inaccuracies in sink strengths are not likely to perturb the general picture of the circulation.

By feeding ANCISTRUS with identical trace gas fields for the beginning and the end of the time interval under consideration, the equilibrium circulation was inferred, where sinks are completely balanced by advection (right panels). For this purpose we have used annual mean mixing ratio distributions. Here the general picture changes dramatically. Without information on monthly changes of the atmospheric state, the inferred circulation is fairly symmetrical, regardless if sinks are estimated with lifetimes typical for March/April (Fig. 1, bottom panel) or September/October (Fig. 2, bottom panel). With this setup,

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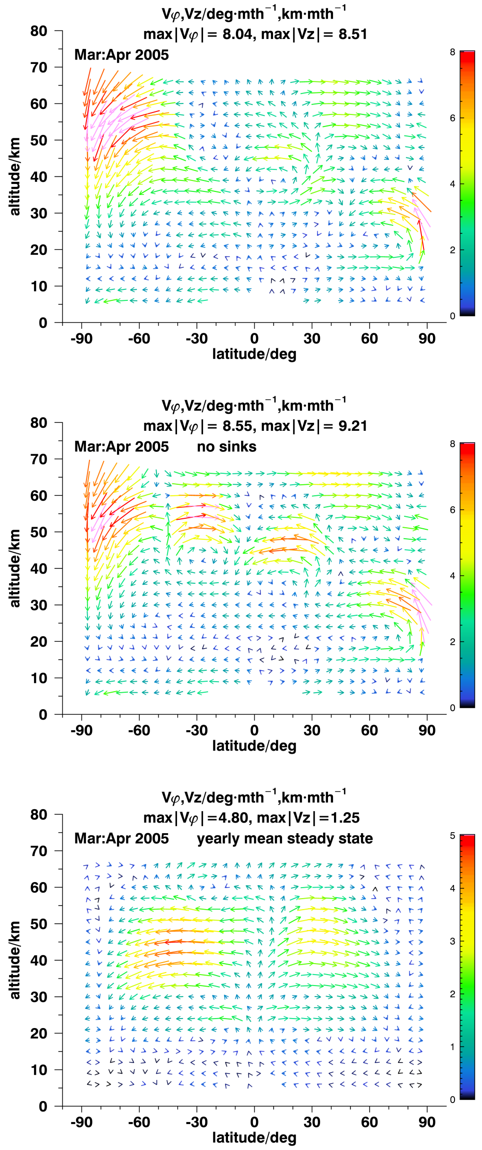

Figure 1. : The meridional middle atmospheric circulation as retrieved with ANCISTRUS for March-April 2005 under realistic assumptions (upper panel), without consideration of sinks of trace gases (middle panel), and for sinks perfectly balanced by transport (lower panel). The colour scales refer to $\sqrt{(v_\phi \mathrm{deg}^{-1}\mathrm{mth})^2 + v_z \mathrm{km}^{-1}\mathrm{mth})^2}$ for v_ϕ and v_z in units of deg mth^{-1} and km mth^{-1}. Pink arrows refer to velocities higher than representable by the colour scale chosen.

the tropical pipe reaches up into the mesosphere, and no pole-to-pole circulation is retrieved within the analysis domain. In summary, it is evident, that both sources of information have to be exploited to infer a realistic circulation field.

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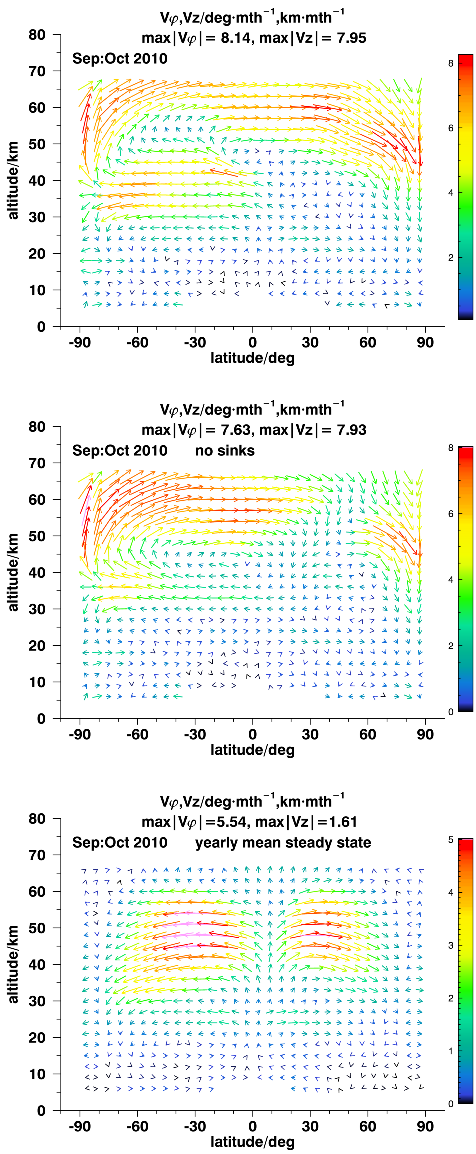

Figure 2. : The meridional middle atmospheric circulation as retrieved with ANCISTRUS for September-October 2010 under realistic assumptions (upper panel), without consideration of sinks of trace gases (middle panel), and for sinks perfectly balanced by transport (lower panel). For details, see Fig. 1

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3 Model recovery tests

vCG16 have presented two series of tests. In a first step, they tested the implementation of the transport scheme used. Tests were chosen intentionally simple in order to make it possible to judge if the algorithm does what it is supposed to, without involving the need of a separate model. If a structure, e.g., a mixing ratio maximum is transported northward by 5 degrees in one month when the assumed uniform velocity field is 5 degrees per month, the success of the test can be directly judged. Diffusive and dispersive characteristics can be tested by analysis of the size of the transported maximum and side wiggles created during the transport. Neither indication of any malfunction nor otherwise conspicious features were found in a long series of these forward model tests of which a small subset was shown in vCG16. This kind of test is considered as severe in the sense of Mayo (1996) because the probability that a flawed transport scheme would be detected is large. Thus, the likelihood that a model which passes these tests is flawed is small. Despite their simplicity, these tests are also general because the operations of the transport scheme are the same everywhere in the analysis space.

vCG16's second series of tests focused on the inversion scheme. Tests fully based on trace gas real measurements suffer from the fact that the corresponding true velocity fields are not known and it is thus not clear what the resulting effective velocity fields should be compared to. Tests based on assumed velocity fields used as surrogate truth along with simulated measurements avoid this problem. Such a test is organized as follows. The assumed velocity field is applied to a measured initial atmospheric state. The resulting solution of the forward transport problem renders the simulated state at a later time. Then the measured initial and the simulated later atmospheric state are fed into the inversion scheme as surrogate measurements, and the resulting velocity field, recovered without using any information on the surrogate truth, is compared to that one used to simulated the later atmospheric state.

For these tests, a sensible choice of the assumed velocity field is essential. Related tests by vCG16 are based on an ad hoc choice of the velocity field. Again, the broad functionality of the inversion scheme could be demonstrated but a closer look revealed that these tests were only partially successful. The cause of problems encountered was that the velocity fields used for testing were not solutions of the continuity equation. An inversion scheme that is based on the hard-wired constraint that the results must comply with continuity cannot reproduce velocity fields which were chosen in an *ad hoc* manner and are not compliant with continuity. Thus, spurious test results at the boundaries of the analysis field did not come unexpected and could not refute the validity of the algorithm.

More severe tests thus must use a velocity field that satisfies the continuity equation. On the face of it, tracer and velocity fields from a climate model would serve the purpose. The comparison of ANCISTRUS results with those from a climate model, however, suffers from the fact that 2D velocities cannot be unambigously compared to 3D model results because there is some room for interpretation of the 2D effective velocities. The latter include contributions from eddy transport and eddy mixing (See appendices in vCG16 and vC19). Furthermore, there exist some more technical problems: Often the zonal mean mixing ratio fields from the climate model deviate in a sizeable way from the MIPAS profile. In this case it is not clear what uncertainties shall be assigned to these mixing ratios from the model. Any rescaling of the assumed error variances would substantially change the weights of the measurements in the inversion, and the results would no longer be representative for the application

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of ANCISTRUS to MIPAS zonal means. Beyond this, modelled trace gas fields are often less structured than the measured ones. The absence of prominent structures, however, means the absence of some useful information for ANCISTRUS, again leading to results not directly comparable to the application of ANCISTRUS measurements to MIPAS trace gas fields.

Our way out is to use ANCISTRUS-generated effective velocity fields to simulate trace gas and density fields, apply ANCISTRUS to them, and test the resulting velocity field by comparison to the initial velocity field. The ANCISTRUS-generated effectice velocity fields satisfy the continuity equation. One might argue that this type of model recovery test is circular, but the circularity is related only to the forward transport model which has already been tested independently. This test of the inversion scheme takes fully place in a two-dimensional world and thus avoids any complication by the interpretation of 2D effective velocities and their relation to 3D model results.

Results of our model recovery tests are shown in Figures Fig. 3 for March–April 2005 (left panels) and for February–March 2010 (right panels) and in Fig. 4 for August–September, 2010 (left panels) and September–October 2010 (right panels). Figures 5 and 6 with their reduced altitude range permit a closer look at the lower stratosphere.

For the September–October 2005 case (Fig 3, left panels), ANCISTRUS reproduces all the patterns of the reference case: subsidence of mesospheric air into the stratosphere at Antarctic latitudes, stratospheric effective upwelling over the North pole, the bifurcation of an upwelling circulation branch at 30°N, 45 km altitude, and the stratospheric branches of the Brewer-Dobson circulation. At Antarctic latitudes around 55 km altitude effective velocities are over-estimated by about 15-20% and and at tropical latitudes around 45 km altitude by about 40%. Largest relative deviations are found where the reference case contains circulation branches in opposite directions at adjacent altitudes. The Tikhonov regularization chosen is designed to keep velocity differences between adjacent model gridpoints small. Thus, this kind of smoothing error observed where the inversion cannot fully resolve the reference field does not come unexpected. Also the slow circulation patterns in the tropopause region and the lower stratosphere are well recovered (Fig 5, left panels).

For the February–March 2010 test case, the situation is very similar to the one discussed above (Fig 3, right panels). All major circulation patterns are recovered. Peak velocities in the mesospheric branches of the circulation are underestimated by about 25% but broadly speaking, the inversion is successful also in quantitative terms. Again, largest discrepancies are found where opposite circulation directions are found at adjacent gridpoints: The inversion does not resolve the small circulation feature at 20°S, 45 km altitude. A more detailed view on the lower altitudes (Fig 5, right panels) shows that the branches of the Brewer-Dobson circulation are well recovered.

Tests for August–September 2010 and September–October 2010 confirm the findings of the first two tests (Figs 4 and 6). All patterns and structures are recovered. Peak velocities are slightly underestimated. Quantitative deviations between the reconstructed field and the reference field are largest where velocity gradients are largest. Most importantly, in none of the tests, the inversion scheme has created artificial patterns which were not present in the reference case.

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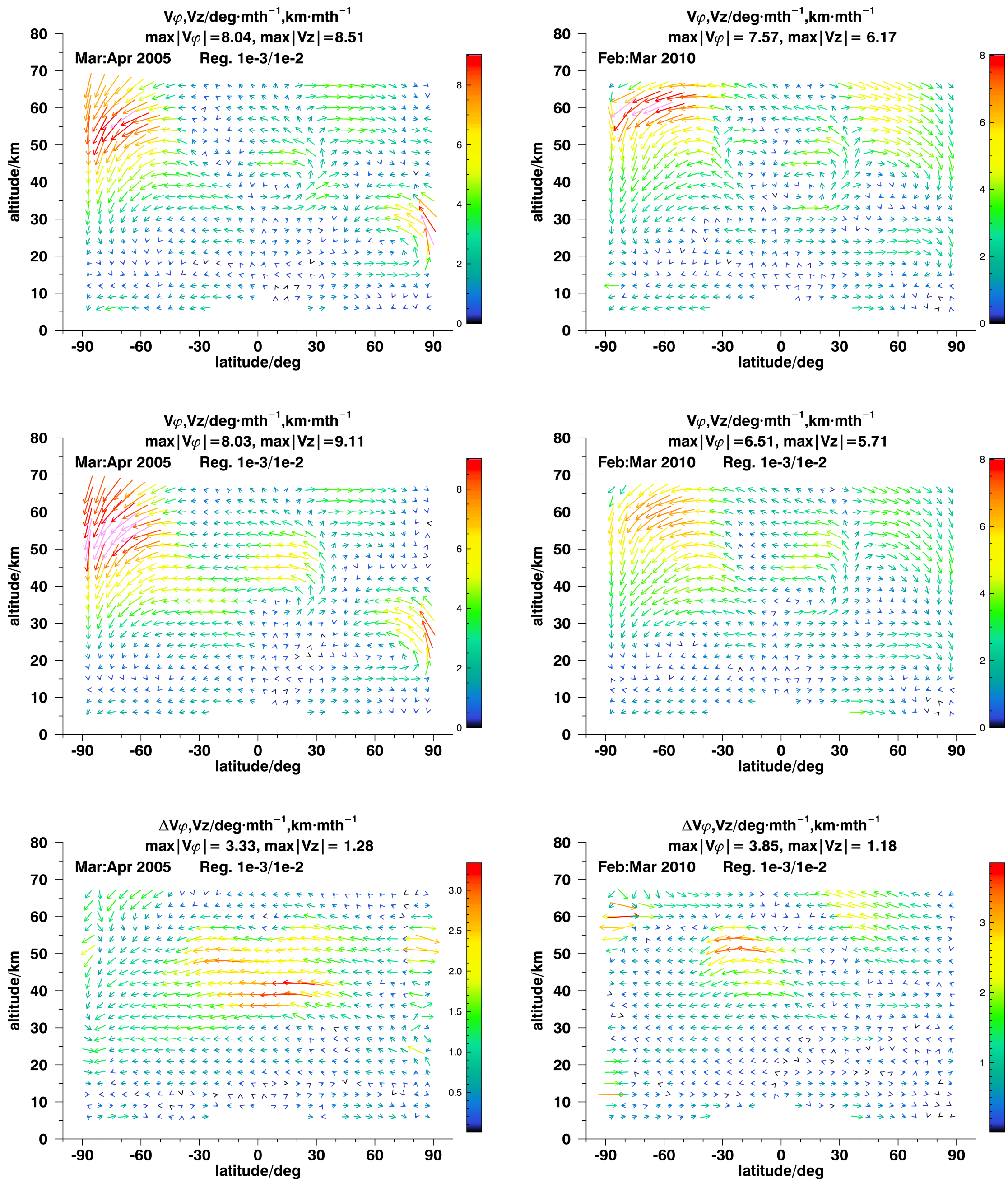

Figure 3. : Model recovery tests for March–April, 2005 (left panels) and February March, 2010 (right panels), reference fields (top panels), results (middle row) and differences (bottom panels). Note the different colour scales of the difference plots. For details, see Fig. 1.

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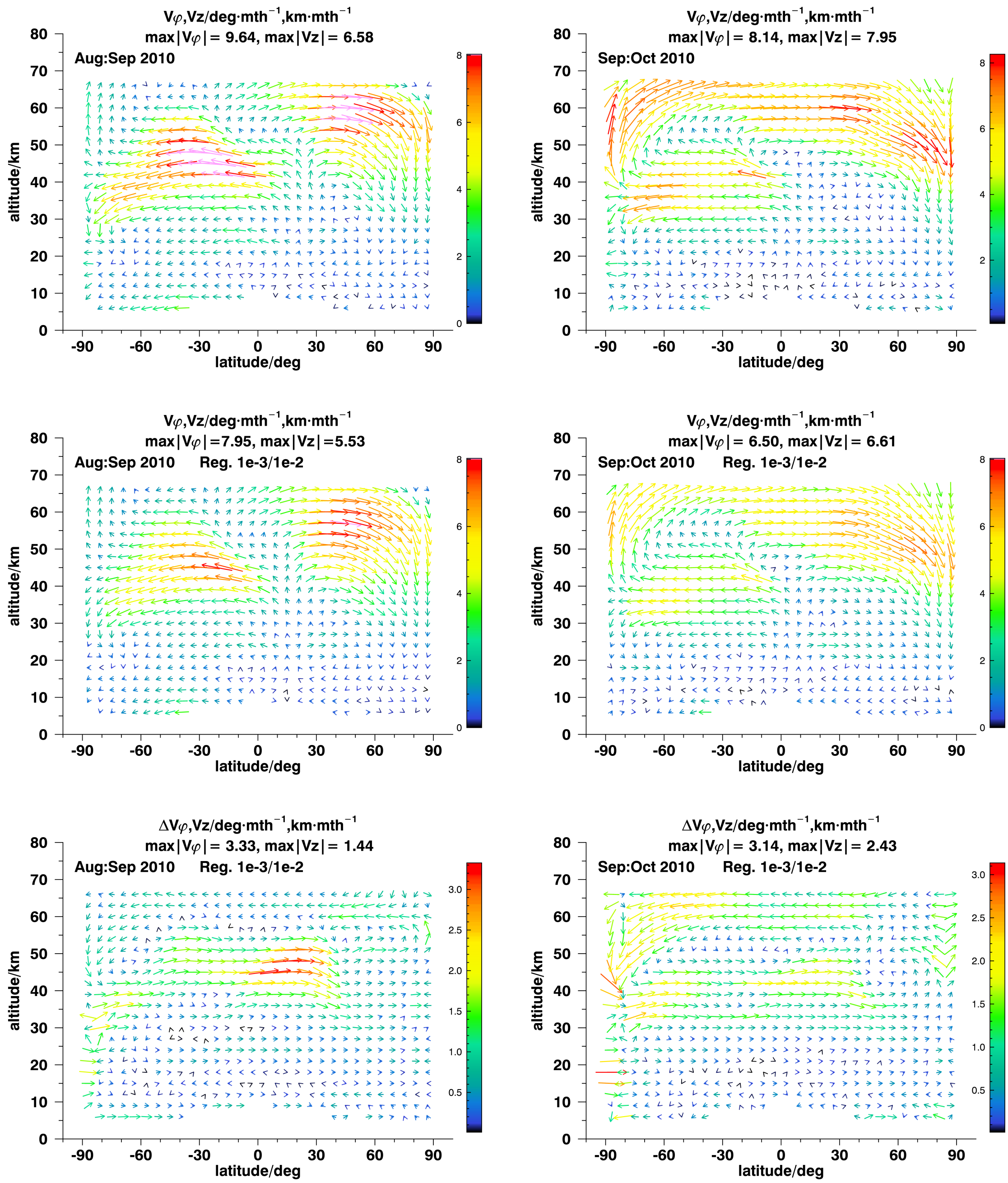

Figure 4. : Model recovery tests for August–September, 2010 (left panels) and September–October 2010 (right panels). For details, see Fig. 3.

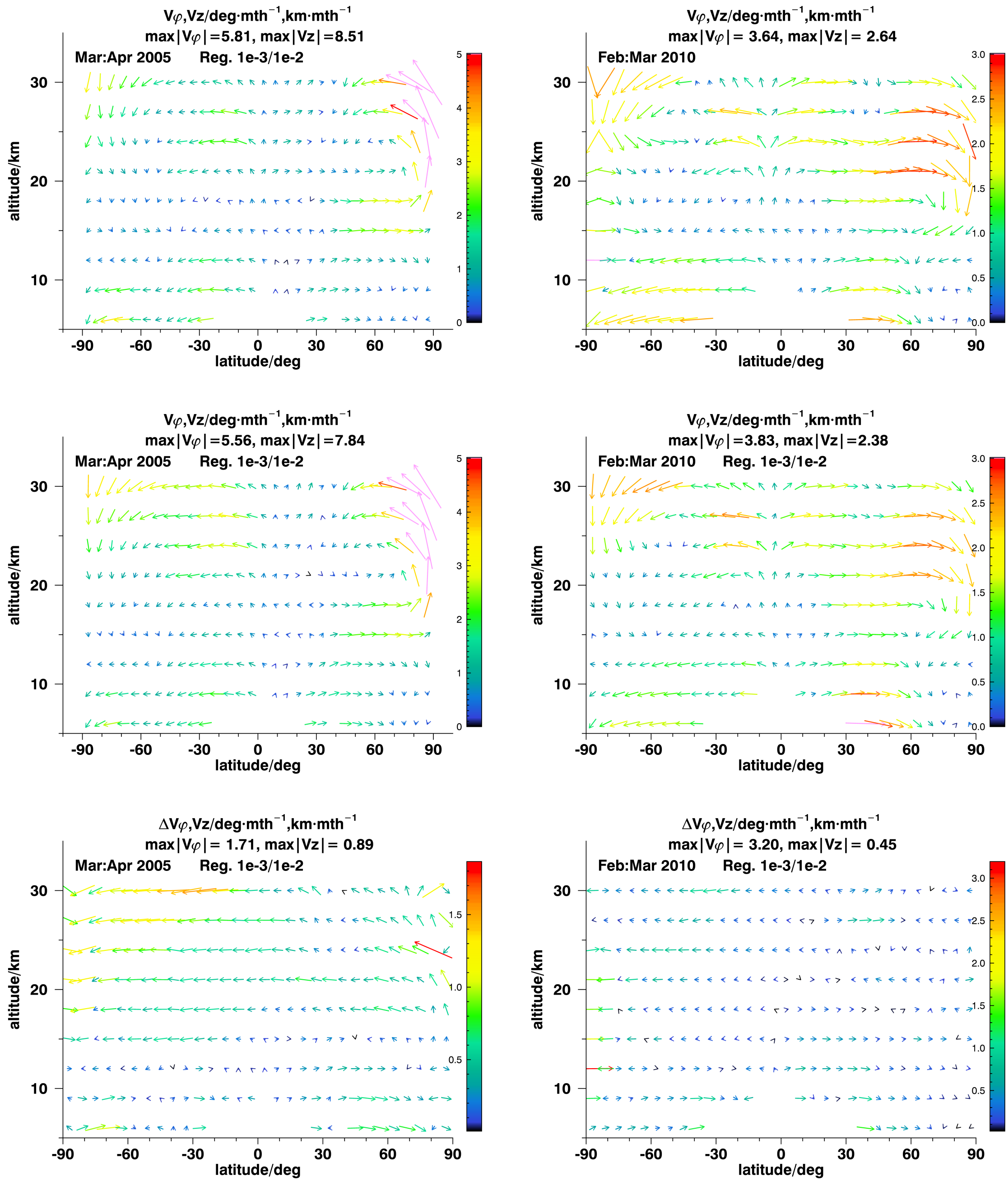

Figure 5. : As for Fig. 3 but with a reduced altitude range for clearer representation of lower altitudes.

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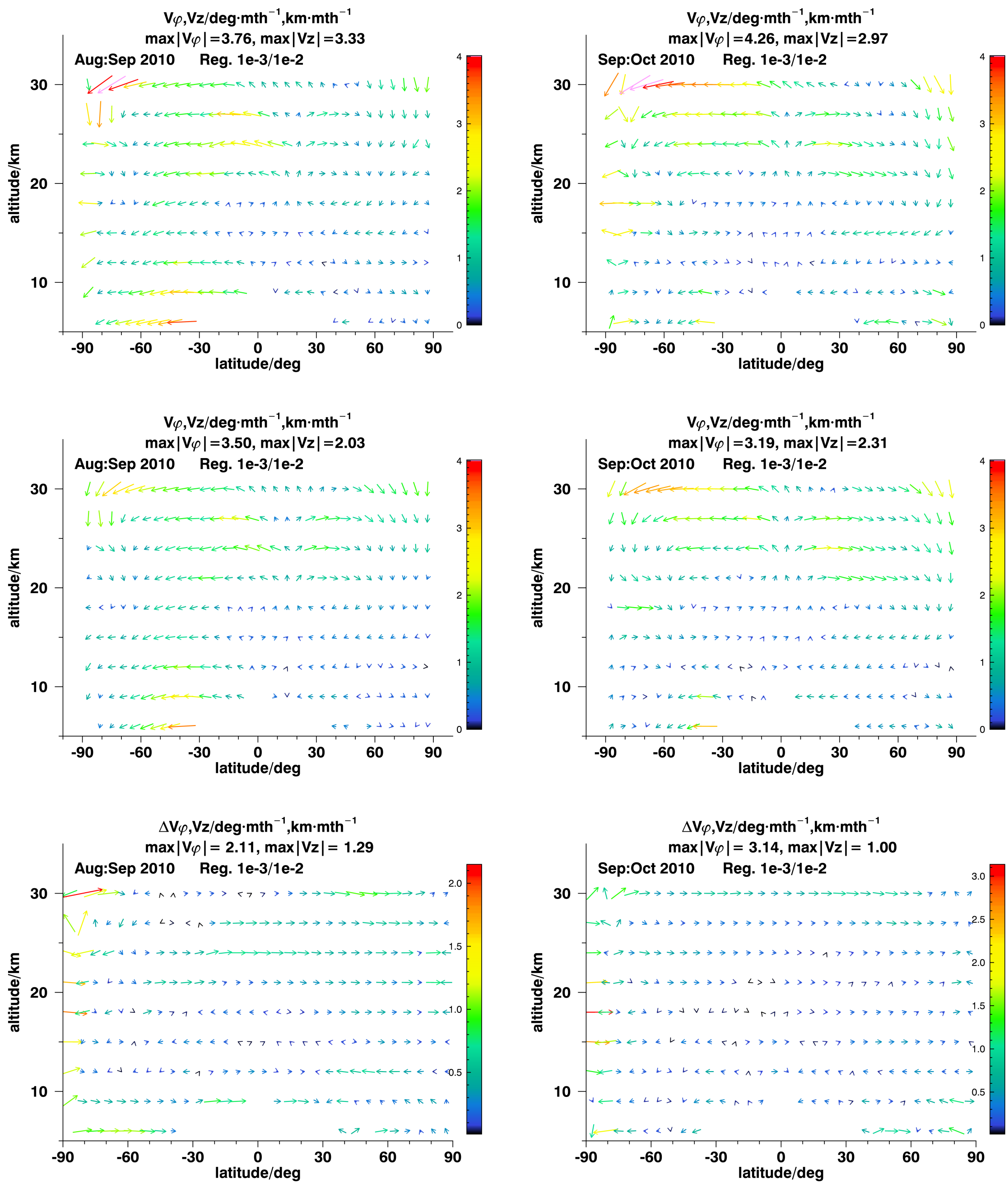

Figure 6. : As for Fig. 4 but with a reduced altitude range for clearer representation of lower altitudes.

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4 The role of the regularization strength

In the previous section, the fact that large velocities are not fully recovered is attributed to the regularization of the inversion. ANCISTRUS uses a Tikhonov (1963) type regularization which leads to the following object function to be minimized:

$$(\boldsymbol{x}-\boldsymbol{F}(\boldsymbol{q};\boldsymbol{x}_0))^T\,\mathbf{S}_{\mathrm{r}}^{-1}\,(\boldsymbol{x}-\boldsymbol{F}(\boldsymbol{q};\boldsymbol{x}_0))+\boldsymbol{q}^T\mathbf{L}_1^T\boldsymbol{\Gamma}\mathbf{L}_1\boldsymbol{q} \tag{1}$$

$(\boldsymbol{x}-\boldsymbol{F}(\boldsymbol{q};\boldsymbol{x}_0))$ is the residual between the measured field $\boldsymbol{x}$ of atmospheric state variables and those predicted using the initial field $\boldsymbol{x}_0$ and an assumed field of velocities $\boldsymbol{q}$. All these fields are expressed as vectors of length m. $\mathbf{S}_{\mathrm{r}}$ is the $m\times m$ covariance matrix characterizing the uncertainties of the residual, under consideration of uncertainties of $\boldsymbol{x}$ and $\boldsymbol{x}_0$. $\mathbf{L}_1^T\boldsymbol{\Gamma}\mathbf{L}_1$ is the $n\times n$ regularization term, where $\mathbf{L}_1$ is a first order difference matrix of dimension $(n-1\times n)$, expressing the vertical and horizontal differences of adjacent values of horizontal and vertical velocities. These velocities are represented by the n-dimensional vector $\boldsymbol{q}$. $\boldsymbol{\Gamma}$ is a diagonal $(n-1)\times(n-1)$ matrix and controls the strength of the regularization and balances the units. The purpose of the regularization term is to prevent horizontal or vertical gradients of horizontal and vertical velocities from becoming unreasonably large, a typical characteristic of instable, oscillating solution of ill-posed inverse problems. It goes without saying that the choice of the entries of $\boldsymbol{\Gamma}$ directly affects the solution. Thus it is in order to test how sensitive the resulting velocity fields are on the choice of $\boldsymbol{\Gamma}$. We use September-October 2010 as a test case.

The model recovery test presented in the previous section relied on regularization strengths of $(c_1\times 1.0\times 10^{-3})^2$ for all entries of $\boldsymbol{\Gamma}$ operating on horizontal velocities and $(c_2\times 1.0\times 10^{-2})^2$ for those operating on vertical velocities. c_1 and c_2 were 7.0×10^4 m^{-1}s and 1.0×10^6 m^{-1}s respectively. In addition, the following pairs of regularization strengths were tested:
$\left((c_1\times 5\times 10^{-3})^2;(c_2\times 5.0\times 10^{-1})^2\right)$,
$\left((c_1\times 1\times 10^{-2})^2;(c_2\times 1.0\times 10^{-1})^2\right)$,
$\left((c_1\times 5\times 10^{-4})^2;(c_2\times 5.0\times 10^{-3})^2\right)$ and
$\left((c_1\times 2\times 10^{-4})^2;(c_2\times 2.0\times 10^{-3})^2\right)$.
Results are presented in Fig. 7.

For the two strongest regularizations the main circulation is qualitatively reproduced but velocities are underestimated by a factor of two to three. Details of the field are not well resolved. With regularization strengths $(c_1\times 1.0\times 10^{-3};\ c_2\times 1.0\times 10^{-}2)$, which is the one usually applied, all patterns are well resolved, and approximate quantitative agreement is found almost everywhere, except for the peak velocities, which are underestimated by several ten percent. With regularization strengths of $(c_1\times 5.0\times 10^{-}4;\ c_2\times 5\times 10^{-3})$ the agreement is even better, but there are many cases for other months where no convergence of the iterative inversion could be obtained. Thus, we consider the nominal regularization strengths as adequate for routine processing. The damping of peak velocities is the price to pay for a robust inversion. With rare cases of non-convergence a good data coverage can be achieved, structures and patterns can safely be recovered, and outside the regions of peak velocities the results are robust even in a quantitative sense.

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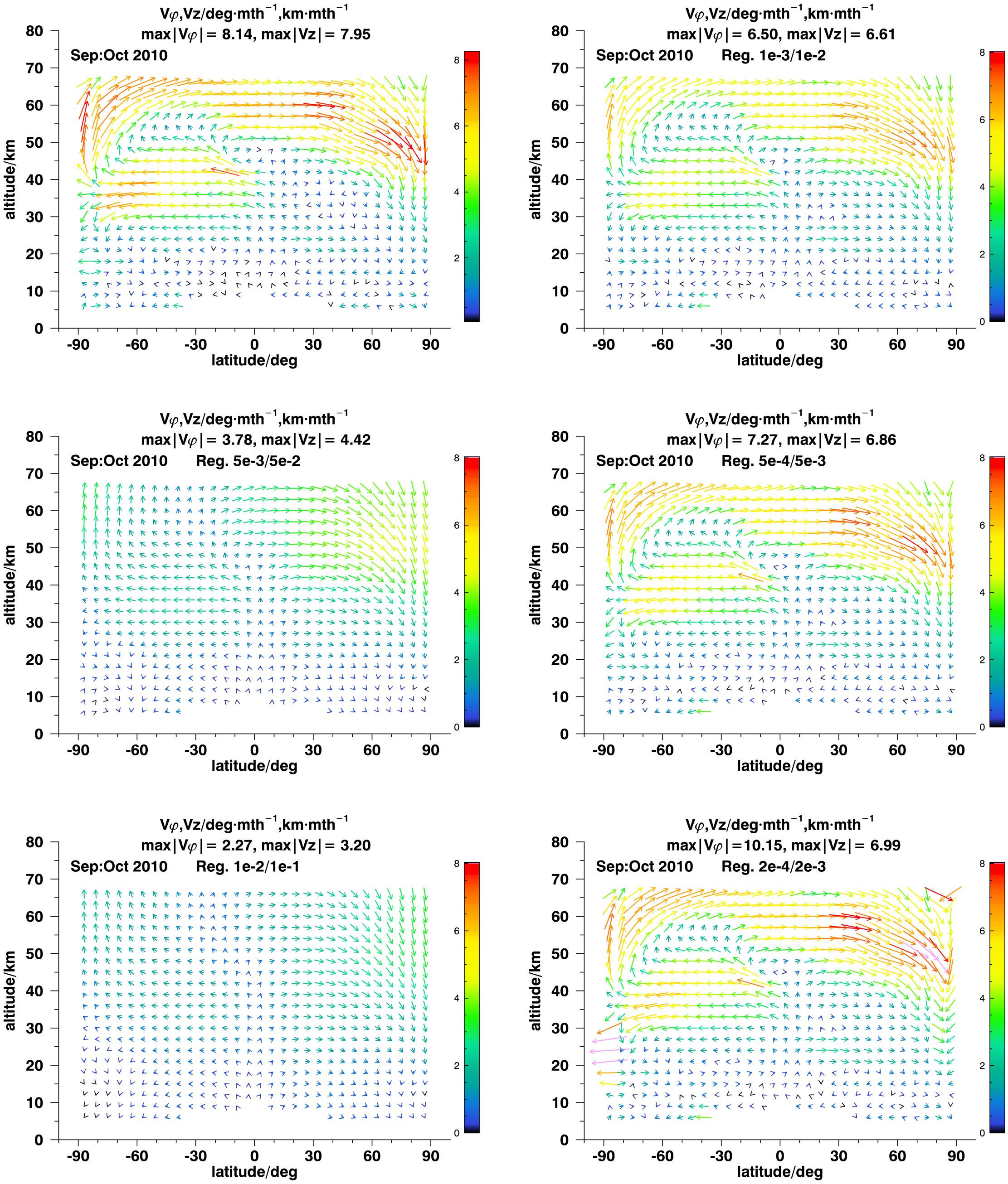

Figure 7. Resulting fields of effective velocity for different regulalization strengths. The upper left panel shows the reference velocity distribution and the upper right panel the model recovery test for the nominal regularization strength of $(c_1 \times 1.0 \times 10^{-3})^2$ for horizontal velocities and $(c_2 \times 1.0 \times 10^{-2})^2$ for vertical velocities. The left middle and lower panels show results for stronger regularization of $((c_1 \times 5.0 \times 10^{-3})^2; (c_2 \times 5.0 \times 10^{-2})^2)$ and $((c_1 \times 1.0 \times 10^{-2})^2; (c_2 \times 1.0 \times 10^{-1})^2)$, respectively. The right middle and lower panels show results for weaker regularization of $((c_1 \times 5.0 \times 10^{-4})^2; (c_2 \times 5.0 \times 10^{-3})^2)$ and $((c_1 \times 2 \times 10^{-4})^2; (c_2 \times 2.0 \times 10^{-3})^2)$, respectively.

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5 Sensitivity tests

For several reasons, ANCISTRUS results are expected to depend on the selection of species used. First, species with different concentration profiles carry information on the circulation at different altitudes. Thus, omitting, e.g., CO and CH_4 and using only species with sizeable concentrations in the lower stratosphere, like CCl_4 or CFC-11, will lead to heavily degraded results in the mesosphere. Second, the more species we have in general, the weaker the effect of regularization will be and thus more information can be retrieved, even if the additional information is fully redundant. Thus, the sensitivity of results with respect to the omission of single species is worthwhile testing. In general, robustness of the retrieval with respect to the omission of a single species is desirable.

The respective test was set up as follows: First an ANCISTRUS run was performed for a complete set of species. Then a series of ANCISTRUS runs was performed, each with one gas omitted, similar as to a jackknife method. The difference of velocities caused by the omission of a candidate species is a measure of the sensitivity of the retrieval to this species. These tests were performed for March–April 2005 (Figs. 8–10) and for September–October 2010 (Figs. 11–13). CFC-11, CFC-12, and HCFC-22 contribute most in the Arctic spring stratosphere, where gradients of regions between old air depleted in these species and young air rich in these species are large (Fig. 8). Conversely, these species contain appreciable information in the Antarctic stratosphere in September–October (Fig. 11). Since mixing ratios of these species are low in the upper stratosphere and above, these species contribute most information below about 40 km. CCl_4 and SF_6 broadly contribute in the same regions as the species discussed before, but their contribution is smaller, because measurement uncertainties are larger for these species and their weight in the inversion is thus lower (Figs. 9 and 12, upper and lower panels). N_2O contributes considerably in the entire altitude range (Figs. 9 and 12, middle panels; note compressed colour scale due to the large amplitude of values). CH_4 and CO provide the bulk of information on the circulation in the upper stratosphere and mesosphere (Figs. 10 and 13, upper and middle panels). However, similar as N_2O, they do also provide a lot of information at lower altitudes, which can hardly be appreciated due to the compressed colour scales of the figures. Also H_2O provides a considerable amount of information (Figs. 10 and 13, lower panels). Its contributions are largest where its gradients are largest, namely in the upper troposphere/lower stratosphere and in the mesosphere.

One might argue that inclusion of species which contribute only little information, such as SF_6 or CCl_4 is useless. Admittedly the information provided by these species is largely redundant with that provided by the other species. However, inclusion of these species reduces the estimated uncertainty of the retrieved effective velocities. Figure 14 shows the estimated standard deviations, representing the uncertainty of the retrieved horizontal and vertical velocities due to the propagated uncertainties of the mixing ratio fields, for an ACISTRUS run without CCl_4 compared to a run where all nine species were included[1]. The estimated uncertainties are reduced by an appreciable amount, mainly in the lower tropical stratosphere.

[1] A similar test, but with an older ANCISTRUS version, has already been performed by Eckert (2018)

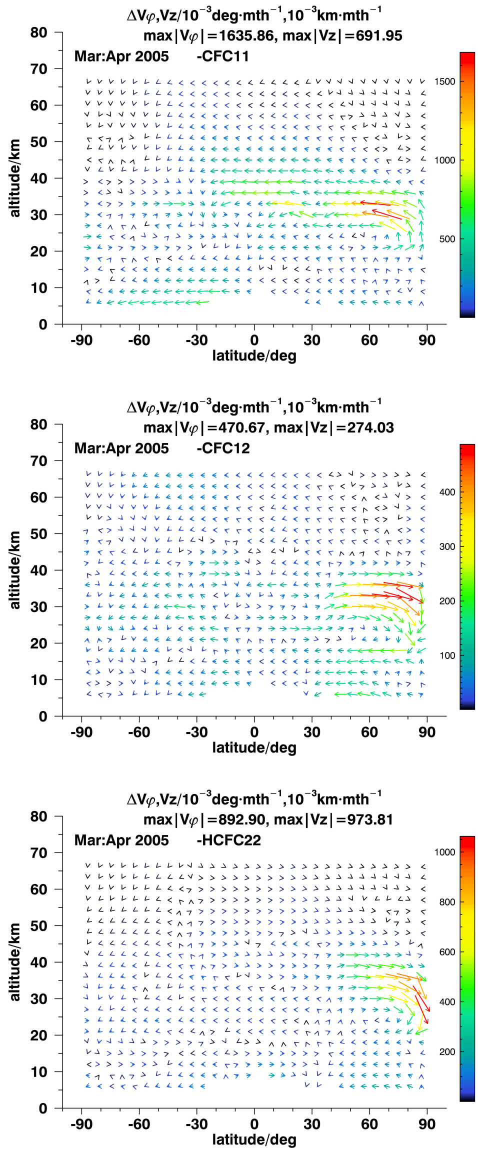

Figure 8. : Differences between ANCISTRUS runs with one species omitted and all nine species included for March–April 2005. The missing species are CFC-11 (top panel), CFC-12 (middle panel), and HCFC-22 (bottom panel). Note the scaling by a factor of 10^{-3}.

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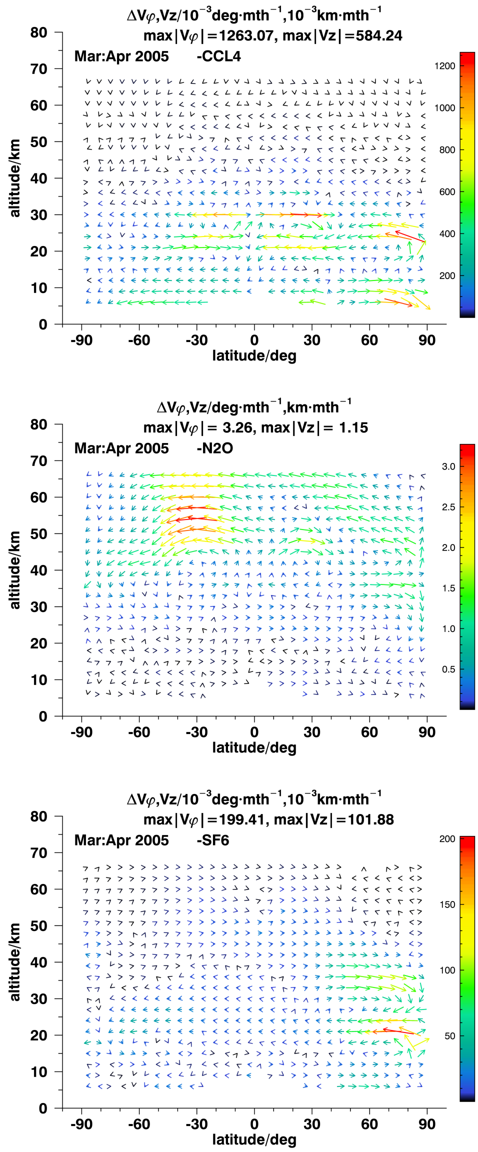

Figure 9. : Differences between ANCISTRUS runs with one species omitted and all nine species included for March–April 2005. The missing species are CCl_4 (top panel), N_2O (middle panel), and SF_6 (bottom panel).

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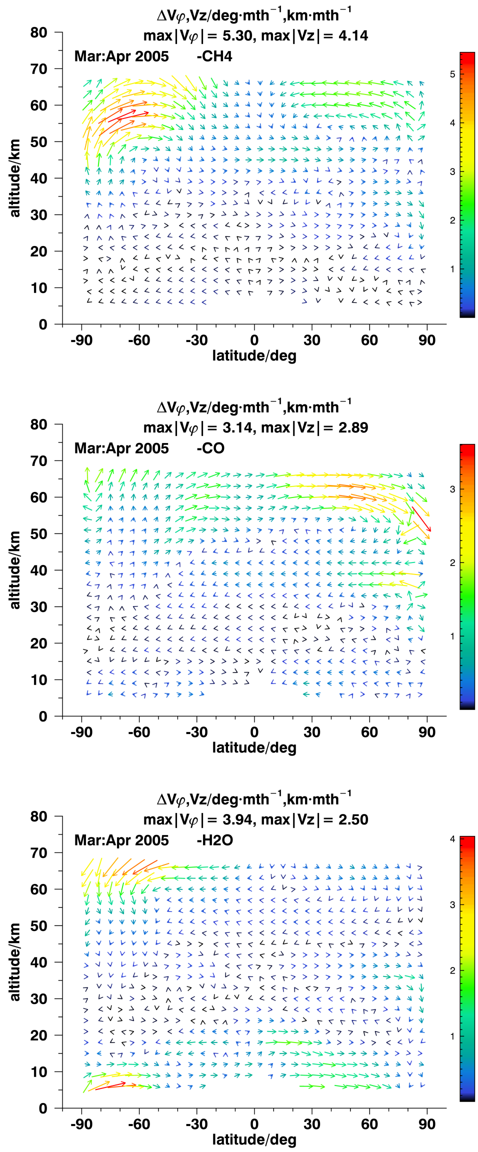

Figure 10. : Differences between ANCISTRUS runs with one species omitted and all nine species included for March–April 2005. The missing species are CH_4 (top panel), CO (middle panel), and H_2O (bottom panel).

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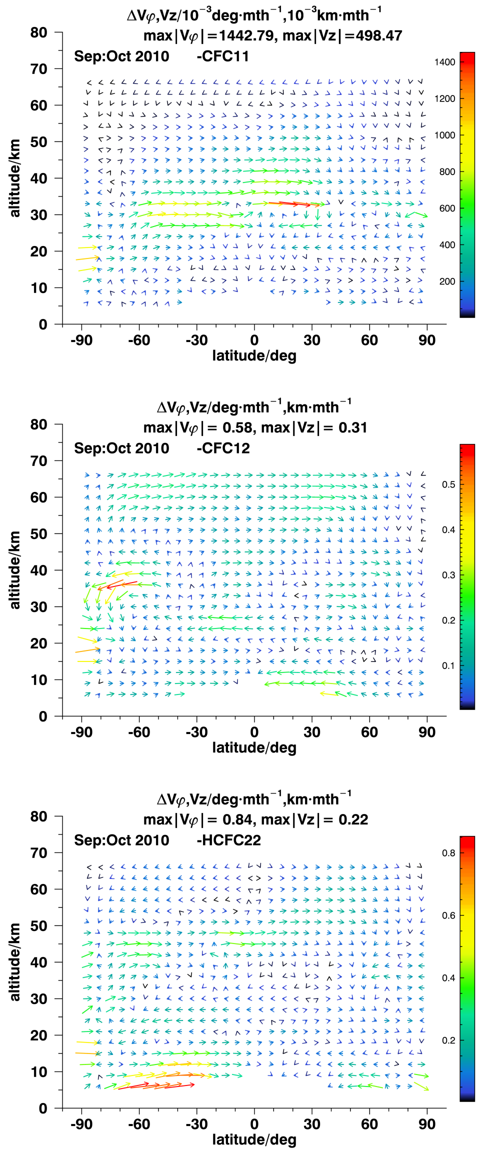

Figure 11. : Differences between ANCISTRUS runs with one species omitted and all nine species included for September–October 2010. The missing species are CFC-11 (top panel), CFC-12 (middle panel), and HCFC-22 (bottom panel).

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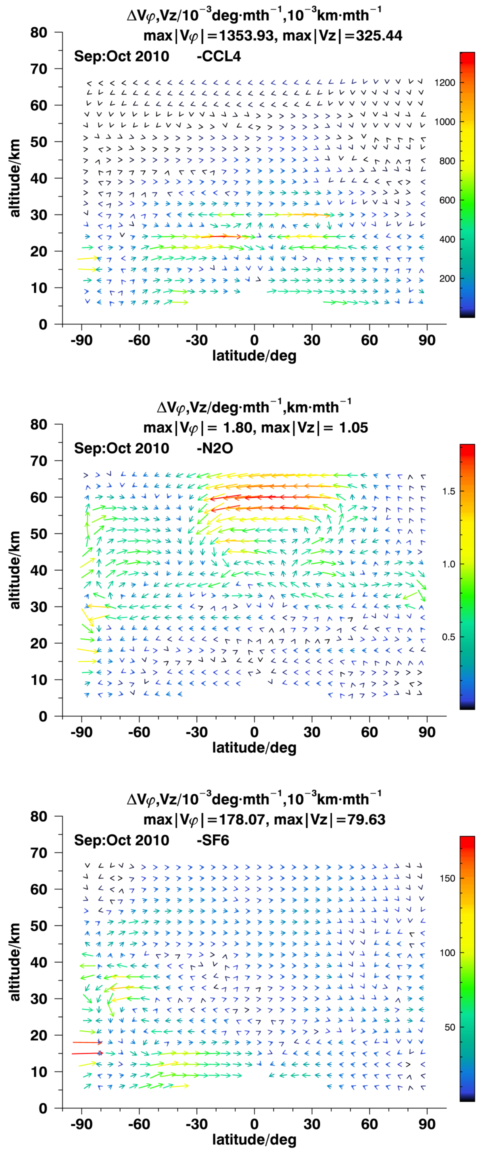

Figure 12. : Differences between ANCISTRUS runs with one species omitted and all nine species included for September–October 2010. The missing species are CCl_4 (top panel), N_2O (middle panel), and SF_6 (bottom panel).

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Atmospheric Chemistry and Physics
Discussions

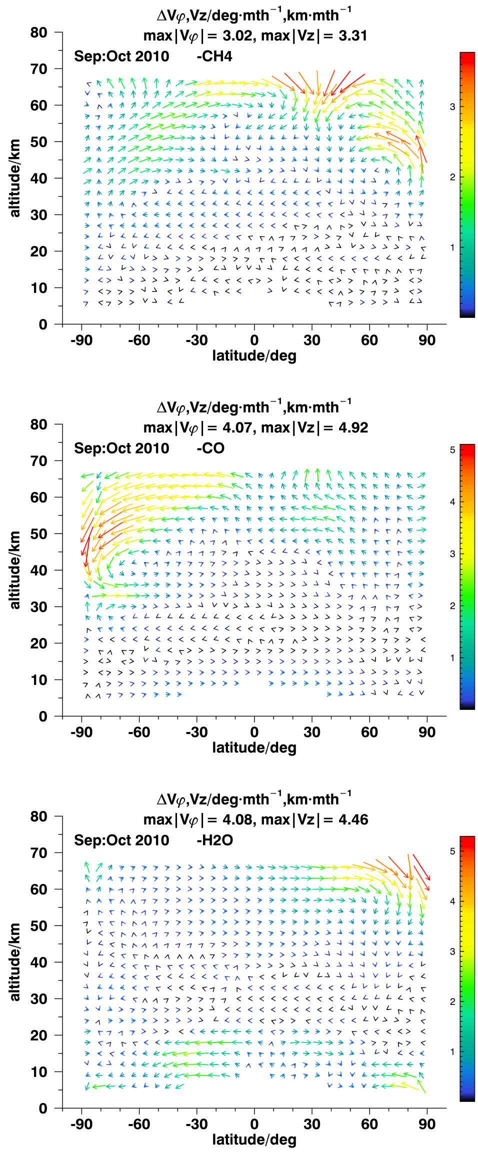

Figure 13. : Differences between ANCISTRUS runs with one species omitted and all nine species included for September–October 2010. The missing species are CH_4 (top panel), CO (middle panel), and H_2O (bottom panel).

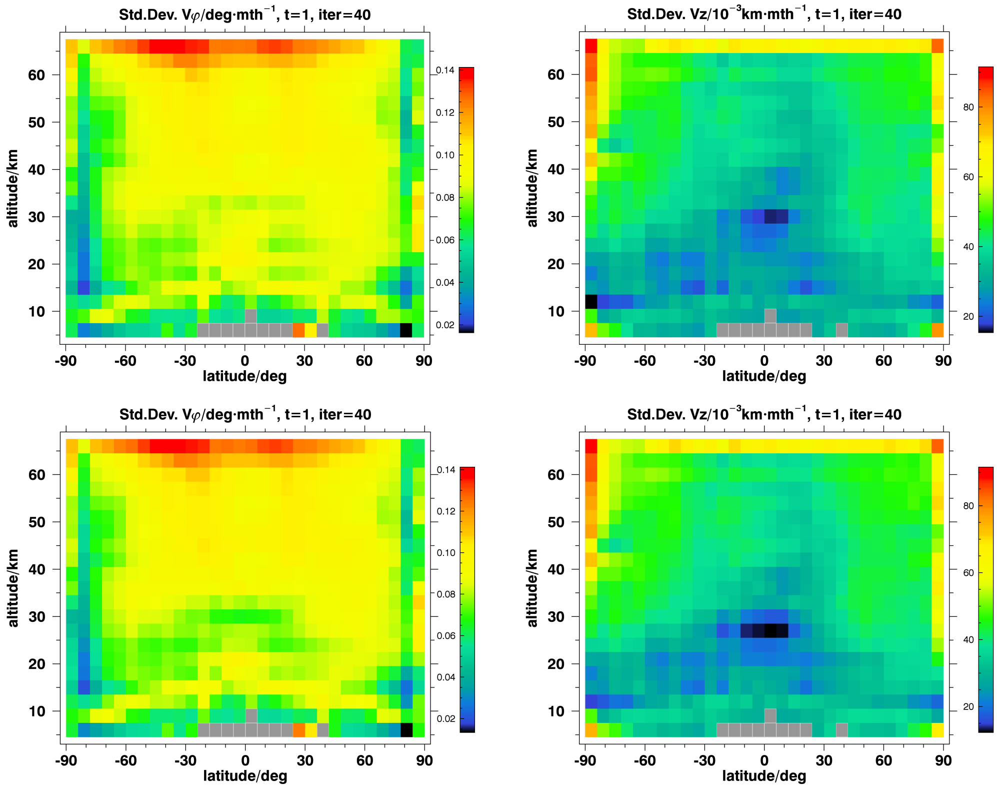

Figure 14. : Estimated standard deviations of horizontal (left panels) and vertical (right panels) effective velocities for ANCISTRUS runs with CCl_4 omitted (upper panels) and all nine species (lower panels) for March–April 2005.

6 Conclusions

Up to about 30 km altitude, ANCISTRUS results have shown to be fairly accurate in a fully quantitative manner. Above, less measurement information is available, and the peak effective velocities deviate from the reference velocities by up to several ten percent. Still structure and patterns are perfectly reproduced and can be considered as robust. Only patterns of very small scales are not resolved. In no case did ANCISTRUS generate artificial structures not present in the reference data. The prevailing underestimation of peak velocities is attributed to the regularization term in the retrieval equation, which pulls values towards zero in the case of insufficient measurement information. The choice of the regularization strength in the ANCISTRUS version tested here was conservative. A rather strong regularization was chosen to avoid ANCISTRUS to produce artificial circulation patterns and to safely achieve convergence of the iteration. According to the terminology of test theory, it had been decided to rather accept type I errors, i.e., to reject a true result, and to safely exclude type II errors, i.e., non-rejection of a false result. The results of this study, however, indicate that there may still be room to fine-tune the regularization in order to better retrieve larger velocities at higher altitudes in a fully quantitative sense. This, however, is deferred to a future

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paper. ANCISTRUS results might also benefit from inductive debiasing. With respect to the scientific analysis of patterns and structures we consider the ANCISTRUS algorithm in its current setup as fit for purpose.

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