The calculation of stratospheric air parcel trajectories using satellite data

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Summary

Air parcel trajectories are calculated for the mid-stratosphere using data from the stratospheric sounding unit on board NOAA-6. In the analysis method all the orbital data for each 24 h period are combined into a single global analysis. Three trajectory methods are used—Isobaric, isentropic and quasi-isentropic—and the results are compared and contrasted. For the quasi-isentropic method a radiation model is used, via the thermodynamic equation, to imply cross-isentrope flow at regular intervals along the trajectory. The positions of the parcels, computed using the three methods, are found in general to be in good agreement when projected on to a horizontal plane. However, the altitude varies according to the trajectory method used and changes by about 1 km along a quiescent trajectory and as much as 2 km along a disturbed trajectory, during a 10-day period. This has important implications in the study of chemistry along parcel trajectories during disturbed periods since the temperature- and pressure-dependent reactions will proceed at different rates under the different assumptions. Also, the high lapse rate in the vertical mixing ratio profile of ozone implies that the detailed photochemistry will depend critically on the height of the air parcel.

Further, potential vorticity and potential temperature are used as quasi-conservative Lagrangian tracers, to try to determine which trajectory method is most realistic. For the quiescent period studied (June 1979 in the southern hemisphere) the isobaric and isentropic methods produced similar results throughout the ten days of the trajectory but the quasi-isentropic method was clearly superior. A disturbed period was also studied (the February 1979 stratospheric warming), but the results from the trajectories studied were consistent with the Lagrangian conservation laws for only 6 days, at most. These results illustrate the need for caution, particularly with regard to sensitivity to initial horizontal position, in using trajectories calculated for disturbed periods.

1. Introduction

Trajectory analyses have traditionally been a tool of atmospheric scientists for studying the physical or chemical history and evolution of the properties of an air mass. Before the availability of satellite data trajectory analyses tended to concentrate on the tropopause region and in a sequence of papers Danielsen (1961, 1974) and Djuric (1961) have demonstrated many of the practical difficulties which arise in the calculation of trajectories. Briefly, there are two main problems. Firstly, lack of resolution of wind data in both space and time restricts the analysis to persistent, large-scale flows. In particular, radiosonde-derived winds contain components from gravity waves etc. which must be filtered to give a large-scale mean analysis. Secondly, because of the absence of reliable measurements of vertical wind velocities, analyses have to be performed on surfaces which can be shown theoretically to have small wind components across them. For example, it is sometimes assumed that an air parcel is only slowly approaching radiative equilibrium so that in the absence of condensation and turbulent mixing the parcel would be expected to remain near an isentropic surface for a period of days. An isobaric assumption is less justifiable but isobaric trajectories are easier to compute than isentropic trajectories and if the geopotential height field is changing slowly and vertical velocities are small may be equally good.

The existence of global upper atmospheric analyses of geopotential from satellite data has enabled trajectories to be computed for the stratosphere. McIntyre and Palmer (1983, 1984), for example, used trajectories to try to understand the breaking of planetary waves in the stratosphere during late January 1979. In addition, the potential value of trajectories in understanding the chemistry of the stratosphere has been indicated by Solomon and Garcia (1983) and Callis et al. (1983), although in both papers isobaric streamlines are used to approximate actual trajectories.
Moreover, in calculating trajectories, lack of resolution in the wind data is less restrictive for the stratosphere where the disturbances are generally of larger scale than in the troposphere, as shown for a stationary, linear atmosphere by Charney and Drazin (1961) and Simmons (1974). Certainly, very small-scale disturbances do exist in the stratosphere but these are believed to be dominated by gravity waves and tides which have their largest effect in the upper stratosphere and mesosphere (Holton 1982). Additionally, during highly transient periods small-scale structures may be produced nonlinearly by an enstrophy cascade. Nonetheless in the absence of information on small-scale dynamics we cannot be certain that these features are unimportant. Even the higher wavenumber disturbances (zonal wavenumbers 4 or 5) which appear in the data can have a significant influence on air parcels on timescales of the order of 5 days although waves with a smaller scale than this generally have too small an amplitude to be significant. Therefore it is advisable to calculate trajectories from an ensemble of parcels with initial positions arranged closely around the position of interest and then to use their dispersion as representative of the trajectory uncertainty due to mixing and dispersive disturbances smaller than the planetary scale.

This approach is adopted in the current work in which 10-day stratospheric trajectories are calculated for a quiescent dynamical situation (June 1979 in the southern hemisphere) and a disturbed dynamical situation (February 1979 in the northern hemisphere). During the quiescent period wave amplitudes were small and slowly varying in time. The disturbed period includes the stratospheric warming discussed by Butchart et al. (1982). Three methods of trajectory calculation are studied: isobaric, isentropic and quasi-isentropic. In the third method the trajectory is taken to be isentropic with the potential temperature value re-adjusted by diabatic heating or cooling at regular intervals along the trajectory. Because this method attempts to allow for the flow across the isentropic surface it would be expected to yield superior results. However, in the absence of knowledge of actual air parcel trajectories there is no rigorous way of demonstrating this hypothesized superiority. Nonetheless some guidance may be obtained by considering potential vorticity, which is approximately conserved following parcel motions. Danielsen (1968) for example found potential vorticity to be a very useful quasi-conservative quantity for studying stratospheric–tropospheric exchange. Moreover it is possible to calculate the expected change in potential vorticity arising from radiative effects using the Lagrangian conservation law presented in section 3.

In section 4 examples of trajectories in the mid-stratosphere using the three methods are presented and compared in order to establish the likely errors in using each method. Finally, the results are summarized in section 5 and guidelines are suggested for the use of mid-stratospheric trajectories computed from satellite data.

2. METHODS OF CALCULATING TRAJECTORIES

In calculating a trajectory it is usually assumed implicitly that the computation refers to an infinitely small air parcel. In practice this is not a very useful assumption because wind observations have a finite scale so that in principle one is calculating trajectories for broad air parcels. This has the major difficulty that wind shears across the parcel may deform the shape to such an extent that the parcel trajectory, or strictly speaking the trajectory of its centre of mass, may have little physical meaning. In general, the larger a single air parcel is, the more it is likely to deform under the action of a given wind field. The degree of deformation of the parcel may be estimated from the dispersion of a set of trajectories the initial positions of which define the edges of the parcel. Using an ensemble of parcels we can thus estimate the largest size of air parcel for which
trajectories can be computed confidently with given wind data. In the current work the resolution in the data is approximately 15° of longitude, 5° of latitude and 8 km in the vertical. This is sufficient to define accurately the large-scale planetary waves which dominate the dynamics of the stratosphere. In the middle and upper stratosphere, under steady, linear conditions the smaller-scale planitary waves, i.e. those with wavenumbers >3, do not propagate (Charney and Drazin 1961; Simmons 1974) and even during transient or nonlinear periods waves 6 and above usually have amplitudes rather smaller than 100 m, if high resolution primitive equation global models are to be believed (O'Neill, personal communication); such waves would have a negligible effect on our trajectory computations. Gravity waves, which are present in the atmosphere, are not represented in the data because the height scales are much smaller than the width of the SSU weighting functions. However, because they are small amplitude waves they are likely to affect the trajectories only on a very local scale. For example, Barat (1982) shows observations made in April 1978 which describe a wave in the zonal wind speed with a vertical wavelength of 0.8 km and an amplitude of 2–3 m s⁻¹. If this were to be maintained (unlikely) in the same direction for a whole 10-day trajectory, it would result in a position error less than 2500 km. This is very much an upper bound to the error associated with small-scale disturbances, and yet is comparable with the error in trajectory position caused by large-scale uncertainties discussed in section 3. We therefore conclude that if, for an individual case, the largest parcel size for which dispersion is unimportant is much smaller than 5° longitude × 5° latitude × 2 km vertically, the calculated trajectory must be considered doubtful since the problem demands greater resolution than is available.

In this section three trajectory methods are described—isoobaric, isentropic and quasi-isentropic—and examples are given in section 4.

(a) Isoobaric trajectories

Thickness fields (Miller et al. 1980; Pick and Brownscombe 1981) were obtained from the stratospheric sounding unit (SSU) on NOAA-6. The thickness fields were obtained by combining all the orbital data for each 24 h period into a single global analysis at a representative synoptic hour in the centre of the period—0001 GMT. The orbits are sun-synchronous, so diurnal variations are removed from the fields by the analysis method. Geopotential height analyses at daily intervals were then obtained by combining 100 mb National Meteorological Center (NMC) analyses with the thickness fields. Available channels peaked at 1.5 mb, 5 mb and 15 mb approximately although the 1.5 mb channel was not functioning correctly during February 1979. Gradient winds on the 10 mb pressure surface were obtained from the geopotential analyses using centred finite differences of second-order accuracy. The gradient wind calculation requires knowledge of the radius of curvature of the air parcel trajectories at each point of the grid. This information is not available at the analysis stage, and must be approximated in some way. The radius of curvature of the trajectory $R_T$ is related to the radius of curvature of the streamline $R_S$ by Blaton’s equation, see for example Haltiner and Martin (1957) pp. 184–194:

$$1/R_T = 1/R_S + (1/V) \partial \psi/ \partial t$$

where $V$ is wind speed and $\partial \psi/ \partial t$ is the local rate of turning of the horizontal wind direction. By substituting typical values during a sudden warming, when $\partial \psi/ \partial t$ might be expected to have its largest values and hence maximize the differences between $R_T$ and $R_S$, it can be shown that $R_T \sim 0.7 R_S$, resulting in a correction of order 3% to the wind speed. $R_T = R_S$ should be a good approximation under circumstances encountered by
the air parcel trajectories computed here at middle and high latitudes in winter; under these conditions, errors from other sources, particularly from transient terms, are larger. Nevertheless it is clear from Blaton's equation that a combination of low wind speed and large \( \partial \psi / \partial t \) would invalidate the approximation \( R_T = R_\psi \). The winds were linearly interpolated in time and linearly interpolated in position to the trajectory coordinates. The interpolation error is likely to be due mainly to transients with a timescale shorter than one day which cannot be quantified in the absence of more detailed information. The gradient wind is a good approximation to the actual wind (\( \sim 10\% \) error, from scale analysis), although it neglects the local acceleration of the wind. The effect of including this term is to change the direction of the wind slightly without changing its strength (to first order). Thus the wind does not blow along the geopotential height contours but at an angle \( \alpha \), measured towards low pressure, where \( \tan \alpha \sim (D_u / D_t) / f \mid u \) (McIntyre and Palmer 1984), \( f \) being the Coriolis parameter, \( u \) the wind velocity and \( D_u / D_t \) the rate of change of wind speed along the trajectory. These terms are easy to evaluate along a trajectory and \( \alpha \) is typically 2–3°, although it may be as large as 20° during disturbed conditions. The unimportance of omitting the \( V^2 / R_T \) term in the denominator of the above equation was confirmed by rerunning all trajectories with this term included; the maximum differences in the resulting trajectories were 0.1° latitude and 0.1° longitude, or about a factor of 50 less than our typical parcel size. Danielsen (1961) included the effects of the local acceleration by appeal to the energy equation, an approach which is not practical for the stratosphere because the errors in the satellite-derived terms are too large.

The air parcel trajectories were computed using the following finite-difference scheme:

\[
x_{n+1} = x_n + \frac{1}{2} \Delta t \{ u(x_n, t + \frac{1}{2} \Delta t) + u(x_{n+1}, t + \frac{1}{2} \Delta t) \};
\]

(1)

\( x_n \) is the position of the air parcel at time \( t \); \( x_{n+1} \) is the position of the air parcel at time \( t + \Delta t \); and \( u \) is the velocity field in the plane of the trajectory, corrected for the local acceleration.

Equation (1) represents an implicit scheme and typically four iterations were required for convergence of \( x_{n+1} \). Experiments were performed with Eq. (1) using \( \Delta t = 0.1 \) days and \( \Delta \tau = 0.01 \) days and the differences in the resulting trajectories for a quiescent period were approximately 2° of latitude and 5° of longitude after 10 days, although larger differences occurred for a sample trajectory calculated during disturbed conditions. The trajectories in section 4 were all calculated with \( \Delta t = 0.01 \) days although a larger timestep would certainly be justified. Similar results were also obtained using \( \Delta \tau = 0.01 \) days and an explicit finite difference scheme of first order but the implicit scheme was used for higher accuracy. These insensitivities are a result of the large-scale slowly varying fields which are imposed. In contrast, for trajectory calculations in the upper troposphere, both the finite difference scheme and the timestep have to be chosen with especial care (G. Vaughan, personal communication, 1983).

(b) Isentropic Trajectories

Geopotential analyses were obtained as above and differentiated with respect to log(pressure) to yield temperature analyses. Next, the Montgomery streamfunction for the 850 K potential temperature surface was constructed (Reiter 1972), using cubic splines for the vertical interpolation. From the gradient winds, calculated as in subsection (a) and corrected for the local acceleration, isentropic trajectories were calculated using the finite difference scheme in Eq. (1).
(c) Quasi-isentropic trajectories

In this method the trajectory is constructed from a sequence of isentropic trajectories (sub-section (b)) of 0-1-day duration joined together. In the calculation of a quasi-isentropic trajectory, however, the isentropic surface is adjusted every 0-1 days using the thermodynamic equation (see Holton 1972, p. 48–9):

$$D\theta/Dt = Q(p_0/p)\kappa.$$  \hspace{1cm} (2)

$\theta$ is potential temperature = $T(p_0/p)\kappa$, where $T$ is temperature; $p_0$ is a standard atmospheric pressure = 1000 mb; $p$ is the ambient pressure; $\kappa$ is a constant, 0-287; $Q$ is the ratio of the heating rate to the specific heat at constant pressure.

Equation (2) is a Lagrangian equation which can be integrated directly along the trajectory to yield

$$\theta_{n+1} = \theta_n + Q(p_0/p)\kappa \delta t.$$  

$\theta_n$ and $\theta_{n-1}$ are successive values of potential temperature and $\delta t = 0.1$ days. $Q$ must include terms due to solar heating and ozone cooling (9.6$\mu$m band) and CO$_2$ cooling (15$\mu$m band). In this paper instantaneous rates of ozone heating were calculated along the trajectories using the Lacis and Hansen (1974) scheme. The ozone amounts were taken from solar backscattered ultraviolet (SBUV) data for the appropriate days. The heating scheme takes into account ground reflection and reflection from clouds with the following fixed parameters: ground albedo 0.5, cloud amount 0.5 and cloud optical thickness 10.0. The ozone cooling term, which represents typically about 30% of the total infrared cooling, was obtained from the parametrization of Harwood and Pyle (1975) and the CO$_2$ cooling rates were calculated with a Curtis matrix (Haigh 1980) assuming a volume mixing ratio of 320$\times$10$^{-6}$. The net radiative heating rates were found to be consistent with values from the Oxford 2-D model (Haigh, personal communication). Essentially the same results were obtained with the Schoeberl and Strobel (1978) scheme replacing the Lacis and Hansen (1974) scheme. This was also true when the overhead ozone column was varied within the range indicated by the SBUV error bars (7–15%). This insensitivity to the choice of radiation scheme is to be expected during winter when solar heating is relatively small. During summer, both terms are relatively large, and computing an accurate difference may prove difficult.

3. Lagrangian conservation laws

It is not possible to establish conclusively which trajectory method yields results closest to the actual air parcel trajectory. Nonetheless some guidance can be obtained by calculating quasi-conservative Lagrangian tracers, the evolution of which can be determined relatively easily from theoretical considerations. In particular, we may be able to establish whether the trajectory methods have general weaknesses. Two tracers of particular interest are potential temperature ($\theta$) and potential vorticity on the potential temperature surface ($P_\theta$). The (frictionless) equations they satisfy (Staley 1960) are (together with Eq. (2))

$$\theta = T(p_0/p)\kappa$$

$$P_\theta = - (\zeta_\theta + f) \partial \theta / \partial p$$  \hspace{1cm} (3)

$$DP_\theta/Dt = -(\zeta_\theta + f) \partial (\theta Q/T) / \partial p + (c_p/fT)(\partial \theta / \partial p) \nabla_\theta T \cdot \nabla_\theta Q.$$  

$c_p$ is the specific heat capacity at constant pressure of dry air; $\nabla_\theta$ is the gradient operator.
acting on the horizontal projection of the $\theta$ surface; and $\xi_\theta$ is the vertical component of the relative vorticity measured on the local $\theta$ surface. All other variables have been defined previously. Equation (3) can be written

$$DP_\theta/Dt = P_\theta X$$

(4)

where

$$X = [\delta(\theta Q/T)/\partial \theta - c_\theta \nabla_\theta T \cdot \nabla_\theta Q] / [fT(\xi_\theta + f)]$$.

The term involving $\nabla_\theta T$ is approximately 10% of $X$ and was neglected by Hartmann (1977), although it has been retained in the current work for completeness. This term comes from the horizontal component of the 3-dimensional relative vorticity, and arises from the thermal wind. Equations (2) and (4) were solved along the trajectories for $P_\theta$ and $\theta$ using the radiation scheme described in section 2(c). Equation (4) can be solved given $P_\theta$ at time $t = 0$. We wish to minimize the error in $P_\theta(0)$ which if too large would propagate through all the predicted values of $P_\theta(t)$ making the comparison with data meaningless. We reduce the error by taking as the starting value the averaged value for the first five days of the trajectory of $P_\theta(t)$ corrected for diabatic effects back to time $t = 0$. Suppose for example that $X = -\alpha = \text{constant}$. Then $P_\theta(t) = P_\theta(0) \exp(-\alpha t)$. The starting value is then taken to be

$$\bar{P}_\theta(0) = \frac{1}{5} \sum_{n=1,5} P_\theta(t) \exp(\alpha t_n)$$

where $t_n = (2n - 1)/2$ days.

In order to assess the trajectories using potential vorticity the orders of magnitude of the errors need to be considered. $\partial \theta/\partial p$ is difficult to calculate given the poor vertical resolution of the SSU instrument. However, Clough et al. (1984) note that good agreement (to within 10%) was obtained with a small number of co-located radiosonde and rocket ascents during a period in late November to mid December 1981. They remark, however, that the error might be a significant underestimate where vertical structure is only partially resolved by the SSU. However, this does not appear to be a problem in the trajectories considered in this paper. Although the size of the error in the radiation scheme is unknown it is probable that at this level errors in the net diabatic heating rate and in the vertical gradient do not exceed 30%. In 10 days this would result in a maximum error in the predicted potential vorticity of order 5%. This change could be typically achieved by a horizontal displacement of order three great circle degrees (~300 km) in the direction of the potential vorticity gradient. Since this is smaller than the typical air parcel size being considered, it can be concluded that, in general, errors in the radiation scheme do not influence significantly the horizontal position of the air parcel. On the other hand a typical random error in the potential vorticity (~10–15%) can be accommodated by a horizontal displacement of order 1000 km. In regions of large potential vorticity gradient the random error is also larger so the horizontal displacement needed is not a sensitive function of the potential vorticity gradient. Thus, if for a given trajectory the potential vorticity diverges significantly from the predicted value, the error in the trajectory may be assumed to exceed 1000 km. However, agreement between the predicted potential vorticity and the satellite-derived values does not necessarily imply that the trajectory is accurate to 1000 km because a large horizontal displacement perpendicular to the potential vorticity gradient would clearly have no effect on the potential vorticity value. Finally, because the same radiation scheme has been used to determine both the evolution of potential vorticity and the parcel position for the quasi-isentropic trajectories, the demonstration or otherwise of the conservation of potential vorticity is
not entirely rigorous. Nonetheless the requirement of consistency between theoretical and satellite-derived values is sufficient in practice to afford confidence in most of the computed trajectories.

4. Examples of Trajectories

(a) Southern hemisphere winter

During the period 2–12 June 1979 the geopotential height field at 10 mb was almost zonally symmetric and very nearly centred over the pole. On 2 June wavenumber 1 was dominant with an amplitude of approximately 750 m at 60°S (300 m at 40°S), which decreased gradually to 450 m at 60°S (100 m at 40°S) by 12 June. Wavenumber 2 decreased initially, reaching a minimum on 5–7 June but then increased to about 200 m at 60°S (300 m at 40°S) by 12 June. Figure 1 illustrates the geopotential height field on 7 June.

![Figure 1](image)

**Figure 1.** Geopotential height field (m) at 10 mb on 7 June 1979 (southern hemisphere).

Because the wave amplitudes were small (<500 m) air parcel trajectories would be expected to be almost zonally symmetric. This is demonstrated in Fig. 2 which shows 10-day trajectories starting on 2 June at 0001 GMT from 40°S 0°E. In the figures the numbers along the trajectories represent the date at 0001 GMT. Figure 2(a) gives the 10 mb isobaric trajectory and Fig. 2(b) gives the isentropic trajectory for the 850 K potential temperature surface. Figure 2(c) gives the trajectory for the quasi-isentropic
Figure 2. Ten-day trajectories starting on 2 June 1979. (a) 10 mb isobaric trajectory starting at 40°S 0°E. (b) 850 K potential temperature isentropic trajectory starting at 40°S 0°E.
Figure 2 (contd). (c) Quasi-isentropic trajectory starting at 40°S, 0°E with initial potential temperature 850 K. (d) Ensemble of isentropic trajectories (850 K potential temperature) starting at ■: 37.5°S, 2.5°W; ▲: 37.5°S, 2.5°E; ○: 40°S, 0°E; +: 42.5°S, 2.5°E; ×: 42.5°S, 2.5°W. The same symbols are used to denote the end points of the trajectories.
method (see section 2) for an initial potential temperature of 850 K. Qualitatively the trajectories are very similar when projected on to a horizontal plane. Because the winds were steady and nearly zonally symmetric, differences between the results may be largely attributed to the vertical wind shear. The quasi-isentropic trajectory is lower in the atmosphere than the other trajectories and the average wind speed was about 6% less than on the 850 K potential temperature surface. The average wind speed along the isobaric trajectory was approximately mid-way between the values along the quasi-isentropic and isentropic trajectories as would be expected from the altitude of the trajectory.

Similar tracks are obtained when the starting position is perturbed slightly. Figure 2(d) shows the results obtained for five trajectories starting at 40°S 0°E, 42.5°S 2.5°E, 42.5°S 2.5°W, 37.5°S 2.5°E and 37.5°S 2.5°W; for clarity the dates are not indicated in the figure. The three most southerly trajectories remained within the range 40° to 59°S although at the end of the 10 days the longitude of the air parcels had a range of 150°. This large longitudinal range arises from the large horizontal shear in the wind speed. Whether the difference is serious would depend on the problem being studied. For example, if a chemical model were to be integrated along the trajectories essentially the same results would be obtained. Provided there was negligible net mixing along latitudinal species gradients, the photochemistry would proceed at approximately the same rate because the latitudinal excursions are small. In general, the longitudinal variations in an equivalent calculation for a quiescent period in the northern hemisphere would be smaller because the horizontal wind shears are less. The other two trajectories deviated from a symmetric path, especially the trajectory starting at 37.5°S 2.5°E which encountered a very weak wind region after about four days.

Figure 3. Differences between trajectories of Figs. 2(a)–(c):
--- isentropic minus quasi-isentropic; --- isobaric minus quasi-isentropic.
The horizontal differences between the three trajectories starting at 40°S 0°E are illustrated in Fig. 3, which gives the displacement in great circle degrees of the isobaric and isentropic trajectories, relative to the quasi-isentropic trajectory. As noted previously the isobaric displacement is less than the isentropic displacement and there is very strong qualitative agreement between the two curves. Both displacements are less than $5^\circ$ for about the first four days of the trajectories. In general one would expect individual trajectories, calculated using slightly different methods, to diverge from each other because of systematic differences in the Lagrangian wind field. Danielsen (1961), for example, found differences of greater than 1000 km in 12 hours in an extreme case for the troposphere. For the current trajectories the differences increase to 1000 km only after 5 to 9 days and may be associated mainly with the vertical shear in the zonal wind.

![Figure 4](image)

Figure 4. Geopotential height along trajectories of Figs. 2(a)-(c):

--- isentropic; ---- isobaric; . . . quasi-isentropic.

The values along the isobaric trajectory have been increased by 350 m for ease of comparison.

Figure 4 shows the geopotential height of the air parcels as a function of time. The error bars (about 200 m) include the error in the 100 mb height field (<100 m) and the error in the 100 mb–10 mb thickness field (≈140 m; Pick and Brownscombe 1981). The isobaric trajectory does not quite start at the same level as the other trajectories so for comparison the actual values have been increased by 350 m and the adjusted values are plotted. Qualitatively the isentropic and quasi-isentropic trajectories are quite similar.
with the peaks and troughs almost coincident in time for the first seven days in both graphs. This is because the potential temperature difference increases steadily with time, as described later, while the horizontal positions of the parcels diverge only slowly. In contrast the geopotential along the isobaric trajectory is almost constant, reflecting the steadiness in the geopotential height field described earlier. Along the quasi-isentropic trajectory the geopotential height generally falls. The net fall of approximately 1200 m in 10 days corresponds to a vertical downward velocity of about 1.3 mm/s. This value is entirely consistent with the (Lagrangian) flow patterns at 30 km deduced by Murgatroyd and Singleton (1961) from a study of the radiative heating balance. By comparison the isobaric and isentropic trajectories imply descent at the average rate of only 0.4 mm/s.

Figure 5. Heating and cooling rates along the quasi-isentropic trajectory (Fig. 2(c)): —— infrared cooling rate; —— ozone solar heating rate.

Figure 5 illustrates the heating and cooling rates computed along the quasi-isentropic trajectory using the radiation scheme described in section 2(c). During the period the infrared cooling rate decreases slowly and fluctuates in the range 1.9–2.8 K/day. The peak solar heating rate is approximately 3 K/day so that there is a net cooling except for short periods near local noon on some days. Note that local noon occurs 12 times during the 10-day period because the strong westerly wind implies a reduced length of day in a Lagrangian framework.

Next, we consider the Lagrangian tracers presented in the previous section. Since these quantities are not measured directly they need to be determined from the geopotential height field and its derivatives, which introduces a large random error component. The quantities in question have therefore been averaged over the natural timescale of the observing system (1 day, 10 values along the corresponding trajectory segment) and the attached error bars represent standard deviations of the individual values from the mean.
Figure 6. Lagrangian tracers along the trajectories of Figs. 2(a)-(c).
(a) Potential temperature: —— isentropic; --- isobaric; . . . quasi-isentropic. The values along the iso-
baric trajectory have been increased by 25 K for ease of comparison.
(b) Potential vorticity: —— isentropic; --- isobaric; . . . quasi-isentropic;
--------- theoretical (obtained by solving Eq. (4)).

Figure 6(a) illustrates the potential temperature along the trajectories. Trivially, for the isentropic trajectory this is constant. For the quasi-isentropic trajectory potential temperature was calculated as in section 2 and imposed on the system. The values depend on the radiation scheme and have a diurnal component due to solar heating but otherwise decrease quite steadily. Thus there is a succession of short periods when the potential
temperature stays constant or increases slightly. Overall the decrease in potential temperature is about 6 K per day corresponding to a decrease in temperature of about 2 K per day. The potential temperature of the isobaric surface has been increased by 25 K for the purposes of comparison. The results show that the values are close to the theoretical values (as predicted by Eq. (2)) for the first three days but thereafter do not change systematically. Nonetheless there is a net decrease in potential temperature albeit significantly smaller than for the theoretical curve.

Figure 6(b) shows the potential vorticity calculated from the vorticity and potential temperature gradient \( \partial \theta / \partial p \) using the satellite data at the parcel position. The random errors are large on some days as indicated by the error bars but are typically about 10%. (The error bars for the isentropic and isobaric trajectories are of similar magnitude but have been omitted for clarity.) The quasi-isentropic values are consistent with the theoretical values (obtained by solving Eq. (4)) on most of the days and are only just outside one standard deviation on the other days. The isentropic potential vorticity is equally consistent with theory for the first seven days but diverges rapidly in the last few days. The isobaric values are almost in agreement with theory but whereas the theoretical curve and quasi-isentropic curves indicate a significant decrease of some 16% in nine days, the isobaric values decrease by only about 10% which is not quite statistically significant.

In conclusion, the consistency of the results presented suggests that the quasi-isentropic trajectory is a reasonable approximation to the actual (unknown) trajectory and that in this case the isobaric trajectory was better than the isentropic trajectory.

(b) Northern hemisphere winter

In this section we proceed, as in the previous section, to examine trajectories from a single starting position using the three trajectory methods. We then consider briefly several trajectories of further interest using the quasi-isentropic method only.

The trajectories were calculated for the period 21 February–3 March 1979 when a major stratospheric warming occurred. By the 21st the circumpolar vortex at 10 mb had already split into two vortices. These vortices remained throughout the rest of February and into March and the Aleutian high, situated at 180°E, moved polewards and intensified. The geopotential height field at 10 mb is illustrated in Fig. 7(a) for 21 February when the most rapidly changing events occurred, and in Fig. 7(b) for 26 February in the middle of the warming. Further description of the warming may be obtained from Butchart et al. (1982). A number of trajectories were calculated for the warming starting in the eastern vortex. These trajectories may be broadly classified into three groups: (i) those that remain entirely within the eastern vortex for the duration of the trajectory; (ii) those that transfer to the western vortex after a short period in the eastern vortex; (iii) those trajectories for which slight perturbations to the trajectory position will result in a change from type (i) to type (ii) or vice versa.

The starting time and position (21 Feb. 0000 GMT, 40°N 50°E) of the first trajectory have been chosen to illustrate some of the potential problems in computing trajectories for the more sensitive type (iii) situation. Figure 8(a) gives the 10 mb isobaric trajectory and (b) illustrates the isentropic trajectory. The trajectory for the quasi-isentropic method is shown in (c). As in June 1979 the three trajectories are similar for the first 5 or 6 days when projected on to a horizontal plane but are quite different thereafter. From its position on 21 February the air parcel moved around the eastern vortex and by midday on 22 February had reached high latitudes (79°N), on the edge of the eastern vortex (see Fig. 7(a)). The air parcel then continued in the eastern vortex again reaching high latitudes on 26 February. The horizontal projections of the isobaric and isentropic
Figure 7. Geopotential height (m) at 10 mb in the northern hemisphere: (a) 21 February; (b) 26 February 1979.
Figure 8. 10-day trajectories starting on 21 February 1979: (a) 10 mb isobaric trajectory starting at 40°N 50°E; (b) 850 K potential temperature isentropic trajectory starting at 40°N 50°E;
Figure 8 (contd). (c) Quasi-isentropic trajectory starting at 40°N 50°E with initial potential temperature 850 K; (d) Ensemble of isentropic trajectories (850 K potential temperature) starting at ■: 37.5°N 47.5°E; ▲: 37.5°N 52.5°E; ○: 40°N 50°E; +: 42.5°N 47.5°E; ×: 42.5°N 52.5°E.

The same symbols are used to denote the end points of the trajectories.
trajectories then rapidly diverge as the isentropic trajectory transfers to the western vortex whereas the isobaric trajectory continues in the eastern vortex. The quasi-isentropic and isentropic trajectories are very similar throughout the 10 days, although the differences tend to get larger in the weak wind region near 30°W (see e.g. Fig. 7(b)).

For this situation the initial starting position is critical. Figure 8(d) shows five isentropic trajectories starting from 40°N 50°E, 42.5°N 52.5°E, 42.5°N 47.5°E, 37.5°N 52.5°E and 37.5°N 47.5°E. All five trajectories follow narrowly defined tracks for 5 or 6 days and thereafter three continue along paths similar to that described above. The trajectories starting at 37.5°N stay within the eastern vortex for the whole period and almost complete two circuits. Clearly, a small perturbation to the parcel position has a profound effect on the subsequent trajectory.

![Figure 9. Differences between trajectories of Figs. 8(a)-(c):](image)

--- isentropic minus quasi-isentropic; --- isobaric minus quasi-isentropic.

The horizontal differences between the three trajectories starting at 40°N 50°E are illustrated in Fig. 9. As remarked previously, the horizontal projections of the isobaric and isentropic trajectories are similar. During the first 4 to 5 days of the trajectories the displacements from the quasi-isentropic trajectory are small—less than 5 great circle degrees. From about day 7 onwards the isobaric displacement increases very rapidly when the isobaric and quasi-isentropic trajectories travel in different vortices. In contrast the isentropic displacement remains quite small and is only about 15 great circle degrees at the end of the trajectory.

Figure 10(a) gives the geopotential height along the trajectories given by the three methods. The height of the isobaric trajectory has been increased by 175 m to allow for
the fact that the 850 K potential temperature level was slightly higher than the 10 mb pressure level at the starting point of the trajectories.

During the 10 days the height of the isobaric trajectory remained approximately constant. In contrast the quasi-isentropic trajectory indicated very rapid vertical motion (~1 cm/s) during two periods and the air parcel experienced a range of about 3 km in geopotential height. The isentropic trajectory reflected these features as closely as for the June 1979 trajectories, for the reasons stated previously. The range of heights for the isentropic trajectory (2 km) was much less than for the quasi-isentropic trajectory.

Figures 10(b) to (d) illustrate the projections of the trajectories on to the meridional plane; the date is marked at 0001 GMT. The isobaric trajectory, (b), is quite featureless because of the constancy of the height, remarked on previously. In contrast both isentropic and quasi-isentropic trajectories ((c), (d)) are elliptical for the whole period. For February 1979 the major axis of the first ellipse traced out by the isentropic trajectory slopes slightly downwards towards the pole. The second ellipse has a steeper slope down towards the pole in the middle of the warming. Similar behaviour is also apparent in the quasi-isentropic trajectory for which the ellipses, particularly the second ellipse, have a steeper slope. The results for the isentropic and quasi-isentropic trajectories are consistent with the results of Matsuno (1980) who showed theoretically that particle motions, when projected on to the meridional plane, are elliptical to first order if the
Figure 10. (b)-(d) Projections on to the meridional plane: (b) isobaric trajectory; (c) isentropic trajectory; (d) quasi-isentropic trajectory. The values along the isobaric trajectory have been increased by 175 m for ease of comparison.
diabatic heating is neglected. Hsu (1980) also found air parcel motions to be elliptical during a wavenumber-2 warming simulated by a model which had only Newtonian cooling as the diabatic heating but in which consistent vertical velocities were available. Moreover, the isentropic and quasi-isentropic trajectories presented here, which were computed for an observed wavenumber-2 stratospheric warming, agree qualitatively with Hsu (1980) both as regards the sizes of the ellipses and the vertical slope of their major axes.

![Graph showing heating and cooling rates](image)

**Figure 11.** Heating and cooling rates along the quasi-isentropic trajectory (Fig. 8(c)): --- infrared cooling rate; — — ozone solar heating rate.

The solar heating and infrared cooling rates along the quasi-isentropic trajectory are illustrated in Fig. 11, which may be compared with Fig. 5. The peak solar heating rates varied by a factor of two along the trajectory because of the changing latitude and altitude of the air parcel. The cooling rates were approximately in antiphase with the peak solar heating and attained the highest values when the geopotential height of the air parcel was a minimum.

Figure 12(a) illustrates the potential temperature along the trajectories; the isobaric values have been increased by 8 K and the adjusted values are plotted. The quasi-isentropic values decrease fairly steadily as explained in sub-section (a). For the February 1979 trajectory the solar heating is on average slightly greater than that in sub-section (a) because of the longer daylight period although this is counter-balanced by the effect of lower altitude where solar heating is weaker. However, the cooling is some 30% stronger than in (a) so that there is a net decrease in potential temperature of 74 K, approximately 20% greater than for the June 1979 trajectory. Potential temperature along the isobaric trajectory does not have a net change during the 10 days although the values fluctuate by about 60 K, showing how physically unrealistic an isobaric trajectory is in highly baroclinic conditions.
Figure 12. Lagrangian tracers along the trajectories of Figs. 8(a)–(c):
(a) Potential temperature: ——-isentropic; ——-isobaric; . . . quasi-isentropic.
The values along the isobaric trajectory have been increased by 8 K for ease of comparison.
(b) Potential vorticity: ——-isentropic; ——-isobaric; . . . quasi-isentropic; ——-theoretical (obtained
by solving Eq. (4)).
Figure 12(b) illustrates the daily averaged values of potential vorticity along the trajectories together with the theoretical values obtained by solving Eq. (4). For the first four or five days the quasi-isentropic values are consistent with the theory. On the 6th day the quasi-isentropic values decrease appreciably although they increase again in the last few days of the trajectory. When the Schoeberl and Strobel (1978) solar heating scheme was used the theoretical change in potential vorticity was increased slightly but this was insufficient to account for the discrepancy on days 6 and 8. Likewise changing the radiation parameters (ozone amount, cloud amount and ground albedo) of the Lacin and Hansen (1974) scheme had a small effect on the results.

Potential vorticity along the isentropic and isobaric trajectories has larger values than along the quasi-isentropic ones because of the factor $\frac{\partial \theta}{\partial p}$, which increases with height. Consequently, although the isentropic curve is more consistent with the theoretical curve on days 6 and 8, in general both isobaric and isentropic values are less consistent with theory than the quasi-isentropic results.

The above trajectories have quite low potential vorticity values. It is of interest to consider briefly trajectories starting in the eastern vortex with different values of potential vorticity to investigate whether the quasi-isentropic method is accurate for these situations. Figure 13 shows quasi-isentropic trajectories starting on the 850 K potential temperature surface on 21 February at 0001 GMT from (a) 50°N 50°E; (b) 60°N 50°E; (c) 70°N 50°E; (d) 80°N 50°E. Figure 14 gives the daily averaged potential vorticity along the trajectories together with the theoretical values (obtained by solving Eq. (4)) for the trajectory in Fig. 13(b). The trajectories may be compared with the trajectory which starts at the same time but from 40°N 50°E, see Fig. 8(c). From the geopotential height field on 21 February (Fig. 7(a)) it can be seen that the air parcels starting from 40°N 50°E and 80°N 50°E are on the edge of the eastern vortex. Both air parcels (Figs. 8(c), 13(d)) transfer to the western vortex after completing one circuit of the eastern vortex. The trajectory from 80°N reaches 89°N on 26 February and since the cross-polar flow is weak on this day (see Fig. 7(b)), the subsequent behaviour must be considered unpredictable. Although the trajectory until 26 February is qualitatively as expected the potential vorticity values (Fig. 14) decrease significantly on day 4, which cannot be explained by radiative effects. Consequently, in this example we can only be confident of the quantitative aspects of the first three days of the trajectory.

The trajectories starting from 50°N, 60°N and 70°N (Figs. 13(a), (b), (c)) remain entirely within the eastern vortex. The trajectory from 60°N starts close to the centre of the vortex on 21 February (see Fig. 7(a)) and has the largest initial potential vorticity of those trajectories presented. Potential vorticity along the trajectory is consistent with the theoretical values (obtained by solving Eq. (4)) for 4 or 5 days but thereafter decreases appreciably. For the trajectory starting from 70°N the agreement with theory is slightly better. On the other hand the trajectory starting from 50°N has a very rapid decrease in potential vorticity during the first 3 or 4 days which is much more rapid than predicted and the quantitative aspects of the whole trajectory must therefore be considered unreliable.

5. SUMMARY AND CONCLUSIONS

Stratospheric air parcel trajectories have been computed for two dynamically different situations. Firstly a quiescent period (June 1979 in the southern hemisphere) was chosen and trajectories were calculated using three different methods. The first method used the isobaric assumption, in which air parcels were assumed to remain on a constant pressure surface throughout. In the second method the Montgomery streamfunction was
Figure 13. Quasi-isentropic 10-day trajectories starting on 21 February 1979 with initial potential temperature 850 K and the following starting positions. (a) 50°N 50°E; (b) 60°N 50°E; (c) 70°N 50°E; (d) 80°N 50°E.
used to compute an isentropic trajectory. In the third method ('quasi-isentropic') an isentropic trajectory was calculated but a radiation model was used to adjust the entropy of the air parcel at regular intervals along the trajectory. These techniques were then employed to compute trajectories for the major stratospheric warming of February 1979.

During the quiescent period geopotential wave amplitudes were small and all three methods yielded nearly zonally symmetric trajectories which were all close together when projected on to a horizontal plane. In contrast, the heights of the trajectories revealed important differences. The quasi-isentropic trajectory decreased overall by about 1 km in geopotential height and was the most realistic trajectory in this respect, consistent with the vertical (Lagrangian) wind fields deduced by Murgatroyd and Singleton (1961). Further, the Lagrangian tracers (potential temperature and potential vorticity) for the quasi-isentropic trajectory were consistent with the theoretical evolution of the tracers whereas for the isobaric and isentropic trajectories the tracers were not consistent with theory. Thus, for the quiescent period investigated the quasi-isentropic trajectory was consistently more realistic than the other trajectories.

On 21 February 1979 the circumpolar vortex at 10 mb had just split into two at the start of the warming which intensified during the rest of February. As in June 1979 the horizontal projections of the three trajectories, which started on 21 February 1979 at 40°N 50°E, were very similar for the first six days but subsequently differed substantially. The trajectories began in the eastern vortex and had reached high latitudes on 22 February and also on 27 February, after completing one circuit around the eastern
vortex. The isentropic and quasi-isentropic trajectories then transferred to the western vortex for the remainder of the period, while the isobaric trajectory continued in the eastern vortex. As in June 1979 the vertical displacements of the trajectories depended substantially on the method of calculation. For the isentropic and quasi-isentropic trajectories the projections on to the meridional plane were qualitatively similar to the model simulations of Hsu (1980), adding credence to these methods. By comparison the isobaric trajectory was not very realistic in this respect. Further, it could be deduced, using the evidence from the Lagrangian tracers, that the quasi-isentropic trajectory was quantitatively realistic for 4 or 5 days. Other trajectories starting on 21 February from the eastern vortex were also studied briefly using potential vorticity. It was deduced that the trajectory starting from 60°N 50°E was quantitatively realistic for 5 or 6 days. On the other hand the trajectory starting from 50°N 50°E could be described as inaccurate, because potential vorticity was not conserved along it, after allowing for diabatic effects. Both these trajectories had high potential vorticity values. Thus the accuracy of the individual trajectory appears to be independent of the actual potential vorticity value.

For a quiescent period a great deal of confidence can be attached to the trajectories because the smooth slowly varying geopotential fields allow accurate time-interpolated gradient winds to be computed. In contrast, during a disturbed period, the events are changing more rapidly so that time interpolation would not be expected to yield such accurate results. Also, the computation of gradient winds from derivatives in the height field is liable to lead to error particularly in high latitudes. These weaknesses were deliberately exposed for the February 1979 trajectories by careful choice of the starting position and time. For the isentropic and quasi-isentropic trajectories starting at 40°N 50°E the air parcels reached 78°N at about 1900 GMT on 26 February. It was found that the parcel position at this stage was quite critical: a small perturbation might result in the parcel staying within the eastern vortex or transferring to the western vortex. Such a perturbation might arise because of a slightly inaccurate wind field. Under these circumstances we need to be able to attach some confidence or otherwise to a particular trajectory and quasi-conservative Lagrangian tracers might be used to do this. For example, for the February 1979 trajectories investigated, although the results were physically realistic, the fact that the quasi-isentropic trajectories did not obey the appropriate potential vorticity conservation law after day 6 implies that the trajectories followed by true air parcels may be quite different after six days. Bearing in mind the sensitivity of the trajectory starting from 40°N 50°E it is possible that the true trajectory remained within the eastern vortex whereas the calculated trajectory transferred to the western vortex. Consequently, care must be taken in using the results from trajectories calculated during disturbed conditions.

It is perhaps surprising that some of the trajectories remain realistic for as long as 5 or 6 days. This is mainly because of the large-scale nature of stratospheric disturbances in all three dimensions. Results from the ensemble of parcels suggest that the resolution of the data is sufficient to imply a typical parcel size of 5°×5°×2 km. For June 1979 the large horizontal wind shears imply that in 10 days the parcel had become very stretched along the trajectory track but was not otherwise seriously deformed. Likewise, the ensemble of trajectories starting near 40°N 50°E on 21 February 1979 had very similar tracks until 27 February, again suggesting some stretching of the air parcels. After this day, however, the ensemble of trajectories dispersed rapidly, severely distorting the air parcel shapes to the extent of making the trajectories physically meaningless. Thus the resolution in the data is not adequate to calculate a 10-day trajectory under these conditions. The trajectories had, however, become quantitatively inaccurate by this time suggesting that the resolution of the data in space is not the most limiting feature. It is
quite probable, therefore, that the limiting factor during the stratospheric warming was
the resolution of the data in time. This problem could be alleviated slightly by using a
more sophisticated time interpolation scheme although the basic problem would still
exist. There is a further practical difficulty which is related to the time resolution.
Occasionally stratospheric analyses are unavailable or only a superficial analysis is
possible. For February 1979 this occurred on 18th and 20th. Under these circumstances
trajectory computations are likely to be meaningless so that for an accurate trajectory
it is essential to have consecutive analyses at daily intervals at least.

Finally, although only a small number of trajectories have been presented in this
paper, it is possible on the basis of these results to suggest guidelines, as follows, for the
use of trajectories computed from satellite data:
1. It is suggested that the quasi-isentropic method should be adopted if trajectories are
required for up to 10 days. This method produces the most physically realistic results
particularly as regards the height of the parcel. This is particularly important in the
context of photochemical modelling along trajectories. For example near 30 km ozone
has a steep lapse rate in the vertical profile of the mixing ratio. This has a significant
impact on photochemically active chemical species since ozone strongly attenuates
radiation at important wavelengths, as well as participating in chemical reactions at the
air parcel height.

2. Isobaric or isentropic trajectories may be considered adequate for up to 3 or 4 days
if the horizontal position only is required. This period may be substantially reduced for
the isobaric method during disturbed conditions if the vertical height of the parcel is
important.

3. If the quasi-isentropic method is used potential vorticity should be computed along
the trajectory and compared with the theoretical evolution. Lack of agreement would
indicate possible errors in the computation. During quiescent conditions agreement
might last for 10 days while during very disturbed conditions agreement might typically
last 4 or 5 days.

4. Confidence in the trajectory can be substantiated or otherwise by considering traject-
cories for an ensemble of air parcels the initial positions of which are close together and
equally spaced from the original trajectory. If a large degree of dispersion is noted for
the ensemble, implying large distortions in the air parcel shapes, the central trajectory
should be used with caution.

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