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**Impact of vortex
intrusions on ozone
loss estimates**

J.-U. Grooß and R. Müller

The impact of mid-latitude intrusions into the polar vortex on ozone loss estimates

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Abstract

Current stratospheric chemical model simulations underestimate substantially the large ozone loss rates that are derived for the Arctic from ozone sondes for January of some years. Until now, no explanation for this discrepancy has been found. Here, we examine the influence of intrusions of mid-latitude air into the polar vortex on these ozone loss estimates. This study focuses on the winter 1991/92. It is based on simulations performed with the Chemical Lagrangian Model of the Stratosphere (CLaMS). The simulations for January 1992 show that the intrusions induce a reduction of vortex average ozone mixing ratio corresponding to a systematic offset of the ozone loss rate of about 12 ppb per day. Further, the results of the Match method are influenced by the intrusions, since the intruded air masses are deformed and reach dimensions below the Match radius. From our calculations we deduce a systematic offset of the Match ozone loss rate by about 10 ppb/day, which may explain about 28% of the published discrepancy between Match and box model simulations for the winter 1991/92.

1. Introduction

It is difficult to determine the chemical ozone loss in the Arctic stratosphere because chemical ozone loss is masked by dynamic variability caused by reversible vertical and horizontal transport and mixing of air masses. Different methods are known to derive the chemical ozone loss from observations such as a comprehensive set of ozone sonde measurements (Harris et al., 2002). Here we discuss the so-called vortex average method (Knudsen et al., 1998; EU, 2001) and the Match approach (von der Gathen et al., 1995; Rex et al., 1998). Both methods use ozone sonde data together with meteorological analyses and estimates of the diabatic descent to derive chemical ozone loss estimates for the polar vortex. Briefly, the vortex average approach calculates the average of all vortex ozone data on an isentropic surface as a function of time. Using a correction for diabatic descent, the chemical ozone loss is derived. The Match method

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uses pairs of observations in the same air mass at different times, so called matches. These matches are determined by trajectory calculations on the basis of meteorological analyses and estimates of the diabatic descent. A statistical analysis is conducted to deduce the rate of ozone loss in the vortex from such a dataset. Only matches for which the distance between the positions of the air parcel trajectory and the second observation is below the so-called match radius (typically 500 km) contribute to the analysis.

During January in some years, large discrepancies were found between Match and the corresponding simulated ozone depletion rates (Becker et al., 1998, 2000; Kilbane-Dawe et al., 2001; Rex et al., 2002): e.g. in 1992 the Match results for 24 January \pm 7 days yield ozone loss rates of 10.0 ± 1.3 ppb/sunlight hour (54 ± 7 ppb/day) whereas the corresponding box model simulations yield only 3.3 ± 0.2 ppb/sunlight hour (18 ± 1 ppb/day). Becker et al. (1998) further demonstrated that this discrepancy cannot be explained by known model uncertainties. Rex et al. (2002) show that this is the largest discrepancy of all the Match campaigns between 1992 and 2000: to explain the ozone loss rates in January 1992 with standard photochemistry the amount of active chlorine must exceed the maximum available chlorine Cl_y by a factor of 2.5.

The air masses within the polar vortex in early winter are often viewed as well isolated from mid-latitudes. However, this assumption is not true in in all winters at all times. Plumb et al. (1994) show an example of a large-scale intrusion of mid-latitude air masses into the polar vortex in January 1992. Here, we use simulations of the Chemical Lagrangian Model of the Stratosphere (CLaMS) (McKenna et al., 2002a,b) to investigate the impact of such intrusions in January 1992 on ozone loss estimates because for this time both large scale intrusions took place and the largest discrepancy between Match and model was found.

2. Model simulations

The Chemical Lagrangian Model of the Stratosphere (CLaMS) is described in detail by McKenna et al. (2002a,b). The simulation was performed for the 475 K potential temperature level for the time period between 12 January and 4 February 1992. The horizontal resolution is 90 km between 30° and 90° N and 450 km south of 30° N corresponding to approximately 18 000 air parcels. Mixing between air parcels is induced when a critical Lyapunov coefficient λ exceeds the value of 1.5 using a mixing time step of 12 h (see McKenna et al., 2002a; Konopka et al., 2002, for details). Wind and temperature information was taken from ECMWF data with high spatial and temporal resolution ($1.125^\circ \times 1.125^\circ$, 6 h).

For the problem under investigation, a two-dimensional isentropic simulation is justified, because the simulation period is rather short (23 days). To estimate the amount of diabatic descent that the air parcels would have experienced, 16 600 3-D trajectories were calculated (without mixing) for the simulation period. The diabatic descent was calculated by a radiation scheme (Morcrette, 1991; Zhong and Haigh, 1995) using a 10-year climatology of HALOE ozone data as input (Grooß et al., manuscript in preparation). For this estimate, temperature and wind data were taken from the UKMO analyses that cover the complete stratosphere up to 0.3 hPa. The derived amount of descent for air parcels in the vortex is $21.5 \pm 2.4 \text{ K}(1\sigma)$ in 23 days which is less than 1 km. In the two-dimensional isentropic simulation we do not simulate the exact positions of the air parcels correctly because of the neglect of diabatic descent. Thus, an exact sampling of the match trajectories within the model domain as by Kilbane-Dawe et al. (2001) can not be performed here. However, the simulation still demonstrates the effect of the vortex intrusions very clearly.

To derive an initial ozone field at 475 K for the CLaMS simulation, we used version 5 data from the Microwave Limb Sounder (MLS) on board the Upper Atmosphere Research Satellite (UARS) (Barath et al., 1993) between 8 and 13 January. Using backward and forward trajectories, the locations of the observations were mapped to

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the assimilation time (12 January 1992, 12:00 UT). These data were then combined on a regular grid with 1° latitude \times 3° longitude spacing. Each grid point summarizes all data points within a distance less than 220 km using a cosine-square weighting with 110 km distance half-width. Figure 1 shows the derived ozone mixing ratio. The other species are initialized using the Mainz photochemical 2-D model (Gidel et al., 1983; Grooß, 1996) mapped onto equivalent latitude.

Figure 2 shows an example of the simulated ozone mixing ratio for 22 and 27 January on a stereographic projection. For illustration, Fig. 2 also shows the location of two Match trajectories with over 0.5 ppm diagnosed ozone loss and over 50 sunlight hours (violet symbols). On 22 January, a largely extended area of air masses outside the vortex between Scandinavia and Greenland with ozone mixing ratios below about 2.5 ppmv (blue colors) is visible. These air masses are drawn into the vortex as also simulated by Plumb et al. (1994). They can be seen as green colors over Newfoundland and eastward of Greenland on 27 January. The simulations show that with time the intruded air masses are deformed and elongated. In this context it is important that the horizontal scale of intruded air masses shrinks within one week below about 500 km which is the maximum allowed Match radius. Figure 2 also shows the individual Match radii of selected Match trajectories (≈ 300 km) as violet circles. On 27 January, a second tongue of air around 75° N, 180° E starts to be drawn into the vortex.

Figure 3 shows an enlargement of Fig. 2 over Scandinavia on 27 January around one Match trajectory location. This is within 24 h before it matches the second ozone sonde. The ozone variance within the match radius – 293 km for this trajectory – is evident. The impact of the variability of ozone mixing ratios within the Match radius on the deduced ozone loss rates is discussed below.

To be comparable with the Match analyses, we calculate the vortex average ozone mixing ratio from the model results using exactly the definition of the vortex edge that is used in the Match analysis Rex et al. (1998), i.e. the 36 PVU line from ECMWF data on the 475 K level. Figure 4a shows the ozone mixing ratio averaged over the vortex area defined in this way for the time of this simulation as a blue line. The red line shows the

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vortex average of a passive tracer that was initialized identically to the ozone mixing ratio. As the tracer is not influenced by chemistry, its vortex average should be constant with time. However, from this analysis it is evident that the major fraction of the change in the vortex average ozone mixing ratio is due to the dynamically caused intrusions into the vortex but not due to chemical ozone depletion. The change of the dynamical ozone tracer in this simulation is a measure for the bias in derived chemical ozone depletion. To derive the chemical ozone loss, one should correct for this dynamical effect. In the following, only the simulated passive ozone tracer will be discussed.

In addition to the regular CLaMS simulation described above we performed a “virtual Match” calculation in order to quantify the expected impact of the vortex intrusions on the Match results. Figure 5 illustrates this method: At each CLaMS air parcel within the polar vortex on one day a trajectory (green line) was started to predict the location of the air parcel on a later day (large green circle). For each of the calculated locations, 8 new points were determined with the distance of a given match radius equally distributed in all directions (red circles). If a new point is still within the vortex, it was considered a Match with the first air parcel. The corresponding passive ozone tracer mixing ratios were then determined from the CLaMS simulation using the data from the closest CLaMS point (blue circles) to each new point. The average vortex ozone depletion rate was then determined from these Matches exactly as in the Match analyses.

3. Discussion

From Figs. 2 and 3 it is evident that the ozone mixing ratios in the polar vortex are not necessarily distributed uniformly on a potential temperature surface. Ozone variability within the polar vortex exists because of various reasons. In spring 1997, for example, a particularly pronounced inhomogeneity of ozone depletion within the polar vortex was both observed and simulated (Müller et al., 1997; Schulz et al., 2000; McKenna et al., 2002b; Tilmes et al., 2002). Also inhomogeneous diabatic descent rates and

intrusions at earlier times that have not yet been completely mixed with vortex air are possible reasons for variability of ozone inside the vortex on an isentropic surface.

Principally ozone variability should not significantly influence estimates of vortex averaged ozone loss in a confined vortex except that it increases the statistical error of the result. However, intrusions of a significant amount of air from mid-latitudes into the vortex cause a systematic offset of vortex-averaged ozone mixing ratios. Since the vortex-average method depends on the assumption that the vortex air masses are well isolated from mid-latitudes, it should lead to a bias in the derived ozone loss rate during a time period with vortex intrusions. In mid-January 1992, the ozone mixing ratios below potential temperature levels of ≈ 500 K are lower outside the vortex than inside and vice versa above. Thus, the intrusions into the polar vortex would lead to an overestimate of chemical ozone depletion detected by this method at the 475 K level that is discussed here. Some studies employing the vortex-average method try to correct for cross vortex edge transport by trajectory simulations, e.g. Knudsen et al. (1998) find no significant effect in the year 1997. However, that is clearly not true for other winters, especially for the winter 1991/92 discussed here.

From the time derivative of the vortex average passive ozone tracer mixing ratio (Fig. 4, bottom panel) the bias of derived ozone depletion rates due to vortex intrusions can be estimated. It shows the simulated vortex-averaged depletion rate for ozone (red line) and the passive ozone tracer (blue line) for ± 2.5 days, i.e. for intervals of 5 day length. (We chose this length because it is comparable to the length of the match trajectories, since e.g. the trajectories that contribute to the data point for 24 January have an average length of 4.5 days.) The red line corresponds to the derived ozone depletion rate due to the intrusions only, while the blue line also includes the simulated chemical ozone loss. Around 24 January, the derived dynamical bias is about 11 to 14 ppb/day.

The bias derived from vortex-averaged ozone tracer loss rate depends also on the definition of the vortex edge. If the vortex edge is moved poleward by using a greater PV value, the derived ozone depletion rate is lower and vice versa (e.g. ≈ 8 ppb/day for

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$PV^{\text{edge}} = 40$ PVU and ≈ 24 ppb/day for $PV^{\text{edge}} = 30$ PVU on 24 January). However, the general shape of Fig. 4b does not change significantly.

The Match method is a more sophisticated approach than the vortex average method. It aims at avoiding such errors as discussed above since individual air parcels are examined that have been probed twice by an ozone sonde inside the vortex. It is therefore unlikely that earlier vortex observations match with air masses that have crossed the vortex edge during the time of the Match trajectory. However, there are displacements between the probed air mass and the location of the matching air mass given by the match radius and furthermore by uncertainties induced by the trajectory calculation. The Match trajectory errors due to uncertainties in the wind data can not be examined by this simulation since both the simulation and the Match trajectory calculation are based on the same meteorological analyses (ECMWF).

Figures 2 and 3 show that in 1992 the large-scale intrusions caused filaments with a width below the Match radius (Match resolution) within about one week. Therefore, the systematic offset described above should also influence the Match results in a similar manner. The results of the Match method can only account for vortex intrusions as long as the horizontal scale of the intrusions is much greater than the Match radius. The actual bias of the ozone depletion rate derived by the Match method depends further on the sampling of these filaments by the Match trajectories. If the matches are distributed equally over the vortex domain, the estimate of a systematic offset of vortex average ozone loss due to intrusions such as those discussed in this study should appear as a systematic error of the Match results as well.

In order to quantify the expected impact of the vortex intrusions on the Match results we performed an additional “virtual Match” calculation as described above. The trajectory length was chosen to be 4 days from 22 January to 26 January. The chosen Match radius was 300 km. For this case 3717 trajectories were started within the vortex of which 2978 stayed within the vortex over the 4 day period resulting in 21 768 virtual match events. Here, the dynamical bias was also determined from the passive ozone tracer from which the ozone depletion rate for the passive ozone tracer was derived

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exactly as in the Match analysis. The resulting dynamical bias was 10.0 ± 0.4 ppb/day (1.94 ± 0.07 ppb per sunlight hour) which is 28% of the discrepancy found by Becker et al. (1998). This result does not seem to depend strongly on the chosen Match radius, e.g. for a Match radius of 450 km, the ozone depletion rate derived from the passive ozone tracer is 11.7 ± 0.4 ppb/day.

In the Match analysis for 24 January 1992, there are only 19 Match events. With this simulation we also tested what statistical error one should expect from this number of events. This was done by randomly choosing a subset of 20 Matches out of the 21 768 virtual Matches which was repeated 200 000 times. From each subset of 20 Matches the ozone depletion rate is evaluated exactly as in the regular Match analysis. The standard deviation of the so derived results is 2.9 ppb per sunlight hour which is a factor 2.2 greater than the derived Match error bar for 24 January. Figure 6 shows a histogram of the derived ozone loss rate bias for the subsets of 20 Matches. For 7.8% of the Match subsets, the deduced ozone depletion rate is equal or even larger than the published discrepancy (6.7 ppb per sunlight hour). However, it seems unlikely that an unfavorable sampling of the Match events causes the complete January ozone loss discrepancy because it was found similarly for other years as well (Becker et al., 2000; Kilbane-Dawe et al., 2001; Rex et al., 2002).

4. Conclusions

We have shown that intrusions of mid-latitude air into the polar vortex introduce a systematic offset of vortex average ozone mixing ratios. Estimates of ozone loss rates are influenced by this effect. If the intrusions reach horizontal dimensions below the Match resolution (Match radius) this systematic offset influences also the Match analyses. This effect does not solve the published discrepancy between Match deduced ozone loss rates and those derived from simulations but it may explain about 28% of the discrepancy that was found for January 1992 (Becker et al., 1998). Therefore the estimates of chemical ozone depletion derived from ozone sonde data need to be cor-

rected for this effect. Further it was shown that the error of the Match results derived from only 20 match events in an unhomogeneous ozone distribution caused by the intrusions in January 1992 must be a factor 2.2 greater. Although the intrusions of mid-latitude air into the polar vortex do not explain the discrepancy completely it is a possible reason why for January 1992 the discrepancy is the greatest so far (Rex et al., 2002).

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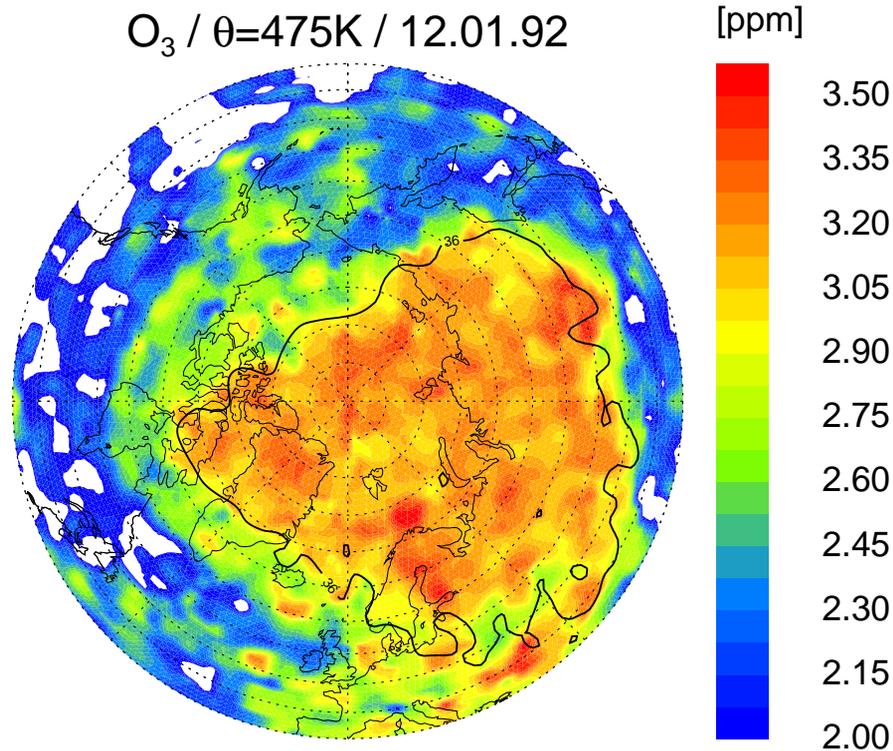


Fig. 1. Initialization for ozone on the 475 K level derived from MLS data. White areas indicate mixing ratios below 2.0 ppm. Also plotted is the PV contour of 36 PVU that is employed here as the definition of the vortex edge.

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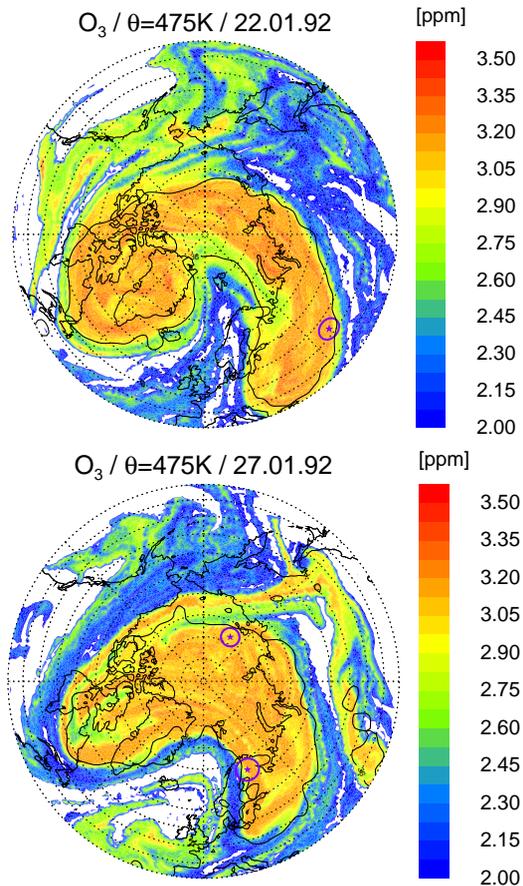


Fig. 2. Simulated ozone mixing ratio for 22 January (top) and 27 January (bottom). The violet stars and circles show the location and Match radius of two individual Match trajectories. The black contour corresponds to the 36 PVU line which is used here as the definition of the vortex edge. White areas indicate ozone mixing ratios below 2 ppm.

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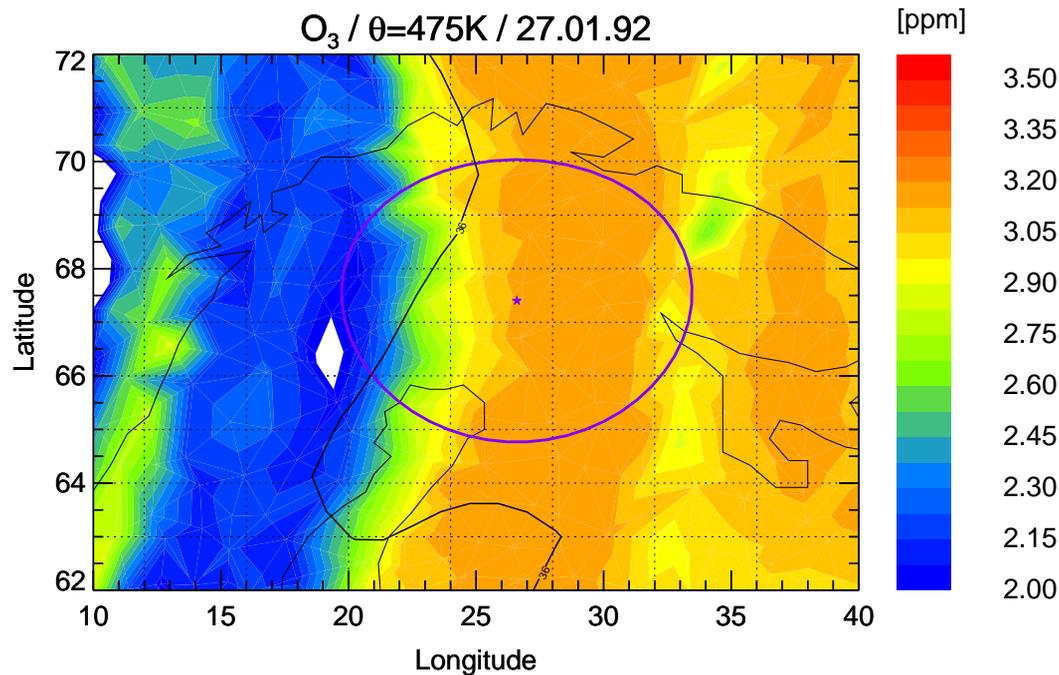


Fig. 3. Enlargement of Fig. 2, bottom panel in the vicinity one Match trajectory location.

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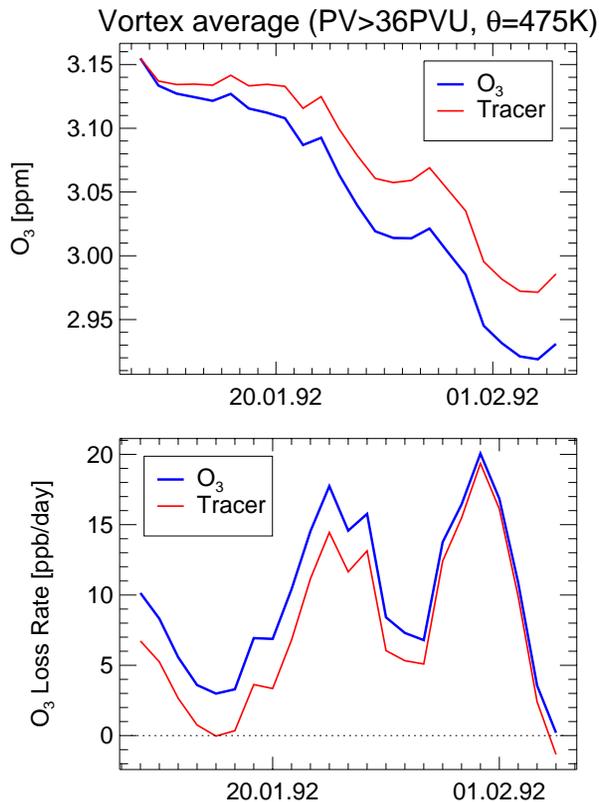


Fig. 4. Vortex average of the simulations. The top panel shows the vortex average ozone mixing ratio (blue line) and the average passively advected tracer that was initialized identically as ozone (red line). The bottom panel shows the time derivative of the top panel, i.e. the ozone (or tracer) change per day for ± 2.5 day intervals.

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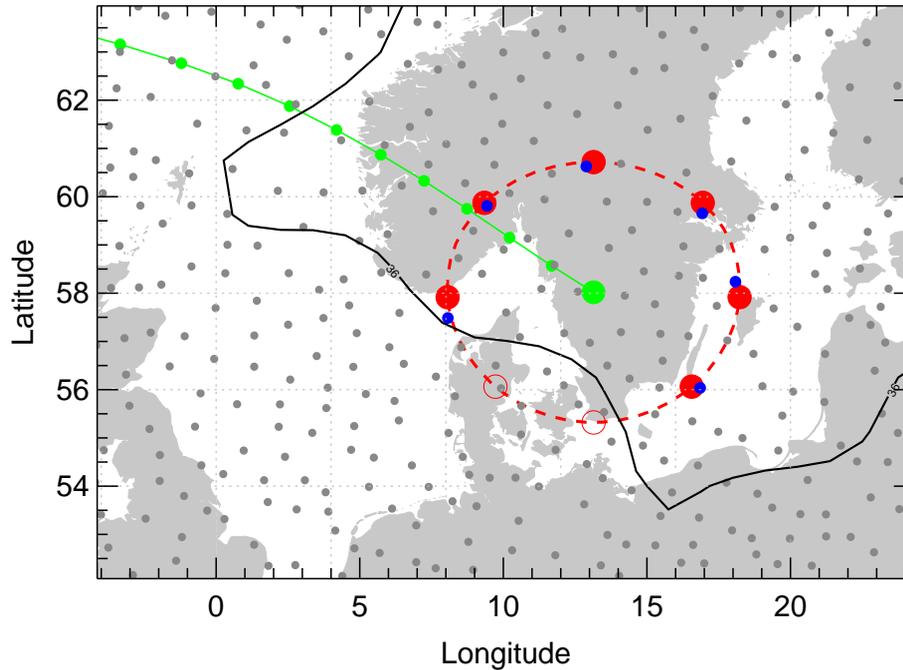


Fig. 5. Sketch of the “virtual Match” calculation. The green line corresponds to one example trajectory ending at the large green circle. The Match radius here is 300 km indicated by the red circle. 8 new locations are marked by the red circles for which only those inside the vortex (filled circles) are considered. The vortex edge is plotted as a thick black line. Grey circles correspond to the individual CLaMS air parcel locations and those chosen for the Match are marked blue.

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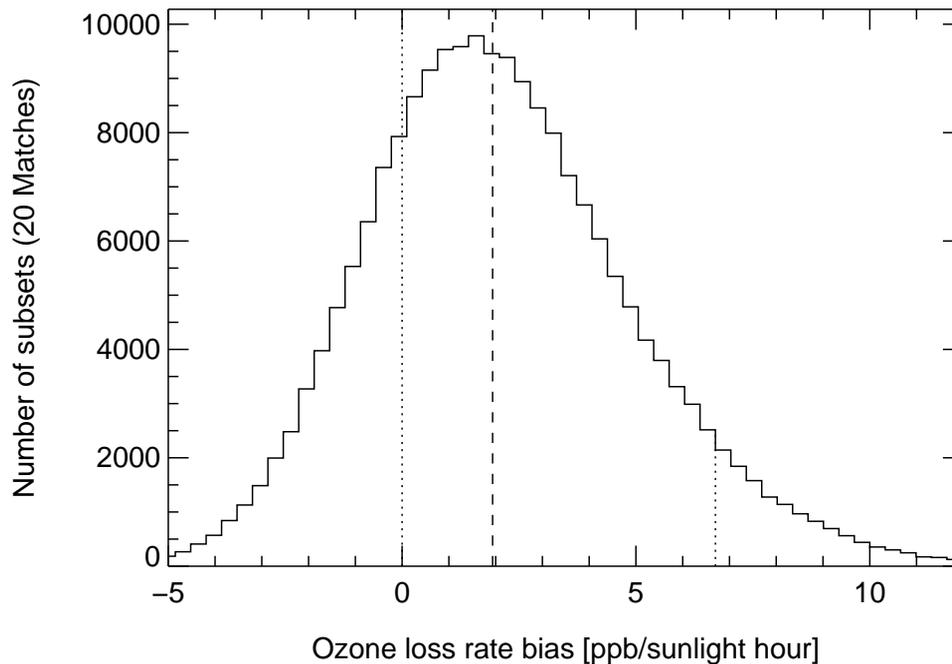


Fig. 6. Histogram of the derived ozone loss rate bias for 200000 subsets of 20 out of 21 768 virtual matches. The solid line shows the ozone loss rate bias derived from the passive ozone tracer for all virtual matches. The right dotted line shows the discrepancy between simulation and Match after Becker et al. (1998). 7.8% of the subsets have equal or larger values than this discrepancy.