Accuracy of trajectories as determined from the conservation of meteorological tracers

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SUMMARY

Dynamical structures as well as transport processes are often investigated using trajectories. Several alternative techniques are currently in use to calculate trajectories, which may produce significantly different results. In this study, three-dimensional, isentropic, isobaric and isoeta (terrain-following coordinate surfaces) trajectories are calculated. In the case of the isentropic trajectories, both the kinematic and the dynamic calculation method are applied.

Using a tracer that is conserved along the real three-dimensional trajectories, it is possible to determine which of these trajectories are the most accurate. Here, conservative meteorological quantities, namely potential vorticity, specific humidity and potential temperature, are used. As these tracers are conserved only in the absence of diabatic processes, regions of the atmosphere where these processes are important, i.e. the boundary layer and moist regions, are excluded. Tracer conservation along the different trajectories is studied to find the most accurate trajectory type.

It is found that three-dimensional trajectories are the most accurate ones, and kinematic isentropic trajectories, affected more by dynamical inconsistencies between meteorological fields, are the second best in the troposphere. In the stratosphere, three-dimensional and isentropic trajectories may be of similar accuracy. Isobaric and isoeta trajectories are much less accurate, both in the troposphere and in the stratosphere. Dynamic trajectories tend to perform unrealistic inertial oscillations and thus give clearly worse results than any of the kinematic trajectories.

Since there exists no direct relationship between the average errors in tracer conservation and average spatial position errors of the trajectories, a transformation of the tracer conservation errors into spatial position errors is difficult.

KEYWORDS: Potential vorticity  Tracers  Trajectories

1. INTRODUCTION

In synoptic meteorology, calculated trajectories are used to explore dynamical processes of the atmosphere (Steinacker 1984), whereas in the environmental sciences they serve the investigation of the transport of air pollutants (Pack et al. 1978; Miller 1987; Stohl 1996a,b). An overview of the calculation, accuracy and applications of trajectories was recently prepared by Stohl (1998). Numerous methods for trajectory calculation have been developed, but a rigorous comparison of the accuracy of different trajectory types is still missing.

The calculation of trajectories is subject to a variety of error sources. Trajectory errors are caused by truncation errors (Walmseley and Mailhot 1983; Seibert 1993), interpolation errors (Kuo et al. 1985; Rolph and Draxler 1990; Doty and Perkey 1993; Stohl et al. 1995; Scheele et al. 1996), inaccurate knowledge of the starting position (Merrill et al. 1985), and analysis or forecast errors in the underlying wind fields (Kahl and Samson 1986; Maryon and Heasman 1988; Kahl et al. 1989; Pickering et al. 1994; Stunder 1996). Investigations and assessments of these errors were presented in the cited literature.

Substantial trajectory errors are also related to different assumptions regarding the vertical wind velocity $w$. In contrast to the horizontal wind, there are no routine observations of $w$, and fields of $w$ are therefore a sole product of meteorological models, e.g. numerical weather-prediction models. Therefore, $w$ is less accurate than analysed horizontal wind.
components. Sardeshmukh and Liebmann (1993) compared circulation analyses of the European Centre for Medium-Range Weather Forecasts (ECMWF) and the US National Meteorological Center for the tropics (30°S to 30°N). They found a signal-to-noise ratio of the divergence of the horizontal wind at 200 hPa of only 2.1. As $w$ is balanced by the vertically integrated horizontal wind divergence, this result underlines the large uncertainty in $w$ at low latitudes. One reason for this uncertainty is the difficulty in the parametrization of cumulus convection which is also of significance at higher latitudes during summer. In addition, Stohl et al. (1995) found that because of the high-frequency variability of $w$, its interpolation produces larger errors than the interpolation of the horizontal wind.

For trajectory calculations, vertical motions can be either neglected (isobaric or terrain-following iseta trajectories), assumed to be adiabatic (isentropic trajectories), or explicitly accounted for (three-dimensional trajectories). Although the third approach is theoretically most sensible, for the reasons discussed above, it is not clear a priori that it really yields the most accurate trajectories. Assuming isentropic flow, it is possible to compute either kinematic (Petterssen 1940) or dynamic trajectories (Danielsen 1961; Petersen and Uccellini 1979; Merrill et al. 1986). Average deviations between different types of trajectories were found by Kuo et al. (1985) and Stohl et al. (1995) to be typically 10 to 30% of the travel distance, but the authors of both studies had no means of finding out which trajectories were actually most accurate.

A possible way of identifying the most accurate type is to compare computed trajectories with the ‘true’ trajectory. The obvious difficulty is to determine this ‘true’ trajectory which requires an air parcel to be tagged by a tracer that is conserved along its trajectory. Tracers of opportunity like Saharan dust (Reiff et al. 1986; Martin et al. 1990), smoke from the Kuwait oil fires during the Gulf war (McQueen and Draxler 1994), non-reactive gases, and radioactive emissions from Chernobyl (Klug 1992) have been used, but all these studies suffered from inaccurate knowledge of the source position, strength and/or release time of the tracer. Balloons (Reisinger and Mueller 1983; Stocker et al. 1990; Kahl et al. 1991; Knudsen and Carver 1994; Draxler 1996; Knudsen et al. 1996; Baumann and Stohl 1997; Stohl et al. 1997) were also used for trajectory validation, but they tend to follow pressure surfaces (constant-level balloons) or actively change height (manned gas balloons and hot-air balloons), whereas real air motions are three-dimensional.

Tracer experiments with controlled releases of inert gases allowed detailed trajectory comparisons (Haagenson et al. 1987; Haagenson et al. 1990; Draxler 1991), but such experiments are expensive and thus only a few cases of long-range transport were studied. Moreover, tracer gases are usually released in the boundary layer, where turbulence complicates their dispersion. Single trajectories are hardly representative of tracer transport under these circumstances, although Stohl and Wotawa (1995) made an attempt to meet this demand by constructing a special boundary-layer trajectory type. Lagrangian particle dispersion models (LPDM) have been developed to simulate transports in the boundary layer by computing a multitude of randomly disturbed trajectories. Tracer experiments are ideally suited to validating LPDMs. Fast and Berkowitz (1997) compared forward particle trajectories computed with an LPDM with mean-wind backward trajectories from the ending points of the particle trajectories. They found large errors of the standard backward trajectories in tracing back the particle’s path, emphasizing that the complexities of dispersion in the boundary layer cannot adequately be described by single trajectories.

An LPDM that is partly based on the trajectory model used in this study was recently validated with data from several large-scale tracer experiments (Stohl et al. 1998). However, the performance of particle models suffers not only from inaccuracies in the mean-wind trajectories, but is also influenced by boundary-layer parameters (surface sensible-heat flux, mixing height, etc.) and the parametrization of the turbulent wind components. Unfortu-
nately, trajectory errors cannot easily be separated from these other influences. Therefore, tracer experiments are also not ideally suited to trajectory validation.

The purpose of this paper is to use three routinely available conservative meteorological quantities, isentropic potential vorticity (PV), potential temperature ($\Theta$) and specific humidity ($q$), to tag air parcels, and to investigate how well these quantities are conserved along six different types of trajectories. Arzt et al. (1985) and Jäger (1992) used PV to study trajectories in individual flow situations, but to our knowledge PV has not yet been used to assess the accuracy of a large set of trajectories yielding statistically meaningful results, and to compare the results obtained with different trajectory types. All three tracers have the disadvantage of not being conserved under all meteorological conditions, but the advantage that they can be calculated along with the trajectories from meteorological analyses, allowing a large data set to be used.

The paper is organized in five sections. Section 2 gives a description of the trajectory model and the types of trajectories that were used. In section 3, the statistical measures applied to describe tracer conservation errors are presented. The results are presented in section 4 and conclusions in section 5.

2. METHODS OF TRAJECTORY CALCULATION

Trajectories are computed with the FLEXTRA model*. A detailed description of this model is given in Stohl et al. (1995), and validations have also been presented by Baumann and Stohl (1997) and Stohl et al. (1997). With FLEXTRA it is possible to compute several types of kinematic trajectories. In this study, constant model level (iseta), isobaric, isentropic and fully three-dimensional (3-d) trajectories are used. The trajectory equation

$$\frac{dX}{dt} = v\{X(t)\}, \tag{1}$$

with $t$ being time, $X$ the position vector, and $v$ the wind vector, is integrated using the iterative scheme after Petterssen (1940)

$$X(t_t) \approx X(t_0) + \frac{\Delta t}{2} \left[ X(t_0) + \dot{X}(t_t) \right]. \tag{2}$$

The integration time-step $\Delta t = t_t - t_0$ is flexible and must fulfill the Courant–Friedrichs–Lewy criterion $C < 1$ with $C = v_t \Delta t \Delta x_t^{-1}$, where $\Delta x_t$ are the grid distances and $v_t$ are the wind components.

For this study, routines to compute dynamic trajectories on isentropic levels were added to the kinematic trajectory model. Dynamic trajectories make use of velocity- and mass-field information and of dynamic equations linking the two. The method of Steinacker (1984) which is based on the integration of the equation of motion for inviscid, adiabatic flow in isentropic coordinates (Petersen and Uccellini 1979) is used in this paper. This equation reads

$$\frac{dv_h}{dt} + \nabla_\Theta M + f{k \times v_h} = 0, \tag{3}$$

where $v_h$ is the horizontal wind vector, $k$ is the unit vector in the vertical direction, $\nabla_\Theta$ is the horizontal gradient on isentropic surfaces, $M = c_p T + gz$ is the Montgomery potential, with $c_p$ being the heat capacity of air at constant pressure, $T$ temperature and $gz$

* The FLEXTRA model source code and a description are available via the internet from http://www.forst.uni-muenchen.de/LST/METEOR/stohl/flextra.html.
geopotential, and $f$ is the Coriolis parameter. Integrating Eq. (3) over the time interval $\Delta t$ and approximating $\bar{v}_h \approx \{v_h(t_0) + v_h(t_1)\} / 2$ gives

$$
\bar{v}_h \approx \left(1 - f \frac{\Delta t}{2} \mathbf{k} \times \right) \left(v_h(t_0) - \frac{\nabla \phi M}{2} \frac{\Delta t}{2} \right) \\
1 + f^2 \frac{(\Delta t)^2}{4}
$$

To compute $\nabla \phi M = \{\nabla \phi M(t_0) + \nabla \phi M(t_1)\} / 2$, $\nabla \phi M$ must be evaluated at times $t_0$ and $t_1$ along the trajectory, which requires an iterative solution of Eq. (4). At the start of a trajectory, the scheme is initialized with the analysed wind. Hereafter, this trajectory type will be referred to as purely dynamic.

Steinacker (1984) found that the resultant trajectories are extremely sensitive to the initial values of wind speed and direction. Petersen and Uccellini (1979) showed that unbalanced ageostrophic components of the initial wind or errors in the Montgomery potential lead to inertial oscillations of the dynamic trajectories. For the special case of a spatially and temporally constant geostrophic wind, Eq. (3) reduces to

$$
\frac{dv_a}{dt} = f v_a \times \mathbf{k},
$$

where $v_a$ is the ageostrophic wind velocity (Jäger 1992). According to Eq. (5), $v_a$ oscillates with a period of

$$
\tau(\varphi) = \frac{12 h}{\sin \varphi},
$$

where $\varphi$ is the geographical latitude.

Jäger (1992) suggested blending the dynamic trajectory wind with the analysed wind at every computational time-step to avoid unrealistic meandering of the purely dynamic trajectory. In this study, the weight for the analysed wind was computed, using a similar method to that of Jäger (1992), as $W_a = \Delta t / \Delta t_w$, where $\Delta t_w$ is the time interval of the wind fields, and the weight for the dynamic-trajectory wind as $W_d = 1 - W_a$. This trajectory type is actually a blend of the kinematic and the dynamic type. Thus, hereafter it will be referred to as the blended-trajectory type.

Meteorological fields from the ECMWF global spectral numerical weather-prediction model with 31 vertical levels and 213 resolvable waves (ECMWF 1989) were used for the trajectory calculations. Initialized analyses (at 0, 6, 12 and 18 UTC) and three-hour forecasts (at 3, 9, 15 and 21 UTC) were available with a horizontal resolution of 1.0°. The three-hour forecasts, for which forecast errors are relatively small, were used to give a higher temporal resolution, as Stohl et al. (1995) found that temporal interpolation is a significant error source for trajectory computations. In the vertical, the original hybrid ECMWF coordinate system was used, where the lowest model levels follow the topography, and the highest levels coincide with pressure surfaces. The computational domain covered the region 50°W to 50°E and 25°N to 80°N. Trajectories were terminated when they left this domain.

Forward trajectories with a length of 144 h were computed twice a day (starting at 0 and 12 UTC) for the period from 11 April 1995 to 24 May 1996, originating at five levels (3000, 5000, 7000, 9000 and 11000 m above sea level) from two locations (20°W, 50°N and 10°E, 47°N). This yielded a total of 7684 trajectories for each trajectory type. The two locations are very different from each other (one above the sea, the other over the Alps) to see whether there are any differences in the results. However, because no clear differences were found, the trajectories starting at both locations were combined into a single data set for the analyses presented in this paper.
3. MEASURES OF TRACER CONSERVATION

The isentropic potential vorticity

$$PV = -g \eta_\Theta \frac{\partial \Theta}{\partial p},$$

(7)

with $\eta_\Theta = \zeta_\Theta + f$, $\zeta_\Theta$ being the vorticity on an isentropic surface, $g$ the gravitational acceleration and $p$ pressure, is conserved along a trajectory for inviscid adiabatic motions (Pichler 1986; Davis 1996). It was calculated by evaluating $\eta_\Theta$ and $\partial \Theta/\partial p$ on a small subgrid and interpolating PV to the trajectory position. The stability term $\partial \Theta/\partial p$ has much larger variability and relative errors than $\eta_\Theta$ (Ziv and Alpert 1993). For this reason, it was found to be beneficial for the conservation of PV to smooth the stability field by a nine-point operator to reduce the noise. In the following, PV is given in PV units (1 pvu = $1 \times 10^{-6}$ m$^2$K kg$^{-1}$s$^{-1}$).

Along isentropic trajectories, potential temperature $\Theta$ is conserved by definition, but for the other trajectories it can be used as a tracer. Yet another tracer is the specific humidity, $q$, that is conserved when phase changes of water vapour are absent. The conservation of all three tracers requires condensation and evaporation not to occur along the trajectories and necessitates frictionless motion. The conservation of PV and $\Theta$ is also disturbed by radiative-flux divergence. Therefore, the tracers were not used when the relative humidity exceeded 90%, when the atmosphere was unstably stratified, or when the trajectories approached the ground (only trajectories above 1000 m above ground level were used).

Nevertheless, a complete conservation of the tracers cannot be expected, not even with the exclusion of conditions under which diabatic processes are important. For instance, turbulent kinetic energy is generated in regions of strong wind shear, and its dissipation produces sensible heat. Radiative-flux divergence is of special importance in the stratosphere, because of the absorption of short-wave radiation. Cumulus convection also causes deviations from adiabatic conditions by friction and condensation processes. However, as long as the disturbances are not too large, partial conservation suffices to investigate which trajectory type conserves the tracers best. The focus of this paper is on PV conservation and the other tracers are used to check the results obtained with PV.

Conservation of the tracers is also obscured by analysis errors in the meteorological fields. Analysis errors might be especially large for $q$ in the stratosphere, because of the poor performance of radiosonde hygrometers in cold, dry environments (Richner and Phillips 1981). Nevertheless, as analysis errors affect the conservation of the tracers for all trajectory types equally, differences found in tracer conservation must be due to different abilities of the trajectories to represent the real air flow.

All investigations were done for the troposphere and for the stratosphere separately, because results were found to be different. To distinguish between these regions, the 1.6 pvu isosurface was used as a dynamical definition of the tropopause (Bethan et al. 1996).

Three statistical measures of tracer conservation along each of the trajectories (averaged over all the trajectories) were used, the absolute tracer conservation error

$$ATE(m) = \frac{1}{N} \sum_{n=1}^{N} \left\{ \frac{1}{(L_n + 1 - m)} \sum_{k=m}^{L_n} \left| T_n(k) - T_n(k - m) \right| \right\},$$

(8)

and the relative tracer conservation error

$$RTE(m) = \frac{1}{N} \sum_{n=1}^{N} \left\{ \frac{1}{(L_n + 1 - m)} \sum_{k=m}^{L_n} \frac{T_n(k) + T_n(k - m)}{2} \right\},$$

(9)
where \( m \) indicates time in hours, \( N \) is the total number of trajectories, \( L_n \) is the length of trajectory \( n \) in hours (maximum length 144 h), and \( T_n \) is the magnitude of the tracer (either PV, \( q \) or \( \Theta \)) along trajectory \( n \). According to Eqs. (8) and (9), all segments of the trajectories are evaluated, not only those originating at the trajectory starting point. This significantly increases the number of effectively available (though not really independent) trajectories. In addition to \( ATCE \) and \( RTCE \), the Pearson autocorrelation coefficient of PV was computed for the different travel-time lags. Evaluations were made only if the local atmospheric stratification was stable, relative humidity was less than 90% and height above ground was more than 1000 m along the whole trajectory segment. Relative humidity was computed using the water-vapour saturation pressure over liquid water for temperatures above 0 °C, the saturation pressure over ice for temperatures below −40 °C, and an interpolated value between 0 and −40 °C.

As supplementary statistics, absolute horizontal \( (AHTD) \) and vertical \( (AVTD) \) transport deviations between 3-d and other trajectories were calculated as

\[
AHTD(t) = \frac{1}{N} \sum_{n=1}^{N} \sqrt{[x_n(t) - X_n(t)]^2 + [y_n(t) - Y_n(t)]^2}
\]

and

\[
AVTD(t) = \frac{1}{N} \sum_{n=1}^{N} |z_n(t) - Z_n(t)|,
\]

where \((X, Y, Z)\) are the locations of the 3-d trajectories and \((x, y, z)\) are the locations of trajectories of any other type at travel time \( t \).

4. Results

(a) The influence of the dynamical inconsistency between analyses

The series of meteorological fields used in this work consists of subsequent pairs of initialized analyses and three-hour forecasts which were used alternately for the trajectory calculations. While the step from an analysis to a forecast is dynamically consistent, the subsequent step from a forecast to an analysis is not, because observational data are used for the analysis.

If there were no diabatic effects and interpolation errors, the tracers should be nearly perfectly conserved along 3-d trajectories during the step from an analysis to a forecast. Contrarily, during the step from a forecast to an analysis, tracer conservation deteriorates due to the dynamical inconsistency of the fields. Whether this could be verified or not was investigated.

In order to study this phenomenon, the trajectory data were split into two subsets, one consisting of 3 h segments ranging from analyses to forecasts (dynamically consistent), the other of 3 h segments ranging from forecasts to analyses (dynamically inconsistent). Table 1 presents absolute tracer conservation errors \( (ATCE) \) for the two subsets. It appears that, over this short distance, about 25–50% of the \( ATCE \) is due to the dynamical inconsistency between analyses. This means that even along a numerically perfect trajectory the values of the tracers change during the step from a forecast (or a previous analysis, if only analysed fields are used) to a new analysis. It is also a confirmation of the suitability of the tracers used that this expected effect can be demonstrated using the \( ATCE \) concept.

(b) Comparison of the different trajectory types

First, the results for trajectories originating in the troposphere will be discussed. Figure 1 shows \( AHTD \) and \( AVTD \) for all trajectory types. Isentropic trajectories agree
TABLE 1. Absolute tracer conservation errors for PV, $\Theta$ and $q$ after 3 h travel time for trajectory segments ranging from an analysis to a forecast (consistent) and for trajectory segments ranging from a forecast to an analysis (inconsistent), using 3-D trajectories in the troposphere and in the stratosphere, respectively.

<table>
<thead>
<tr>
<th></th>
<th>PV (pvu)</th>
<th>$\Theta$ (K)</th>
<th>$q$ ($10^{-4}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Troposphere</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>consistent</td>
<td>0.057</td>
<td>0.33</td>
<td>0.622</td>
</tr>
<tr>
<td>inconsistent</td>
<td>0.084</td>
<td>0.50</td>
<td>1.204</td>
</tr>
<tr>
<td>Stratosphere</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>consistent</td>
<td>0.420</td>
<td>0.54</td>
<td>0.021</td>
</tr>
<tr>
<td>inconsistent</td>
<td>0.571</td>
<td>0.85</td>
<td>0.029</td>
</tr>
</tbody>
</table>

PV = potential vorticity,
$\Theta$ = potential temperature, and
$q$ = specific humidity.

Figure 1. (a) Absolute horizontal transport deviation $AHTD$ and (b) absolute vertical transport deviation $AVTD$ from the respective 3-d trajectories for isentropic (black dashed line), isoeta (black dotted line), isobaric (grey solid line), dynamic (grey dashed line) and blended (grey dotted line) trajectories. Only trajectories starting in the troposphere were considered.

best with 3-d trajectories, especially during the first 24 h of transport. Obviously they partly follow the vertical motions of the 3-d trajectories. Nevertheless, after a few days large transport deviations occur, exceeding 1000 km after less than five days. This demonstrates the significance of choosing the most accurate trajectory type for describing atmospheric flow. The transport deviations found in this study are somewhat larger than those found by Stohl et al. (1995), because the trajectories were calculated at higher levels, where wind speeds are usually larger. $AHTD$ and $AVTD$ for isobaric and isoeta trajectories are larger than for the isentropic trajectories. The blended and the dynamic isentropic trajectories show even larger transport deviations, especially in the horizontal. The reason for these large deviations will be discussed later.

The PV conservation of the different trajectory types is presented in Figs. 2(a)–(c) and Table 2. It is clear that all the kinematic trajectories conserve PV much better than
Figure 2. (a) Absolute tracer conservation errors $ATCE$ for potential vorticity (PV), (b) relative tracer conservation errors $RTCE$ for PV, (c) autocorrelation of PV, (d) $ATCE$ for potential temperature ($\Theta$), (e) $ATCE$ for specific humidity ($q$), and (f) $RTCE$ for $q$ for trajectory segments originating in the troposphere (PV < 1.6 pvu). The lines represent 3-d (black solid line), isentropic (black dashed line), isoeta (black dotted line), isobaric (grey solid line), dynamic (grey dashed line), and blended (grey dotted line) trajectories. Results are only plotted for travel times with at least 10,000 trajectory segments being available.
TABLE 2. Absolute potential-vorticity conservation errors (\( p\nu_u \)) for the different trajectory types in the troposphere at several travel times

<table>
<thead>
<tr>
<th>Time</th>
<th>3-d</th>
<th>isen</th>
<th>isoe</th>
<th>isob</th>
<th>blend</th>
<th>dyn</th>
<th>dyn (start)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.06</td>
<td>0.07</td>
<td>0.07</td>
<td>0.07</td>
<td>0.12</td>
<td>0.34</td>
<td>0.14</td>
</tr>
<tr>
<td>6</td>
<td>0.10</td>
<td>0.11</td>
<td>0.12</td>
<td>0.11</td>
<td>0.21</td>
<td>0.46</td>
<td>0.38</td>
</tr>
<tr>
<td>12</td>
<td>0.14</td>
<td>0.16</td>
<td>0.17</td>
<td>0.17</td>
<td>0.32</td>
<td>0.50</td>
<td>0.66</td>
</tr>
<tr>
<td>24</td>
<td>0.18</td>
<td>0.21</td>
<td>0.25</td>
<td>0.24</td>
<td>0.46</td>
<td>0.61</td>
<td>0.75</td>
</tr>
<tr>
<td>48</td>
<td>0.22</td>
<td>0.28</td>
<td>0.31</td>
<td>0.30</td>
<td>0.63</td>
<td>0.70</td>
<td>0.82</td>
</tr>
<tr>
<td>96</td>
<td>0.26</td>
<td>0.37</td>
<td>0.37</td>
<td>0.35</td>
<td>0.83</td>
<td>0.77</td>
<td>0.89</td>
</tr>
</tbody>
</table>

'isen' denotes kinematic isentropic, 'isoe' isoeta, 'isob' isobaric, 'blend' blended and 'dyn' dynamic trajectories; 'dyn (start)' refers to errors evaluated only for segments beginning at the start of the trajectory.

Blended and dynamic isentropic trajectories. The poor performance of the dynamic and blended trajectories is also confirmed by \( q \) conservation (Figs. 2(e) and (f)).

It is unexpected that dynamic isentropic trajectories are that much less accurate than kinematic isobaric or isoeta trajectories as the latter entirely neglect vertical motions. A closer examination showed that the poor results for the dynamic trajectories are due to their strong tendency to perform ageostrophic inertial oscillations. Figure 3 gives an extreme example for these oscillations: the kinematic and the dynamic trajectory do not agree well right from the start in this case, with obvious deficiencies of the dynamic trajectory occurring after approximately 24 h travel time. After that time, the dynamic trajectory starts to rotate at an increasing, and soon unrealistic, speed. The period of these rotations (which can be estimated in Fig. 3(b) from the height fluctuations of the trajectory caused by the north–south gradient of potential temperature) agrees well with the period of inertial oscillations (see Eq. (6)) of \( \tau \approx 14 \text{ h} \) at a latitude of 60°N.

Although Petersen and Uccellini (1979) and Jäger (1992) were aware of inertial oscillations, they could not recognize their full magnitude, because they used trajectories of less than 24 h duration. It seems that the large oscillations found here are primarily caused by errors in the Montgomery field and not by ageostrophic components of the initial wind. The errors accumulate along the trajectory and introduce growing ageostrophic wind components. This effect is not a numerical instability caused by integration time-steps that are too long. The same result was obtained even with a constant time-step of 40 s.

Merrill et al. (1986) calculated five-day kinematic and dynamic trajectories, but they did not report any difficulties with the dynamic trajectories. However, they used highly idealized flow fields generated by a channel model. When they superimposed an artificial diurnal temperature oscillation, dynamic trajectories calculated with the Petersen and Uccellini (1979) technique started to deviate from the reference trajectories without temperature oscillation. Thus, any disturbance in the Montgomery potential impairs trajectory quality. Here, real meteorological analyses were used, where errors in the Montgomery potential are much larger. Additional errors are caused by its interpolation to the trajectory position.

The quality of the wind value used to advect the dynamic trajectory (see Eq. (4)) deteriorates with travel time. Therefore, the tracer conservation along trajectory segments not initialized at the start of a trajectory is worse than the conservation along segments initialized at the trajectory start. Equations (8) and (9) therefore give estimates of the tracer errors at the trajectory start that are too high. In Table 2 the respective \( ATCE \) at the
trajectory start (only $k = m$ in Eq. (8)) are given, too, although the size of the data sample is much reduced. $\Delta T CE$ at the trajectory start is smaller than that averaged over the whole trajectory length, but still much larger than for the kinematic trajectories.

Blending kinematic and dynamic winds prevents the trajectories from oscillating and keeps wind speeds at realistic values, because errors in the Montgomery potential cannot accumulate that much. Nevertheless, blended trajectories are less accurate than kinematic trajectories.

Some explanatory notes are needed before the results for the kinematic trajectories are discussed. The tracers used in this study have large vertical gradients. On the average, PV and $\Theta$ increase with height, whereas $q$ decreases with height. Therefore, the temporal and spatial variability of a tracer at a fixed level is much smaller than in the whole atmosphere. As tracer autocorrelation decreases along a trajectory (either because the tracer is unsuitable or the trajectory is inaccurate), $\Delta T CE$ and $RT CE$ approach a saturation level
that represents the sampled variability. Isobaric and isoeta trajectories will have smaller $ATCE$ and $RTCE$ than 3-d or isentropic trajectories for travel times longer than a certain critical time, because they sample smaller tracer fluctuations. This critical time depends on the conservation properties of the tracer and the quality of the trajectories. As PV is a better tracer than $q$ and $\Theta$, its critical time is longer than that of $q$ or $\Theta$.

Among the kinematic trajectories, the 3-d trajectories clearly conserve PV best (Figs. 2(a) and (b), and Table 2). Second best are isentropic trajectories; poorer results are obtained for isobaric and isoeta trajectories. The fact that after three to four days isentropic trajectories become worse than isoeta and isobaric trajectories is probably to be explained by the critical time as discussed above. Differences in absolute and relative PV conservation between the isentropic, isoeta and isobaric trajectories are most evident at travel times up to 48 h (Table 2) because afterwards the results are impaired by the effect of sampling height discussed above. The good conservation of PV by 3-d trajectories even for very long travel times, however, clearly demonstrates that this trajectory type is very accurate. In terms of PV autocorrelation (Fig. 2(c)), isentropic and 3-d trajectories perform equally well, whereas isobaric and isoeta trajectories are clearly worse. Tracer values along dynamic and blended trajectories are uncorrelated even for short travel times.

Potential temperature can only be used as a tracer for 3-d, isobaric and isoeta trajectories. The results confirm that 3-d trajectories are most accurate. The effect of sampling height discussed above is more evident for $\Theta$ (see Fig. 2(d)) than for PV. $ATCE$ increases almost linearly with travel time for the 3-d trajectories, indicating a linear growth of trajectory errors. A linear growth is also typical for horizontal trajectory position errors (see, e.g. Baumann and Stohl (1997)). $ATCE$ for the other trajectories grows nonlinearly, fast during the first two days of transport and more slowly thereafter. It seems that after two days the rate of increase of $ATCE$ has reached a saturation value that is typical for the variability of $\Theta$ at a fixed height.

Results for $q$ (Figs. 2(e) and (f)) are rather difficult to interpret. As $q$ is not conserved as well as PV and its analysis is more difficult, all trajectory types have relatively large conservation errors; 3-d trajectories conserve $q$ best only for very short travel times. $RTCE$ for 3-d trajectories is smallest for the first 12 h, $ATCE$ only for the first 3 h. For somewhat longer travel times, isentropic trajectories conserve $q$ better, but for travel times longer than 24 h isobaric and isoeta trajectories perform best. It is likely that the better conservation of $q$ by two-dimensional trajectories is an artifact of sampling in a field with a large vertical gradient.

While the results presented so far refer to the troposphere, Fig. 4 shows the $AHTD$ and $AVTD$ for trajectories originating in the stratosphere. As in the troposphere, the smallest deviations are found for isentropic trajectories, followed by isobaric and isoeta trajectories. Overall, both $AHTD$ and $AVTD$ are smaller than in the troposphere. Dynamic and blended trajectories deviate strongly again.

In the stratosphere, PV is best conserved by the isentropic trajectories, followed by 3-d trajectories (Figs. 5(a) and (b)). Isobaric and isoeta trajectories conserve PV worse and, as in the troposphere, dynamic and blended trajectories do not conserve PV at all. The same ranking is obtained using PV autocorrelation (Fig. 5(c)). Potential temperature is much better conserved by 3-d trajectories than by isobaric and isoeta trajectories, even at the longest travel times used in this study (Fig. 5(d)). During the first day of transport, $q$ is best conserved by 3-d trajectories (Fig. 5(e) and (f)). At longer travel times, isobaric and isoeta trajectories conserve $q$ better. Isentropic trajectories conserve $q$ somewhat worse than 3-d trajectories during the first three days of transport, but better thereafter.

In general, results for the stratosphere resemble those for the troposphere. The main difference is that in the stratosphere isentropic trajectories conserve PV better than 3-d
trajectories after 15 h travel time. Contrarily, $q$ is better conserved by 3-d trajectories. Thus, no definite conclusion can be drawn as to whether 3-d or isentropic trajectories are more accurate in the stratosphere. However, both are clearly better than isobaric and isoeta trajectories. One reason for the similar performance of isentropic and 3-d trajectories might be the lower vertical model resolution in the stratosphere, making interpolation of the vertical wind velocity to the trajectory position more inaccurate.

(c) Effect of wind-field time resolution

In order to investigate the effect of time resolution of the wind fields on the accuracy of trajectories in terms of PV conservation, the time resolution of the wind fields was degraded artificially. Three-dimensional trajectories originating in the troposphere were calculated based on three-hourly wind fields (analyses plus 3 h forecasts, i.e. the reference case), six-hourly analyses, six-hourly 3 h forecasts, and 12-hourly and 24-hourly analyses.

The AHTDs after 96 h travel time are approximately 600 km for both six-hourly analyses and forecasts, 1000 km for 12-hourly analyses and 1200 km for 24-hourly analyses (Fig. 6). Thus already, with a resolution of 6 h, significant horizontal deviations from the undegraded trajectories occur. These values are similar to those found by Stohl et al. (1995). Nevertheless, in terms of PV conservation, a reduction of the time resolution from 3 h to 6 h has little effect on the overall accuracy of trajectories, except during the first 3 h travel time (Table 3). Trajectories calculated from six-hourly analyses as well as trajectories calculated from six-hourly 3 h forecasts conserve PV nearly as well as trajectories calculated from both data sources together with a 3 h time resolution. Unexpectedly, PV conservation is slightly better for the 3 h forecasts than for the analyses, which is probably related to the spin-up time of the ECMWF model. Vertical wind velocities might need some hours of model integration to strengthen to realistic values.

A reduction in wind-field time resolution to 12 h has a more significant impact on trajectory accuracy (Table 3), and a degradation to 24 h impairs PV conservation even
Figure 5. (a) Absolute tracer conservation errors $ATCE$ for potential vorticity (PV), (b) relative tracer conservation errors $RTCE$ for PV, (c) autocorrelation of PV, (d) $ATCE$ for potential temperature ($\Theta$), (e) $ATCE$ for specific humidity ($q$), and (f) $RTCE$ for $q$ for trajectory segments starting in the stratosphere ($PV \geq 1.6$ pvu). The lines represent 3-d (black solid line), isentropic (black dashed line), isoeta (black dotted line), isobaric (grey solid line), dynamic (grey dashed line), and blended (grey dotted line) trajectories.
more, especially during the first 24 h of transport. However, comparing results in Table 3 and Table 2 shows that at travel times longer than 24 h, 3-d trajectories based on 24-hourly wind fields are more accurate than any other trajectory type based on 3-hourly wind fields. Thus, in terms of PV conservation it is beneficial to calculate 3-d trajectories even if wind fields are available only at relatively low temporal resolution. Figures 1 and 6 show that $AVTD$ is smaller for poorly resolved 3-d trajectories than for highly resolved other trajectory types, while $AHTD$ is comparable. The better PV conservation is obviously due to the more realistic representation of vertical motions by 3-d trajectories, even if the time resolution of the available wind fields is rather low.

The less realistic representation of vertical motions by isentropic trajectories as compared to 3-d trajectories is not only caused by diabatic effects, but also by the dynamical inconsistencies between subsequent analyses. Table 4 presents $ATCE$ for three-hourly segments of isentropic trajectories ranging from analyses to forecasts (dynamically consistent) and from forecasts to analyses (inconsistent). Comparing Tables 1 and 4, it can be
seen that isentropic trajectories are more affected by dynamical inconsistencies than 3-d trajectories. The reason for this is clear: for the isentropic trajectories, the vertical trajectory position is directly affected by dynamical inconsistencies between two consecutive fields, whereas for the 3-d trajectories only the vertical wind is affected by inconsistencies, which less immediately influences subsequent trajectory positions. Isentropic trajectories can thus experience unrealistic shifts of their vertical position during time-steps from one analysis (or forecast) to another analysis. This effect might also contribute to the large inaccuracies of the dynamic trajectories. On the other hand, using only consecutive fields of the same dynamically consistent forecast run, kinematic isentropic trajectories might have accuracies similar to those of the 3-d trajectories.

\((d)\) Position errors

Horizontal and vertical trajectory position errors are of more practical relevance than tracer conservation errors. However, a transformation of the tracer conservation errors into position errors of the trajectories is difficult. One possibility would be to check the spatial structure of the tracer fields around each trajectory location and find the points and their distance from the trajectory position, where the tracer has the same value as at the beginning of the trajectory. However, since there are always many such points which may be found at very different distances, a unique relationship between tracer deviation and distance cannot be constructed for individual cases. On the other hand, if probabilities are calculated for these distances based on many cases, there is the problem of how to weight different possible distances within one case. Assigning the same probability to all of them is obviously not realistic.

In this study it is not possible to check the spatial structure of the tracer fields around each trajectory location. However, as a simple indicator for the spatial tracer structures, the average difference in tracer values at two locations separated by some distance is calculated. This is done for many points separated by various distances and for a long time period to obtain the climatological increase of tracer difference with distance.

The spatial absolute tracer deviation, \(ATD\), is computed for 40 distances \(\Delta x_i\) from 48 reference points uniformly distributed in the computational domain at heights of 4000, 6000 and 8000 m

\[
ATD(\Delta x_i) = \frac{1}{N} \sum_{n=1}^{N} |T_n(\Delta x_i) - T_n(0)| ,
\]

where \(\Delta x_i\) gives either longitudinal or latitudinal distance in steps of 50 km or vertical
distance in steps of 100 m (both upward and downward from the reference points), $T_n(0)$ and $T_n(\Delta x_i)$ are the tracer magnitudes at the $n$th reference point and at distance $\Delta x_i$ from the reference point, and $N = 48K$ is the total number of reference points, with $K = 812$ being the number of meteorological fields used. The fields were in 12-hourly intervals during the same period as that used for the computation of the trajectories.

Figure 7 shows $ATD$ for PV, $q$ and $\Theta$ as a function of distance. $ATD$ grows fast for small and more slowly for longer horizontal distances, whereas the vertical growth is closer to linear, especially for $\Theta$. A PV deviation of slightly less than 0.3 pvu as found, for example, in 3-d trajectories after 120 h travel time, corresponds to a distance of 400 km horizontally (that is less than 20% of the travel distance) or 1300 m vertically. However, this value cannot be regarded as the true average position error of the trajectories, because of the problems discussed above and also because there might be a correlation between the PV deviation along a trajectory and the PV structure expressed by the ATD.
5. Conclusions

Several techniques are often used and certain assumptions are made to calculate trajectories. Their accuracy is, however, largely unknown and it is also not always clear which method yields the most accurate trajectories. In this study, three-dimensional, isentropic, isobaric and isoeta trajectories were intercompared. For the calculation of the isentropic trajectories three techniques were used: the kinematic, the dynamic and a blend of these. The accuracy of these six different types of trajectories was investigated using conservative meteorological quantities, namely potential vorticity, potential temperature and specific humidity, as tracers. The aim was to rank the accuracy of the trajectories in terms of tracer conservation. Conclusions that can be drawn from this study are:

- Isentropic trajectories are strongly affected by dynamical inconsistencies between consecutive analysis fields which can result in unrealistic shifts of their vertical position.
- Dynamic isentropic trajectories tend to perform unrealistic inertial oscillations due to accumulating ageostrophic wind components caused by inexact determination of the Montgomery potential and dynamical inconsistencies between consecutive analysis fields. These oscillations are especially important for travel times longer than 24 h. Dynamic trajectories are less accurate than any other trajectory type, including isobaric trajectories. This is valid in the troposphere as well as in the stratosphere, and based on PV as well as on $q$ conservation. The dynamic computation technique was invented before high-resolution weather-prediction models became available. Now that data from such models are readily available, the dynamical method is outdated and kinematic trajectories are superior.
- Only marginally more accurate are trajectories for which dynamic trajectory winds are blended with interpolated analysed winds. Although they do not oscillate, their accuracy is clearly lower than that of kinematic trajectories.
- Isobaric and isoeta kinematic trajectories are much more accurate than dynamic and blended isentropic trajectories, but less accurate than 3-d and kinematic isentropic trajectories.
- 3-d trajectories are clearly the most accurate trajectories in the troposphere. Isentropic trajectories are less accurate. However, when using dynamically consistent fields of a single forecast-model run for the trajectory calculations, isentropic and 3-d trajectories might be of similar accuracy.
- Stratospheric 3-d trajectories are less accurate than kinematic isentropic trajectories in terms of PV conservation, but more accurate in terms of $q$ conservation. Thus, no definite conclusion is possible as to whether 3-d trajectories are the most accurate in the stratosphere.
- A reduction in the time resolution of the meteorological fields impairs trajectory accuracy. However, 3-d trajectories calculated from fields with 24 h resolution are still more accurate at long travel times than any other trajectory type calculated from fields with 3 h resolution. This is especially true for their vertical position.
- From our investigations, it appears that PV is a much better tracer of air motion than both $\Theta$ and $q$, since it is conserved better along the trajectories.
- A transformation of the tracer conservation errors into average position errors of the trajectories is very difficult.
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