Some aspects of simulating large scale atmospheric mixing

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ABSTRACT

The classical picture of one-dimensional diffusion in a homogeneous fluid results in a symmetrical distribution of the conservative property around the peak concentration while the latter remains fixed in space. This paper examines the asymmetry and movement of the peak resulting from mixing in a non-homogeneous fluid.

A one-dimensional model comprising 21 boxes permits the diffusive flux across the wall of each box equal to the coefficient of eddy diffusion times the air density multiplied by the gradient of (mixing ratio) concentration. The end boxes are half the volume of the others and there is no flux across the ends of the model. The divergence of this flux creates the change in concentration in each box.

With constant diffusion coefficients and density, the peak (mixing ratio) concentration initially in the center of the model remains fixed and symmetry exists for all times as theory predicts. Firstly, placing the point source near either edge produces asymmetry due to reflection of the Gaussian curve, also in accord with theory. The peak concentration actually shifts with time, its movement depending on the magnitude of the eddy diffusion coefficient and proximity to the edge.

Secondly, the peak concentration initially in the middle of the model moves upward for the case of a constant diffusion coefficient but with density decreasing as in the standard atmosphere. For example, for a coefficient of 10^4 cm^2 sec^{-1}. The rate of rise increases with an increasing coefficient and vice versa. When the model contains a strong diffusion regime, or a troposphere, to about 9 km and a transition to smaller coefficients above 17 km, the stratosphere, then the rate of rise of the peak concentration increases (rising from 20 to 40 km in 24 rather than 30 months for a stratospheric coefficient of 10^4 cm^2 sec^{-1}). The removal of tracer material from below also increases the ascent rate of the peak concentration.

Thirdly, models with constant density but variable coefficients of diffusion produce considerable asymmetry and some drift of the peak concentration with altitude.

Finally, the one-dimensional model may be adapted to a spherical earth with constant horizontal air density. Material added at the equator diffuses symmetrically into both hemispheres as expected. But injections at other latitudes produce asymmetries such that, for example, the peak concentration shifts from 45° to the pole in 30 months if the coefficient of horizontal diffusion is 10^9 cm^2 sec^{-1}.

An attempt will be made to explain the asymmetries and try to distinguish between possible real atmospheric effects and those due to the model simulation. The artificial substitution of a three dimensional world by a one dimensional model must be recognized.

Introduction

Classical diffusion theory in a homogeneous fluid predicts a peak concentration which remains at the same place in time. Material (or conservative properties) diffuses away from the source producing a symmetrical picture. It is the purpose of this paper to present illustrations of the movement of the maximum concentration and the development of concentration asymmetries in a non-homogeneous fluid. These results may help interpret the findings of more complex two or three dimensional models.

First, it is appropriate to describe the numerical model. Twenty-one equi-spaced boxes are arranged along a straight line. The bottom and top boxes are one half the volume of the other 19 boxes, as is evident in Fig. 1. The flux across the interface between each box is calculated from the formula.

$$F = -K\varrho\partial q/\partial s$$

where F is the flux (grams of matter per unit area per unit time); K, the diffusion coefficient (in cm^{-2} sec^{-1}); ϱ, the density (grams of air

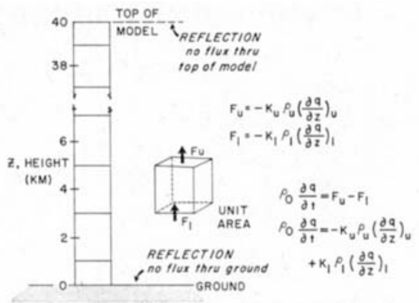

FIG. 1. The one-dimensional diffusion model.

cm^{-3}); q, the concentration (grams of matter per gram of air); and s, the direction of the coordinate system. In the one dimensional model, either or both the eddy diffusion coefficient or the density can vary. The difference between influx and efflux determines the change of concentration in each box. In all the examples but one, a fixed input is placed only in one box at the initial time, the changes are computed in each box in time steps and after a given number of such iterations, one views the new concentration distribution.

As in most numerical calculations, the substitution of finite differences for continuous functions introduces errors. Fig. 2 illustrates the magnitude of these errors for a very simple case of a tracer added to the middle of the model and in which the space and time steps have been successively reduced. The continuous line depicts the theoretical distribution, a Gaussian curve with a standard deviation equal to the square root of twice the eddy diffusion coefficient multiplied by the elapsed time. It is clear that as the time and space steps become smaller, the fit to the theoretical curve improves. The reason for the lack of fit below 18 and above 22 kilometers for the smaller time and space step profile is the proximity to the boundary for these runs. Despite the errors introduced by the 2 kilometer space and one day time step, this grid has been used in all subsequent illustrations in order to permit the model to extend from the ground to 40 km. One might note that the error attributed to coarse grid becomes smaller with time.

Boundary effects

The first type of asymmetry to be discussed exists even for a fluid with both constant density and constant eddy diffusion coefficients. If the insertion takes place close to the edge of model and if one assumes reflection at either boundary, then obviously an asymmetry will result. This is illustrated in Fig. 3 in which the input occurs at 4 kilometers (between 3 and 5 kilometers), with a diffusion and density field identical with the previous case. The saw-tooth profiles after 1 and 4 months illustrate the computed asymmetry. The displacement of the peak concentration after 4 months brings it to the ground. It is to be noted that the highest concentration at the ground is only slightly

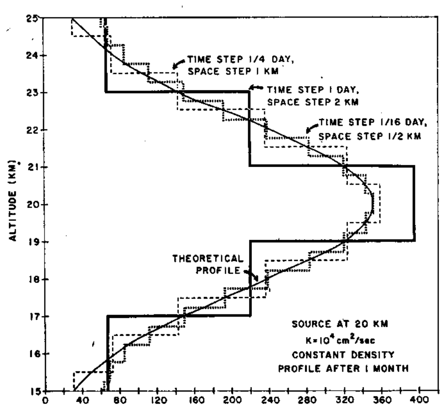

FIG. 2. A comparison of theoretical profiles with model computed profiles using successively finer time and space grids.

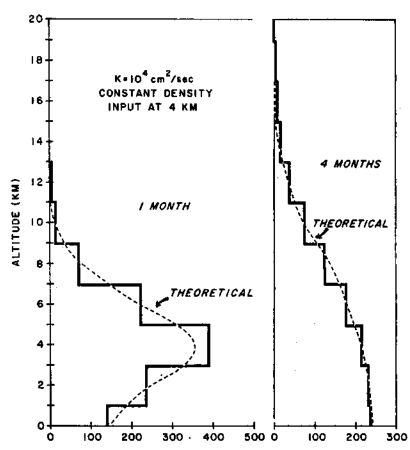

FIG. 3. The migration of peak concentration to the lower boundary of the model.

greater than that in the next higher box. The movement of the peak toward the boundary can be determined theoretically using the conventional methods of images. In fact, the continuous curves on Fig. 3 show the theoretically determined profiles. The discrepancy between the theoretical and model computed profiles results from the coarse finite difference grid in the latter.

Fig. 4, a graph determined from theory, shows the time, along the abscissa, it takes for the peak concentration to reach a boundary from an initial source at a distance from the boundary given in kilometers on the ordinate and in a field of constant eddy diffusion given by the sloping lines. Thus, at a distance of 4 kilometers from the boundary, using a coefficient of diffusion of 10^4 cm^2/sec, it takes about three months for the peak to reach the boundary. The previous figure showed that a month later, at four months, the machine computation already brought the peak to the ground.

This migration of the peak concentration probably possesses little significance in the real atmosphere because one is rarely interested in the position of the peak concentration after extended times, that is, months in the troposphere. But it may introduce misleading results for models in the stratosphere where a source is introduced near the upper artificial boundary and then followed for long times.

Variable density

Fig. 5 plots the altitude of the peak concentration as the ordinate vs time, expressed as months, along the abscissa. The numbers adjacent to the dots signify the percentage excess of the peak, concentration over the average concentration on either side of the peak or the peakedness. Thus, if the peak concentration is 100 units at 22 kilometers and the concentration at 20 kilometers is 97 and that at 24 kilometers is 99 units then the percentage excess will be denoted as 2.0%. In all cases, except as noted, concentrations are expressed as mixing ratios not as concentration in per unit volume.

The horizontal dashed line and dots correspond to the previous case of 10^4 cm^2/sec for the diffusion coefficient and a contant density. The solid line corresponds to the same diffusion coefficient but with density decreasing with altitude in accordance with the standard atmosphere. It

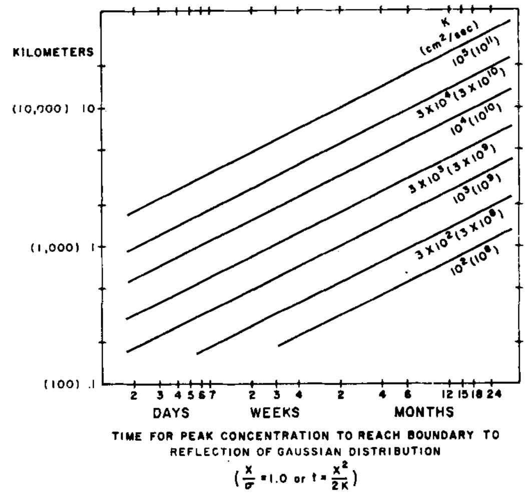

FIG. 4. A nomogram to determine the time it takes for the peak concentration to migrate to a boundary. This nomogram is obtained from theoretical calculations.

is clear that the peak concentration rises in altitude with time and at a significant rate; reaching the top of the model in about 30 months. The reason for the non-smooth curve on this and successive figures lies in the fact that the vertical profile from the machine output happens to be printed out at three month intervals. Fig. 6 shows that the increase in height will occur at either nearby altitudes with the same rate of rise when the density decreases with altitude. Finally, the last of this series of figures, Fig. 7, demonstrates the dependence of the rate of rise on the coefficient of diffusion. The rate of ascent increases with increasing diffusion coefficients and vice versa.

Why should the peak concentration rise? Table 1 illustrates the sense and reasons for the asymmetry. At the initial time, we consider a mixing ratio concentration of 1000 marked atoms per gram of air in one box and zero in all other boxes. The second and third columns provide the constant values of the coefficient of diffusion and the decreasing values of air density with altitude. The fourth column converts the concentration per gram of air into atoms per cm^3 by multiplying the mixing ratio by the air density in each box and assuming the boxes to have a cross section area of one cm^2. The fifth column indicates the number of atom in each box, obtained from column four by

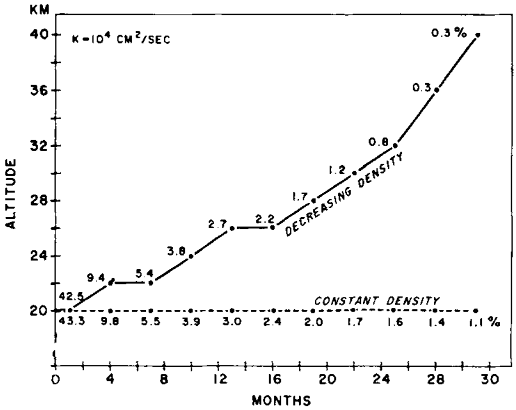

Fig. 5

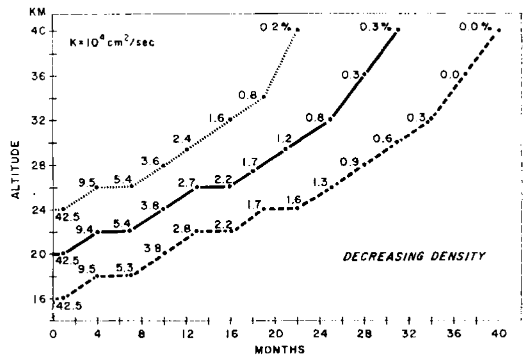

Fig. 6

FIG. 5. The time history of peak mixing ratio concentration for a model with a constant coefficient of diffusion and decreasing density.

FIG. 6. The time history of peak mixing ratio concentration for a model with a constant coefficient of diffusion and decreasing density; source altitude at 16, 20 and 24 kilometers.

multiplying by 2 kilometers, the depth of the box. The sixth column provides the flux across each interface using the indicated formula and allowing the flux to act over a period of 10^5 seconds or a little over one day. This flux removes atoms through each interface reducing the number of atoms in the source box by exactly the number added to the adjacent boxes. These atoms per box are then converted back to concentration per cm^3 in column 8 and to concentration per gram in column 9. In column 9, it is evident that even though more atoms moved downward (column 6), the concentration per gram is considerably higher above than below the source. Carried through many iterations, the peak concentration of mixing ratio actually migrates upward. However, one may also note that when the concentration is expressed per cm^3, as in column 8, the higher values are at a lower altitude and the peak concentration per cm^3 moves downward. Thus, figure 8 shows the relative vertical distribution of concentration expressed per unit mass or the mixing ratio illustrating the upward movement of the peak mixing ratio concentration after 10 months and the downward movement of the peak concentration of the concentration in per unit volume under the same conditions.

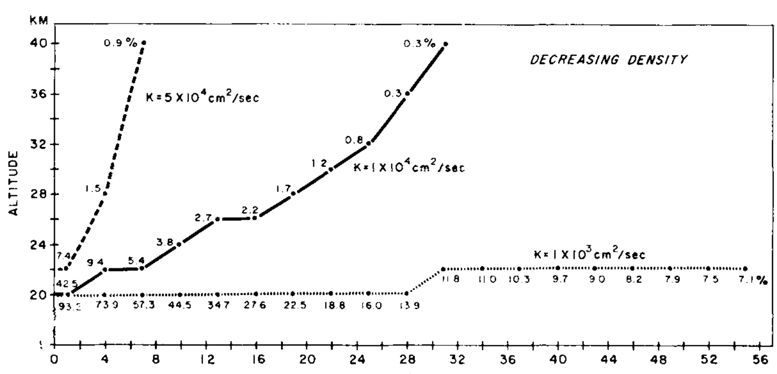

FIG. 7. The time history of peak mixing ratio concentration for a model with a constant (but different for each case) coefficient of diffusion and decreasing density.

TABLE 1. *The explanation for asymmetry in an atmosphere with decreasing density. The time step, Δt, has been chosen as 10^5 seconds.*

ALT. (KM)	1 q CONC. ATOMS/GM	2 K $CM^2\ SEC^{-1}$	3 ρ GM/CM^3	4 $q \times \rho$ CONC. $ATOMS/CM^3$	5 # OF ATOMS IN BOX OF $1\ CM^2$ AREA	6 FLUX $-K\rho \frac{\partial x}{\partial z} \Delta t$	7 # OF ATOMS IN BOX	8 $q \times \rho$ NEW CONC. $ATOMS/CM^3$	9 q NEW CONC. ATOMS/GM
		10^4							
22	0		$.0628 \times 10^{-3}$	0	0		367.	.00184	29.24
21		10^4	$.0734 \times 10^{-3}$			↑ 367.			
20	1000		$.08593 \times 10^{-3}$	.08596	$\times 2 \times 10^5$ 17191.		16321.	.08160	949.4
19		10^{4*}	$.1006 \times 10^{-3}$			↓ 503.			
18	0		$.1176 \times 10^{-3}$	0	0		503.	.00252	21.38
		10^4							

In some problems, meteorologists assume that the Austausch ($K\rho$) rather than the coefficient of eddy diffusion remains constant with height. Fig. 9 shows that the rate of ascent of the peak concentration (of mixing ratio), the dashed line, is very rapid if the Austausch is kept constant. The Austausch in this example corresponds to an eddy diffusion coefficient of 10^4 cm²/sec and the density at 20 kilometers. The rate of ascent can be compared with the rate of rise of the peak concentration with a constant coefficient of eddy diffusion (the solid line). It is thus seen that if one desires to avoid the rising peak concentration, substitution of a constant Austausch in lieu of a constant eddy diffusion coefficient is not the solution. In fact there is no way of keeping the peak at exactly the same altitude or of maintaining a symmetrical distribution in the presence of a decreasing density field. Low rates of diffusion slow the rate of ascent. A decrease of the coefficient with altitude also tends to maintain symmetry and can alter the ascent as seen below.

Variation of diffusion coefficient with altitude

It is evident that a model in which the coefficient of diffusion changes with altitude will also introduce asymetric distribution from a point source. In this paper, the patterns of vertical distribution will primarily be limited to cases on non-uniform diffusion coefficient in a field of decreasing density. There are a number of peculiar or unexpected findings in the model containing constants density with varying coefficients of diffusion. An example appears as the dashed curve on Fig. 10. This figure compares the rate of rise for a model with constant density and with decreasing density. For both cases, coefficient of diffusion decreases linearly with height from 20×10^3 cm³/sec at 1 kilometer to 1×10^3 cm²/sec at 39 kilometers. The coefficient of diffusion in the vicinity of the source input at 20 km, again, is 1×10^4 cm²/sec. Previously, it was shown that the peak concentration rose to 40 kilometers in about 30 months but in the case of decreasing coefficients of diffusion of Fig 10, the peak does not reach the top of the model by five years.

Of greater interest might be the case of trying to simulate a troposphere and stratosphere in a one dimensional model. Both examples of

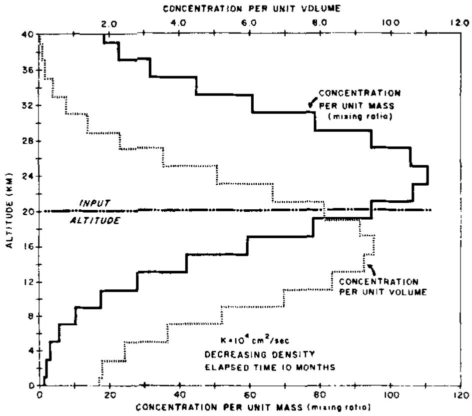

FIG. 8. A comparison of vertical profiles expressing the concentration as per unit mass and per unit volume.

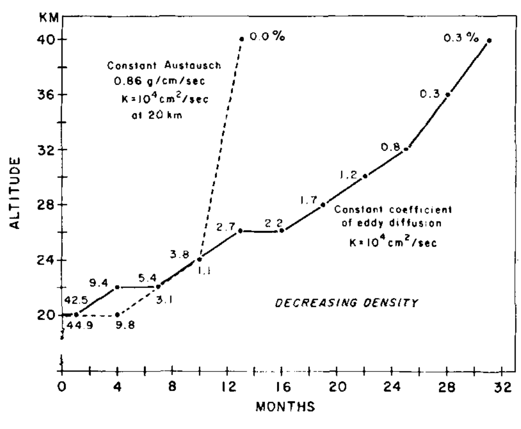

FIG. 9. A comparison of the history of the peak mixing ratio concentration for an atmosphere with decreasing density but with either a constant coefficient of diffusion or constant Austausch.

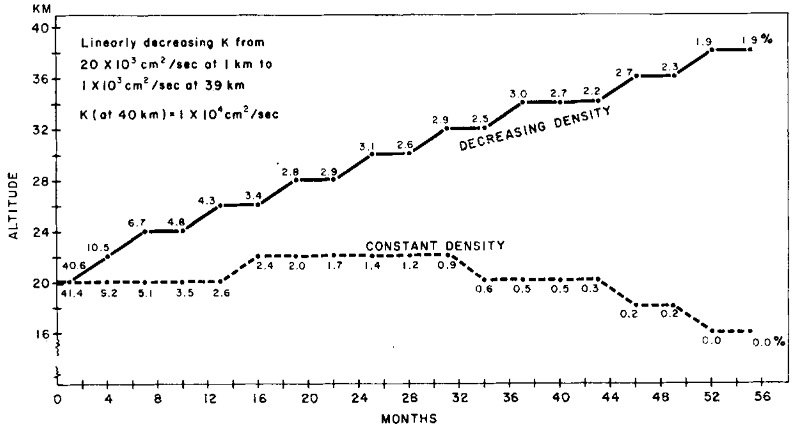

FIG. 10. The history of peak mixing ratio concentration for a model with linearly decreasing coefficients of eddy diffusion; a comparison between constant and decreasing density.

Fig. 11 are based on a density decrease with altitude. The first, solid line, repeats the ascent rate of peak concentration for a diffusion coefficient equal to a constant 10^4 cm²/sec. The second, the dashed line, depicts the rise in altitude of peak concentration in a model with a tropospheric mixing coefficient of 5×10^5 cm²/sec to 9 kilometers, a stratospheric coefficient of 1×10^4 cm²/sec beginning at 17 kilometers and a transition between 11 and 15 kilometers. Note that in both curves the coefficient is 10^4 cm²/sec in the region around and above 20 kilometers, the input altitude. It is evident that the presence of a troposphere increases the ascent rate of the peak concentration. It also increases the descent rate for the peak concentration expressed as per unit volume.

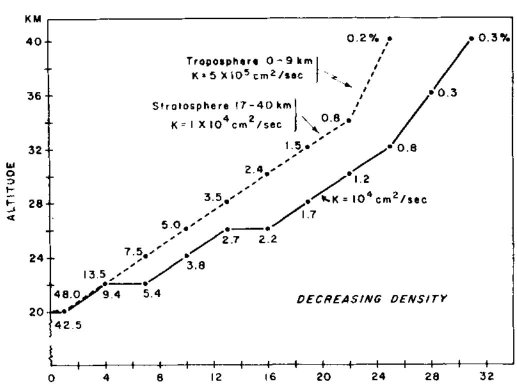

FIG. 11. The time history of a model with decreasing density but a simulated troposphere and stratosphere; a comparison with a model containing a constant coefficient of eddy diffusion.

Sink at the ground

The reason for the enhanced upward migration of the peak concentration when one introduces a troposphere lies in the more rapid downward movement of the tracer material which "eats away" the material in the lower stratosphere. This is further illustrated by introducing a sink at the ground in a model with a troposphere and stratosphere as shown in Fig. 12. One finds that the rate of ascent of the peak increases when a sink is present in the troposphere. Thus, in this example, the peak reaches the model top almost a year earlier with a sink than without one.

Spherical earth

The one dimensional model just described may be modified and scaled to simulate north-south horizontal diffusion on a spherical earth. One finds that the convergence of the meridians as well as the boundaries at the poles introduces assymmetry and migration of the peak concentration towards the poles. Thus, Fig. 13 illustrates north-south profiles after 13 months for a coefficient of eddy diffusion equal to 10^{10} cm²/sec. The distribution about the equatorial source is symmetrical, as expected, but

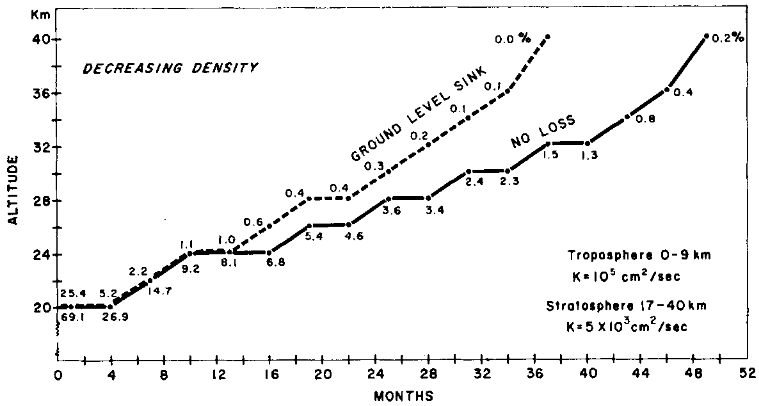

FIG. 12. The time history of a model with decreasing density for a simulated troposphere and stratosphere; a comparison with and without a sink at the ground or at the bottom of the model.

as the source moves from 9° to 45° to 72°N, the resulting pattern becomes more and more distorted and in each case the peak has shifted from the source latitude to the north pole. It is of interest to note that the boundary effect alone would have shifted the peak from 9°N to the pole in about 16 months, whereas the sphericity of the earth speeded up this displacement to less than a year.

Discussion and conclusion

Certain of the model features producing asymmetry may be artifacts while others must, in part, be viewed as real atmospheric features.

1. Asymmetries due to the lower boundary are real but those due to the upper are artificial.
2. The decreasing density must be viewed as a real cause of asymmetry but when one uses a more realistic eddy diffusion coefficient in the stratosphere of about 5×10^3 rather than the 10^4 cm²/sec used for most of the examples, the rate of development of the asymmetry, although still present, may be too slow to be significant.
3. The presence of a troposphere and especially a ground level sink tends to enhance the asymmetry and upward motion of the peak concentration in the stratosphere and is a real feature of the atmosphere for some tracers.
4. The convergence of the meridians on a spherical earth in creating asymmetries must also be viewed as a real atmospheric feature.

On the other hand, many of the exact details of the asymmetry illustrated in this paper may be quantitatively in error because of too large a grid spacing. One should also consider that the magnitude of many of the features of asymmetry may easily be lost in the real and instrumental noise of the tracer measurements. In conclusion, this paper has illustrated models of atmospheric diffusion in one dimension containing asymmetrical distributions from point sources.

A final caution should be noted. The atmosphere is three dimensional, not one dimensional as treated in the paper. In the case of vertical mixing, the sources should be contained in a horizontally uniform area. In the case of diffusion on a spherical earth, the results are most applicable if the tracer material is quickly spread in the vertical and in the east-west plane compared with north-south diffusion.

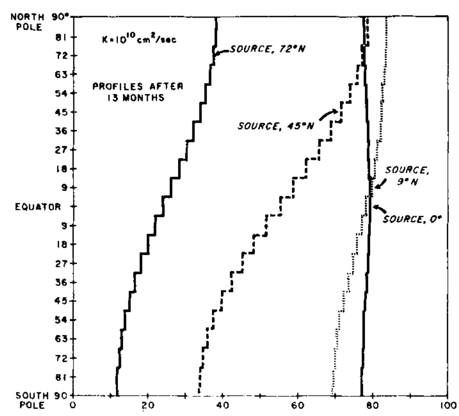

FIG. 13. North-south concentration profiles for an atmosphere on a spherical earth; a comparison of distributions from different source latitudes.

НЕКОТОРЫЕ АСПЕКТЫ МОДЕЛИРОВАНИЯ КРУПНОМАСШТАБНОГО ПЕРЕМЕШИВАНИЯ АТМОСФЕРЫ

Классическая картина одномерной диффузии в однородной жидкости проявляется в симметричном распределении сохраняющихся характеристик вокруг пика концентрации, в то время как последний остается фиксированным в пространстве. Эта статья посвящена исследованию ассимметрии и движения пика в результате перемешивания в неоднородной жидкости.

Одномерная модель, содержащая 21 элементарный объем, допускает диффузионный поток поперек стенки каждого объема, равный коэффициенту турбулентной диффузии, умноженному на плотность воздуха и на градиент (или отношение смеси) концентрации. Дивергенция этого потока создает изменения в концентрации в каждом объеме. Объемы на концах выделенного столба равны половине обычного объема, поток через границы модели отсутствует.

При постоянных коэффициентах диффузии и плотности пик (отношение смеси) концентрации первоначально остается фиксированным в центре модели и, как предсказывает теория, для всего времени существует симметрия. Во-первых, помещение точечного источника вблизи какого-либо турбулентного вихря вызывает ассимметрию, обусловленную отражением гауссовской кривой, что также находится в согласии с теорией. Пик концентрации действительно сдвигается со временем, его движение зависит от коэффициента турбулентной диффузии и от близости к краю.

Во-вторых, вначале пик концентрации в середине модели движется вверх для случая постоянного коэффициента диффузии, но при этом уменьшается плотность, также как и в стандартной атмосфере. Например, для коэффициента 10^4 см^2 сек$^{-1}$ скорость подъема увеличивается с увеличением коэффициента и наоборот. Когда модель содержит сильный диффузионный режим, или тропосферу до 9 км, а затем переход к меньшим коэффициентам выше 17 км (стратосфера), то скорость подъема пика концентрации увеличивается (время подъема от 20 до 40 км в 24 раза дольше времени подъема, равного 30 месяцам для коэффициента 10^4 см^2 сек$^{-1}$ в стратосфере).

Удаление трассирующего материала снизу также увеличивает скорость подъема пика концентрации.

В третьих, модели с постоянной плотностью, но переменными коэффициентами диффузии вызывают заметную ассимметрию и некоторый дрейф пика концентрации с высотой.

Наконец, одномерную модель можно приспособить для сферической земли с постоянной горизонтальной плотностью воздуха. Вещество, вводимое на экваторе, диффундирует симметрично, как это и ожидалось, в оба полушария. Но введение вещества на других широтах вызывает ассимметрию, так что, например, пик концентрации сдвигается с 45° к полюсу за 30 месяцев, если коэффициент горизонтальной диффузии равен 10^9 см^2 сек$^{-1}$.

Будет сделана попытка объяснить эту ассиметрию и провести различие между реальными эффектами атмосферы и эффектами, обусловленными моделью. Следует иметь в виду искусственную замену трехмерного мира одномерной моделью.