A Method for Calculating Residence Times

ROBERT G. HEWITT AND BRIAN MARTIN

School of Physics, Sydney University, Sydney, N.S.W., 2006, Australia

A straightforward method for calculating residence times from properties of a medium is presented. The method is used to calculate some representative stratospheric residence times.

Consider a region of space containing a system of particles in motion, such as part of the atmosphere. It is often useful to know the average time a particle at a given place takes to move to a certain other place. If this other place is everywhere exterior to the region, we may speak of this average time as the residence time against exit from the system. In this paper, we show how such residence times may be derived from properties of the medium, such as winds and diffusion rates, and illustrate the technique by calculating some stratospheric residence times.

Basic Theory

To begin, let us look closely at how likely a particle is to move from one part of the region to another. Divide the region of space under consideration into a set of N boxes, labeled $i = 1, \cdots, N$, such that every particle is contained in some box. Furthermore, divide the time dimension into a number of equal intervals of duration τ. In principle these boxes and τ can be made arbitrarily small.

Let A_{ij} be the probability that a particle in the ith box moves to the jth box and B_i be the probability that the particle moves out of the set of boxes during any time interval τ. The A_{ij} and B_i will depend, for example, on winds, diffusion, and chemical processes; B_i represents removal of a particle in box i from the region either by simple movement, rainout, absorption on the surface of the earth, chemical destruction, or the like.

By conservation of particles during a time interval,

$$B_i + \sum_{j=1}^{N} A_{ij} = 1 \qquad i = 1, \cdots, N \qquad (1)$$

Let n_i be the average number of time intervals before a particle in the ith box exits from the region, including the interval when the exit takes place. A relation between the n_i may be written using the transition probabilities:

$$n_i = B_i + \sum_{j=1}^{N} A_{ij}(n_j + 1) \qquad (2)$$

$$i = 1, \cdots, N$$

Physically, this means that for a particle in a given box i the average number of time intervals for removal from the system is the sum of the probabilities of moving to each box j times the average number of time intervals for removal from that box plus one. The one represents the interval needed for movement to the box j. If the n_i are written as a column vector and the A_{ij} as a matrix, then by means of (1) the solution of (2) is

$$\mathbf{n} = (\mathbf{1} - \mathbf{A})^{-1}\mathbf{U} \qquad (3)$$

where $\mathbf{1}$ is the unit matrix and $\mathbf{U}$ is a column vector with every element equal to unity. Hence, given the transition probabilities $\mathbf{A}$ for a time interval τ, the average time for removal from the region of a particle beginning in any box i, $n_i\tau$, may be calculated by using (3). These times are referred to as the residence times of the system.

It is important to note that the solution (3) holds only if the probabilities $\mathbf{A}$ are constant in time. If $\mathbf{A}$ varies in time, the solution will be accurate to the extent that the time for change in $\mathbf{A}$ is large compared to the times $\mathbf{n}\tau$.

The usefulness of the concept of residence time is well known. For example, the total equilibrium mass in a region may be simply calculated if the residence time is known throughout the region. If each box i has a constant source S_i (mass added in a time interval), in equilibrium the region contains a total mass

$$\sum_{i=1}^{N} n_i S_i \tag{4}$$

The term exchange is often used in the same sense as residence time. However, it sometimes refers to a particular exit from the region, where more than one exit exists [e.g., *Pressman and Warneck*, 1970]. One particular case is the exchange time for transfer between the northern and southern stratospheres, or the time for interhemispheric mixing; in such a case, transfer to the troposphere may also occur. The neat solution given in (3) for residence times applies only when all sinks are included. When this is not done, there is no simple way of getting transfer times. (See Appendix 1 for details.)

Transition Probabilities

The matrix of box transition probabilities **A** is derived from the properties of the system that cause movement of a particular species from one part to another. For the atmosphere such mechanisms are either bulk motions, as from mean winds and gravity, or mixing, as from molecular and eddy diffusion.

The transition probability A_{ij} equals the fraction of the mass in box i that moves to box j in the time τ. The mass transfer equation may be written

$$m_j[n+1] = \sum_{i=1}^{N} m_i[n] A_{ij} + S_j \tag{5}$$

$$j = 1, \cdots, N$$

where $m_j[n]$ is the mass in box j at the nth time interval and S_j is the mass introduced into box j in a time interval. For any particular system the mass continuity equation may be reduced to some linear numerical form involving masses in boxes; comparison with (5) then determines the A_{ij}.

The easiest way to get a useful but simple expression for A_{ij} is to take a small interval τ and assume that the mass in box i does not change significantly during this time. Then physically a particle can only move to a box j that is adjacent to box i. In the absence of diffusion, A_{ij} is approximately given by the fraction of the volume of box i that moves into box j:

$$A_{ij} = \frac{\langle \mathbf{v} \cdot \mathbf{n} \rangle \sigma_{ij} \tau}{V_i} \tag{6}$$

σ_{ij} is the surface area common to boxes i and j, V_i is the volume of box i, and $\langle \mathbf{v} \cdot \mathbf{n} \rangle$ is the component of velocity of the particles perpendicular to the surface σ_{ij} averaged over that surface and over the time interval τ. To include contributions such as diffusion, $\langle \mathbf{v} \cdot \mathbf{n} \rangle$ may be replaced by a similar but more comprehensive term. The most drastic assumption used to derive (6) is that the mass in box i is uniformly distributed at any time. This gives rise to the denominator V_i. A more detailed analysis of mass distribution makes determination of **A** excessively complicated. Accuracy is more easily increased by increasing the number of boxes in the region, and thus the assumption of uniformly distributed masses is made more valid. The size of τ can be chosen arbitrarily, provided every A_{ij} is nonnegative and large enough to avoid numerical difficulties.

Sample Calculation

The method outlined above has been used to determine a set of representative stratospheric residence times against exit into the troposphere. A grid was assigned in the two dimensions of latitude and altitude (Figure 1). The boxes are formed by sweeping this grid around the earth longitudinally along the lines of latitude.

Solid lines represent impenetrable barriers, whereas boxes with surfaces generated by dotted lines contain sinks (i.e., mass flow into the troposphere). The transition probabilities were obtained by using the mean winds and eddy diffusion coefficients derived by *Reed and German* [1965], interpolated in space to give values at the box faces. (Since Reed and German's data were derived from winds and heat flux data, they may not be appropriate for particulate matter often traced in bomb blast studies. See also *Gudiksen et al.* [1968].) The matrix **A** was that proposed by *Bassett et al.* [1973]. Its detailed form is outlined in Appendix 2. Other forms of the transfer equation, such as those derivable from equation 28 of Reed and German, can also be used to obtain the matrix **A**.

Once **A** was determined, stratospheric residence times against transfer to the troposphere were obtained by using (3). The method by which the large (399 × 399) matrix **1** − **A** was inverted s outlined in Appendix 3. Residence times presented here (Figures 2–5) are for several different sets of velocities and diffusion coefficients. These times are comparable with times cited in the literature (e.g., *Pressman and Warneck* [1970] and references therein).

There are several sources of error present in the course of the calculation of the residence times presented here. Because of the significant contribution to the residence times of the particles that escape only after traveling higher than their original position, it is necessary to extend the upper boundary of the model considerably above any height for which useful results are sought. Reed and German's data extend to 27 km; the upper boundary of our model is 39 km. Residence times at altitudes near 27 km nevertheless are of reduced accuracy because (1) particles cannot move higher than 39 km and (2) the diffusion parameters used in the region above 27 km (in this calculation, the same as those at 27 km) lack detailed physical basis. We do not present residence times for altitudes above 27 km because of the second influence above. On the basis of a few sample calculations, we estimate that at 27 km these errors total to at most 5% and decrease rapidly with decreasing altitude.

At the lower boundary the representation of the tropopause is quite crude. The times presented here may best be considered as the average times to cross the penetrable boundaries indicated in Figure 1, whether or not they coincide with the actual tropopause. The effect of the difference between our simple representation of the tropopause and an accurate representation is rather small at a distance of several kilometers from this boundary. At smaller distances interpretation of our results is difficult and not necessarily meaningful; hence no isolines are presented in Figures 2–5 for times less than 0.3 year. It should be remembered that calculations of residence times for particles at the tropopause or in the troposphere (against contact with the earth's surface, for example) must include averaging over the fraction of particles that pass through the stratosphere before reaching the sink.

Other errors can arise from the finite size

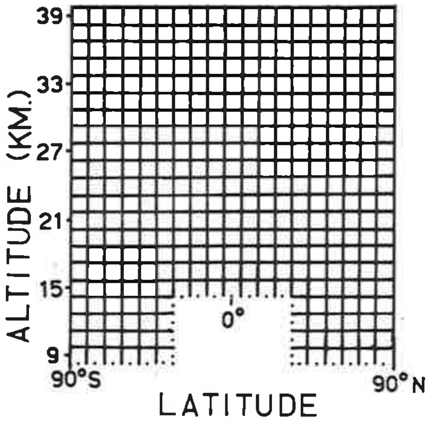

Fig. 1. A grid representing the division of the stratosphere into boxes. The longitudinal direction extends perpendicular to the page.

of the boxes, the particular numerical form of the transfer equation adopted, and computer roundoff. These are small effects, of the order of a few percent at most.

Of most decisive importance in determining the magnitude of the residence times are the values of the winds and eddy diffusion coefficients. In actuality these values change in time, whereas our calculation assumes them to be time independent. In a situation with time dependent parameters the residence times should be bounded by times calculated by using as time independent parameters the highest and lowest rates of diffusion.

Residence times presented in Figures 2 and 3 are based upon Reed and German's transport coefficients for February and May. Times based on the parameters for August and November are

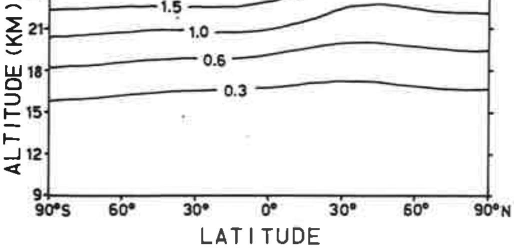

Fig. 2. Contours of stratospheric residence times based on Reed and German's transport coefficients for February. The times are in years.

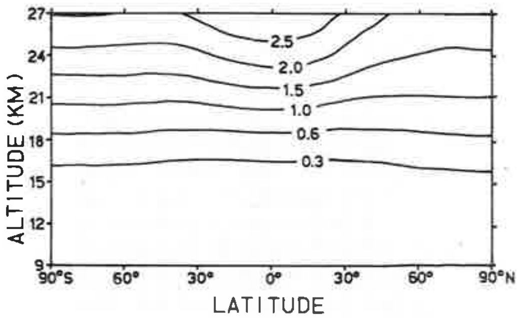

Fig. 3. Contours of stratospheric residence times based on Reed and German's transport coefficients for May. The times are in years.

almost exactly equal to those for February and May, respectively, but with the reversal of the hemispheres. (Parameters for the southern and northern hemispheres were assumed equal for any given season, except for sign reversals, for the purposes of the calculation, of the horizontal mean wind and anisotropic eddy diffusion coefficient.)

If all the winds and eddy diffusion coefficients are multiplied by a constant factor, the residence times are simply divided by the same factor. Thus independent estimates of residence times implicitly determine the transport parameters to a certain extent. If the ratios between the transport parameters are altered, there is no simple scaling method. To illustrate this problem, calculations were made of residence times with horizontal winds and horizontal eddy diffusion coefficients multiplied by 0.1 and are presented in Figures 4 and 5. It is seen that these times are mostly greater than those in

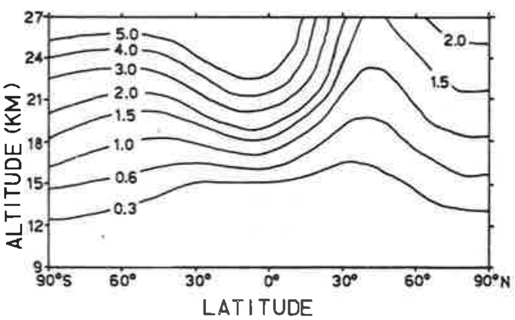

Fig. 4. Contours of stratospheric residence times based on Reed and German's transport coefficients for February with the horizontal parameters multiplied by 0.1. The times are in years.

Figures 2 and 3. A similar calculation, with horizontal transport parameters multiplied by 10, showed only a small decrease from the values in Figures 2 and 3. The scaling method would therefore imply that, if the vertical winds and diffusion coefficients were multiplied by 0.1 and the horizontal parameters left the same, the times in Figures 2 and 3 would be multiplied by a factor only slightly less than 10. This indicates that for Reed and German's data the horizontal motion is rapid enough that vertical motion is the most important determinant of the stratospheric residence times against exit into the troposphere.

APPENDIX 1

If a particle in a box may exit from the region through more than one sink, the average time to reach a particular sink is infinite, since some particles never reach it. We may instead consider the average time to get to the sink for those particles that eventually get there. It is apparent that such a time may be determined for movement to any box as well as to a particular sink.

To analyze the situation, let p_{ik} be the probability that a particle in box i eventually reaches box k (i.e., does not leave the region instead), and let n_{ik} be the average number of steps taken by those particles that do make the journey to box k. Box k may be considered to be a particular sink if desired. Then

$$p_{ik} = \sum_{j=1, j\neq k}^{N} A_{ij}p_{jk} + A_{ik} \qquad i, k = 1, \cdots, N$$

$$n_{ik} = \sum_{j=1, j\neq k}^{N} A_{ij}p_{jk}(n_{jk} + 1) + A_{ik} \qquad i, k = 1, \cdots, N$$

Unfortunately, the solution to this set of equations is at least as difficult to compute as the time evolution of the mass transport equation, which also can give the average times taken to reach various areas.

APPENDIX 2

Presented below is our form of (5), from which **A** may be derived. This form is discussed in *Bassett et al.* [1973]. A representative set of boxes is pictured and labeled in Figure 6; terms not defined explicitly are the same as those used by *Reed and German* [1965].

$$m_5[n+1] = m_5[n]$$
$$-\left[\begin{Bmatrix} C_5\langle V'\rangle & \text{if } \langle V'\rangle > 0 \\ C_6\langle V'\rangle & \text{if } \langle V'\rangle < 0 \end{Bmatrix} - K_{yy}'(C_6 - C_5)\right.$$
$$\left. - \begin{Bmatrix} K_{yz}'(C_3 - C_8) & \text{if } K_{yz}' > 0 \\ K_{yz}'(C_2 - C_9) & \text{if } K_{yz}' < 0 \end{Bmatrix}\right]_{(y+1/2\Delta y,\, z),\, [n]}$$
$$+ R + S_5$$

where R represents terms analogous to the one in large brackets, due to fluxes through the faces of box 5 that border boxes 2, 4, and 8.

In this equation $C_i = m_i/V_i$, where V_i is the volume of box i,

$$\langle V'\rangle = (\langle v\rangle - \Gamma K_{yz}) A\tau$$
$$K_{yy}' = \left(\frac{K_{yy}}{\Delta y} - \frac{|K_{yz}|}{2\Delta z}\right) A\tau$$
$$K_{yz}' = (K_{yz}/2\Delta z) A\tau$$

and

$$A = \Delta z 2\pi a \cos\left(\frac{y + \frac{1}{2}\Delta y}{a}\right)$$

Here $\langle v\rangle$ is the average horizontal velocity.

Within the large square brackets, the wind and diffusion parameters are evaluated at $(y + \frac{1}{2}\Delta y, z)$, i.e., the midpoint of the face between boxes 5 and 6, and the mass at time interval n.

APPENDIX 3

Suppose the time step τ is chosen small enough that the transition probabilities A_{ij} are nonzero only if i and j are the labels of physically neighboring boxes. The matrix $\mathbf{1} - \mathbf{A}$ is then very sparse, having at most nine nonzero elements in any row or column. Before any attempt is made to solve (3), it is clearly advantageous to order the boxes in such a way that these nonzero elements are localized in an ordered pattern of submatrices or blocks.

One way of achieving this is to number the boxes sequentially left to right across the rows of Figure 1, beginning at the bottom of the stratosphere. The matrix $\mathbf{1} - \mathbf{A}$ can then be partitioned so that the i, jth element lies in a block whose dimensions are the number of boxes in the rows containing boxes i and j, respectively. Since the element A_{ij} is nonzero only if i and j lie either in the same or adjacent rows, $\mathbf{1} - \mathbf{A}$ is tridiagonal in blocks; i.e., it has nonzero elements only in a set consisting of diagonal blocks and blocks immediately adjacent to the diagonal.

It is useful for computational purposes to have all blocks the same size. This can be achieved by increasing the size of the matrix by including rows and columns with unity in the diagonal positions and zero elsewhere. This procedure does not affect the inverse of the original matrix. In our computation, 28 such rows and columns were introduced.

All elements in blocks immediately below the diagonal may be successively eliminated by

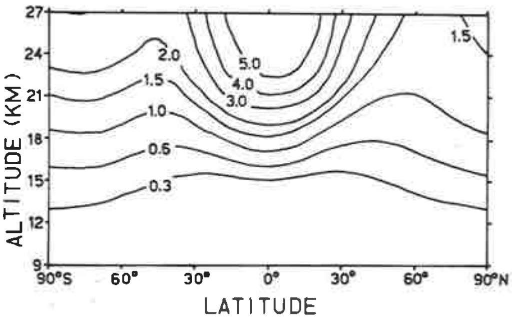

Fig. 5. Contours of stratospheric residence times based on Reed and German's transport coefficients for May with the horizontal parameters multiplied by 0.1. The times are in years.

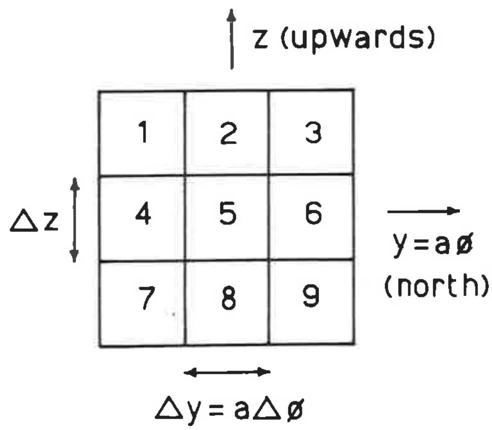

Fig. 6. A grid representing a set of neighboring boxes. The longitudinal direction extends perpendicular to the page.

using pivots selected in the conventional manner from the diagonal blocks. These pivots can also be used to eliminate appropriate nonpivot elements in the diagonal blocks so that the transformed matrix can be solved by using back substitution.

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