NOAA Technical Memorandum ERL ARL-155

DEPARTMENT OF COMMERCE
UNITED STATES OF AMERICA

THE USE OF BACK AIR TRAJECTORIES IN INTERPRETING ATMOSPHERIC CHEMISTRY DATA: A REVIEW AND BIBLIOGRAPHY

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noaa NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION / Environmental Research Laboratories

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ABSTRACT. One of the most important aspects of atmospheric chemistry is interpreting the measurements of different chemical species in terms of their cycles in the earth-atmosphere system. One method--the calculation of single, back trajectories from the point of measurement--has been widely and successfully employed to evaluate transport of chemical substances in the atmosphere. This paper reviews how the single-trajectory analysis has been applied in atmospheric chemistry. It surveys the different models used, the methods of application, and the forms in which the results are presented. Important new analysis techniques have been developed in the last few years, such as flow climatology, automatic computer categorization, the use of meteorological forecast model output, and others. Despite its limitations, the single, back-trajectory analysis method has proved very useful in the interpretation of atmospheric chemistry data.

1. INTRODUCTION

Attempting to describe the path that both natural and anthropogenic substances follow in the atmosphere has become an important area of meteorological research. For the last several decades, scientists have tried to design ways of understanding and measuring these atmospheric pathways. Analyzing such transport requires that the measurements of the structure of the atmosphere be organized in some fashion. This paper is a review of one approach that has proved particularly useful, that is, calculation of single, back trajectories and evaluation of atmospheric chemistry data using these calculations.

Use of the concept of a trajectory has been a standard meteorological technique for over 30 years. In essence, a trajectory is the path of an imaginary air parcel as it is acted on by the winds (Huschke, 1959). Usually this idea has been applied to forward motion; that is, the parcel starts at some point and is pushed by the winds at a given level or surface of interest. One application of single, forward trajectories is to follow a parcel from the source of a given substance and to see where the material could be transported. When continuous or intermittent atmospheric chemistry measurements are made at some point, either on the ground or in the air, then the origin of the path of travel of that sampled air is of interest in interpreting the data. Thus for a chemical measurement at a given time and place, a single, back trajectory can be calculated, giving the path that the air parcel traveled previous to the measurement. An example of several single, back trajectories for one day is shown in Fig. 1, where the time refers to when the imaginary parcel whose path is described by the trajectory passed over the point of interest (the western Mediterranean). In this case, 10-day, 850 mb and 700-mb trajectories are shown. The number refers to the day back in time; that is, 1 is the position of the parcel 24 hours earlier, 2 is 48 hours earlier, etc.

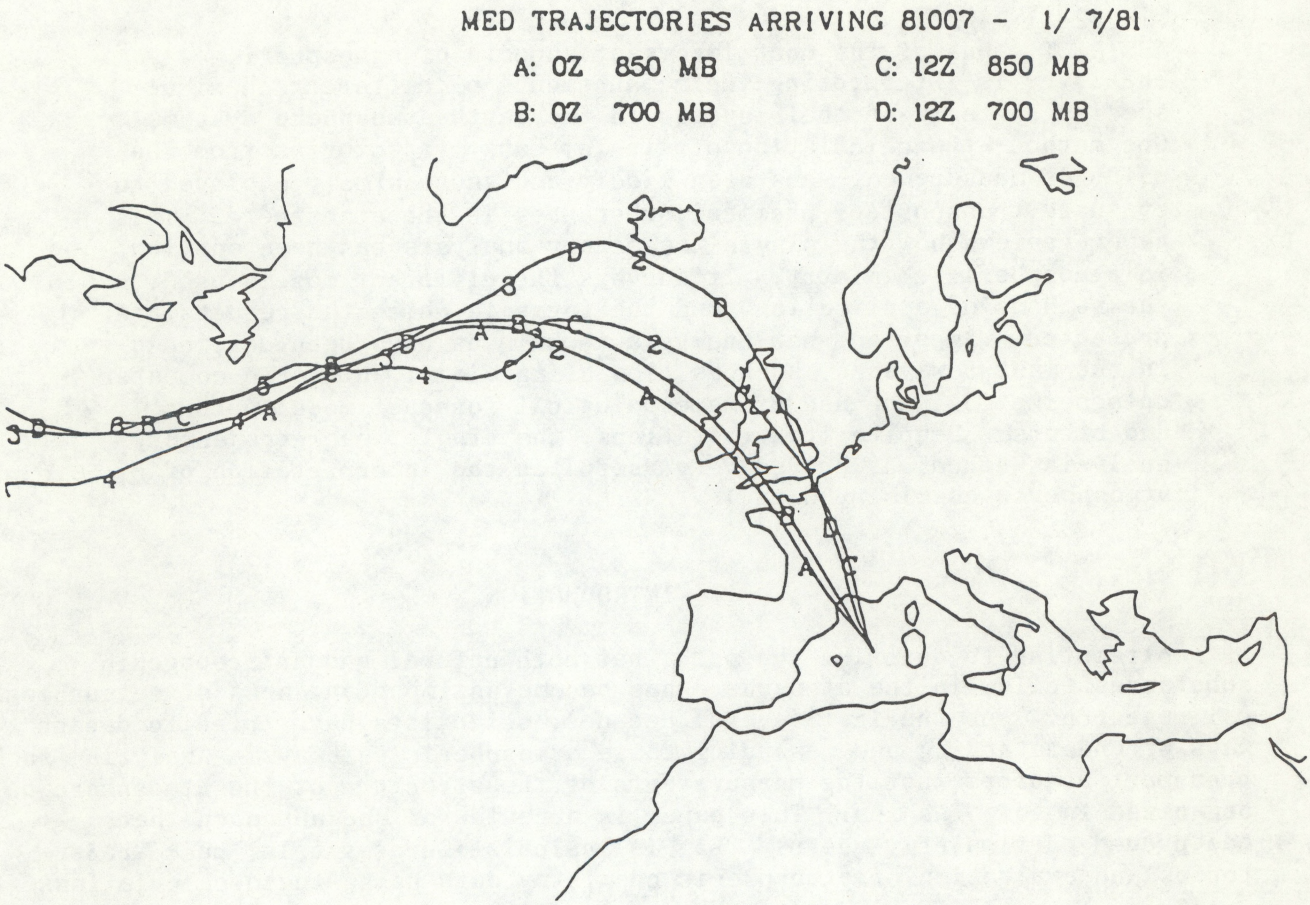

Figure 1. Example of 10-day back trajectories for January 7, 1981, from a point in the western Mediterranean. The 850-mb trajectories are A (00Z) and C (12Z); the 700-mb trajectories are B (00Z) and D (12Z). The numbers (1, 2, etc.) refer to days back in time.

Though the parcel is conceptionally helpful in describing the movement at a given level of the atmosphere, its use in understanding the transport of trace substances in the atmosphere can be very complicated for any single atmospheric event. Most of these materials are released at or near the earth's surface and may be eventually mixed through several kilometers of the atmosphere. If the parcel is restricted to a given level, then such widely dispersed trace materials could be transported by a group of parcels moving in different directions in both the vertical and the horizontal. Naturally, if the flow were unidirectional at several levels with a small vertical component, then describing the transport would be relatively simple. Under chaotic, discontinuous conditions, common in frontal discontinuities, parcels would follow different paths at different levels, and transport would be very complicated. This limitation of applying the parcel method must always be kept in mind when using the back-trajectory technique.

2. APPLICATION OF BACK-TRAJECTORY ANALYSIS TO ATMOSPHERIC CHEMISTRY

2.1 Method

Over a decade ago, objective computer methods (Heffter et al., 1975; Pack et al., 1978) were developed to take different parameters such as pressure, wind or temperature fields and, using interpolation schemes, to calculate trajectories on a given level. One advantage of the computer approach is the ability to make consistent calculations over long periods of time. Also, different fields can be mixed so that, for example, measured winds can be interpolated to an isentropic surface and trajectories constructed (Merrill et al., 1985). Thus the computer allows a broad range of options that can be applied to trajectory calculations and their interpretation.

Before reviewing the application of trajectories to atmospheric chemistry, it is appropriate to discuss the different approaches meteorologists have developed to calculate trajectories from the data, i.e., the twice-a-day vertical soundings. There are two basic kinds of trajectories--dynamic and kinematic. Dynamic calculations are made with such fields as pressure and temperature to draw isobaric or isentropic trajectories, whereas kinematic calculations are made with measured wind fields. A breakdown is shown in Table 1 in which the advantages and disadvantages of the different models are outlined. Though the isentropic dynamic model is more satisfying from a theoretical viewpoint, its added sophistication may not always improve the results because of a variety of factors (Artz et al., 1985; Merrill et al., 1986). When the flow is simple, the isentropic dynamic and the kinematic models track the same paths very well. In more complex meteorological situations, one can assume but not prove that the added calculation used in the isentropic approach gives better, more accurate trajectories.

On the basis of the above discussions, the application of the back-trajectory method is determined by the following factors: (1) the choice of the type of model used (dynamic, kinematic, mixed); (2) the level at which the calculation is made (whether it is a pressure surface, potential temperature field, layer in the atmosphere, etc.); (3) the grid size, which determines the area of interest and the distance back a trajectory can go; (4) the number of days backward; (5) the availability of data; and (6) the computer time required to make necessary calculations. Decisions about these and other practical problems must be made before the first trajectory can be drawn.

Table 1. Singe back-trajectory methods

Kind	Type	Advantages	Disadvantages
Dynamic	Isobaric	Easy to calculate; large data bank; operational	Geostrophic winds not representative; no vertical motion
	Isentropic	Vertical motions taken into account	Large amount of computer time; good only for case studies; not operational
Kinematic	Wind field (real or calculated)	Easy to run; operational	No vertical motion
Mixed	Wind fields on isentropic surfaces	Vertical motion; easier to run than pure isentropic	Not completely operational; misses vertical motion due to adiabatic processes

2.2 Application

After the above decisions are made, the researcher is ready to use trajectories in data analysis. In the single, back-trajectory analysis the usual approach is to compare directly a 5- to 10-day back trajectory with an atmospheric chemistry measurement made over a 12- to 24-h period at the point of origin of the trajectory. If there are only a few measurements at the point, then each can be compared directly with its trajectory, as discussed by Byrd and Andreae (1986), Colbeck and Harrison (1985b), Galloway et al. (1983), Halter and Peterson (1981), and many others. If, however, there are a large set of measurements, a more structured approach must be made, and therefore a method of trajectory classification is required. The two elements in any classification scheme are to account for the direction from which the trajectory came and the distance it took to travel in a given time, i.e., the speed of transport. Direction is usually categorized by some kind of sectoring arrangement. The schemes are either a type of mechanical division, such as 45° quadrants, or are based on a hypothesis that a given sector repesents a special transport zone. Figure 2 shows examples of these two kinds of classification schemes. Each sector may also be divided into distances from the origin so that the probable speed of flow can be determined.

How one does the classification must also be considered. To date, the most usual method is inspection by the individual researcher. This may lead to differences in interpretation, as is the case in analyzing weather maps. However, the approach ensures that each individual trajectory will be handled separately. For large data sets visual classification can be a laborious process. Examples of this method are given, for example, in Kurtz et al. (1984), Merrill et al. (1985), and Munn et al. (1984). An alternate approach is to design a scheme that allows automatic analysis by the computer. Though this saves considerable time, it may also lead to spurious results during complicated weather situations.

3. NEW APPROACHES

Though the methods discussed in Sec. 2 for applying back-trajectory analysis have been useful, researchers have been looking for other ways of extracting further information using this technique. Four methods seem promising: (1) automated long-term analysis of trajectories, i.e., flow climatology; (2) detailed studies of individual trajectories such as including diurnal changes, following layers, and adding extra fields such as rainfall amount along the trajectory path; (3) use of the fields provided by forecast models, to account for vertical motions; and (4) field studies to verify back trajectory calculations. Application of these new approaches could be an aid in establishing further understanding of transport and atmospheric chemistry that was not possible using earlier analysis techniques.

3.1 Flow Climatologies

From daily trajectories, a flow climatology can be constructed for the location of interest. Thus the transport potential of a given substance can be evaluated assuming that the analysis is tailored to the possible source areas. This is illustrated by an example shown in Fig. 3 (Miller et al., 1987). The ARL trajectory model was used to calculate 10 days back from a point in the

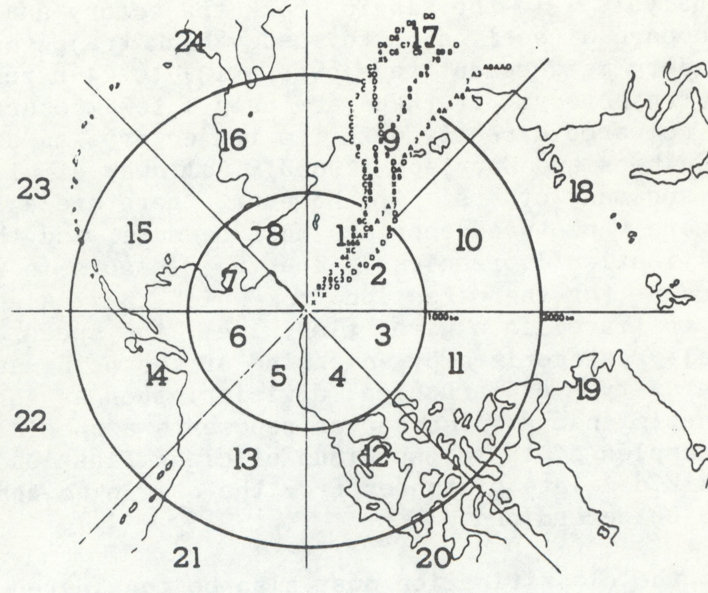

Figure 2(a). A scheme in which distances and speed of flow can be determined for each regularly spaced sector (Miller 1981a).

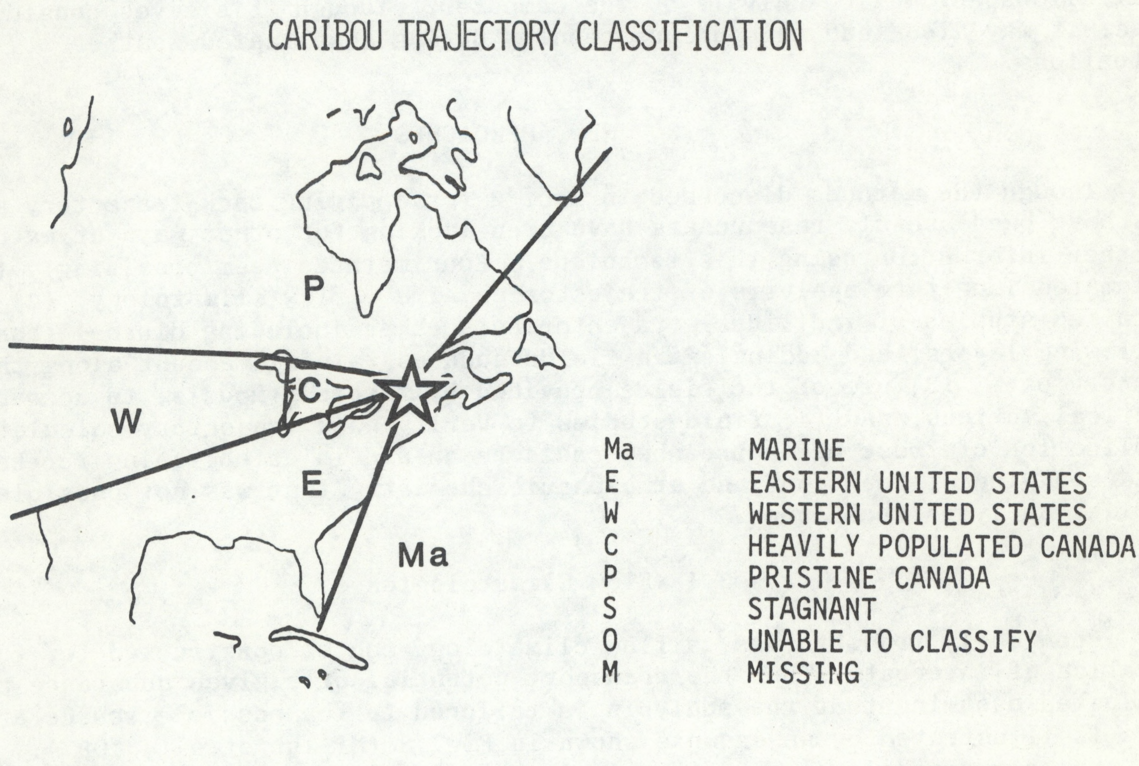

Figure 2(b). A scheme in which categorization is according to pollution sources (Artz and Dayan, 1986).

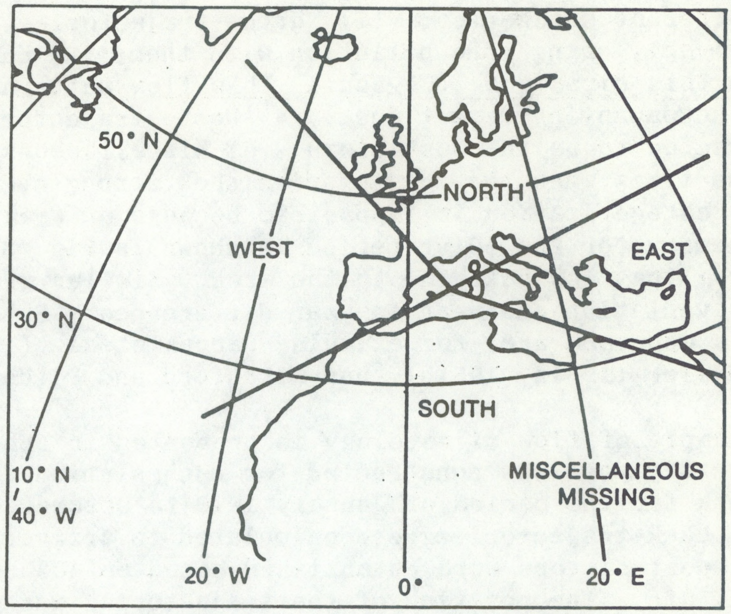

Figure 3(a). The typing scheme used to categorize 10 years (January 1975-December 1984) of 850-mb back trajectories from a point in the western Mediterreanean.

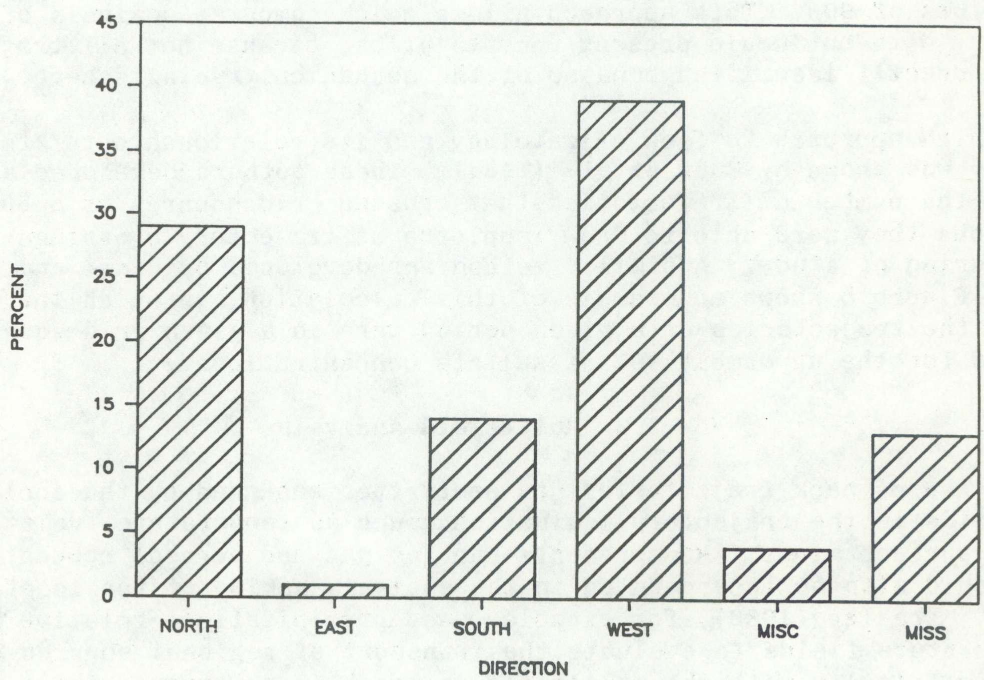

Figure 3(b). The number of trajectories for each type (Miller et al., 1987).

western Mediterranean (40°N, 6°E) for the period from January 1975 to December 1984. This procedure was performed twice a day for the 850-mb level. The trajectories were categorized according to the following scheme (see Fig. 3). There are six different categories: (1) North--trajectories coming from this area would conceivably bring more pollution with them; (2) East--trajectories rarely come from this direction; (3) South--this flow pattern brings air from the Sahara with accompanying desert dust; (4) West--trajectories from this sector could be expected to be the most clean; (5) Miscellaneous--this case includes both the times when the trajectories show strong cyclonic motion and the times when a categorization is impossible because of weak flow; and (6) Missing. The summary for the 10-yr period is shown in Fig. 3, which demonstrates the prevailing flow patterns to the area. Similar graphs can be made showing seasonal variation and year-to-year differences. Publications illustrating this approach are, for example, Pacyna et al. (1984a), Parekh and Husain (1982), Miller (1981a, 1981b), and Pitchford and Pitchford (1985).

A second example of flow climatology is presented in Lehmhaus et al. (1985). A trajectory rose was constructed for each station in the European monitoring network for the period of January 1978 to October 1982 (Fig. 4). Four 96-h 850-mb back trajectories were calculated to arrive at the station each day. Eight transport sectors were established based on 45° sections such as North, Northeast, etc. The position of the trajectories was identified every second hour. If more than half of the positions of the four trajectories in a given day were within a certain sector, then the day was allotted to that sector. A ninth sector was defined when this was not the case. Only trajectories between 150 and 1500 km were considered. An example of the results is shown for one station, F1 at Vert-le-Petit, France. Not only are the number of cases shown for each sector, but they are also compared with the measured and calculated values of SO_2. This approach allows quick computer analysis of the trajectory data but could present uncertainties, because not all trajectories can be correctly identified because of the mechanical typing scheme.

A third approach to flow climatology and its relationship to atmospheric chemistry was shown by Munn et al. (1984). These authors developed a method of counting the number of trajectories that crossed grid squares of a 50 x 50 km^2 area. Thus they were able to draw isopleths of trajectory crossings for the entire period of study. A similar method was developed by Henmi and Bresch (1985). Figure 5 shows an example of this calculation, in which the percentages of times the trajectories of a given period were in a given grid square are displayed for the uppermost 10% of sulfate concentrations.

3.2 Multifield Analysis

The use of back trajectories can be further enhanced by the inclusion of other fields in the trajectory evaluation, such as temperature, relative humidity, and surface winds. Measurements such as gas and aerosol concentration fields could also be incorporated in the analysis upwind of the location of interest. Draxler (1983), for example, used precipitation, relative humidity, and temperature fields to evaluate the transport of regional sources of pollution. A difficulty with the multifield approach is to express these other fields in a form that can be used in the calculations. In addition, the manner in which each field interacts with the other is hard to establish and thus a number of assumptions must be made. Though this approach does present promise, establishing the fields needed for the calculations is a major handicap.

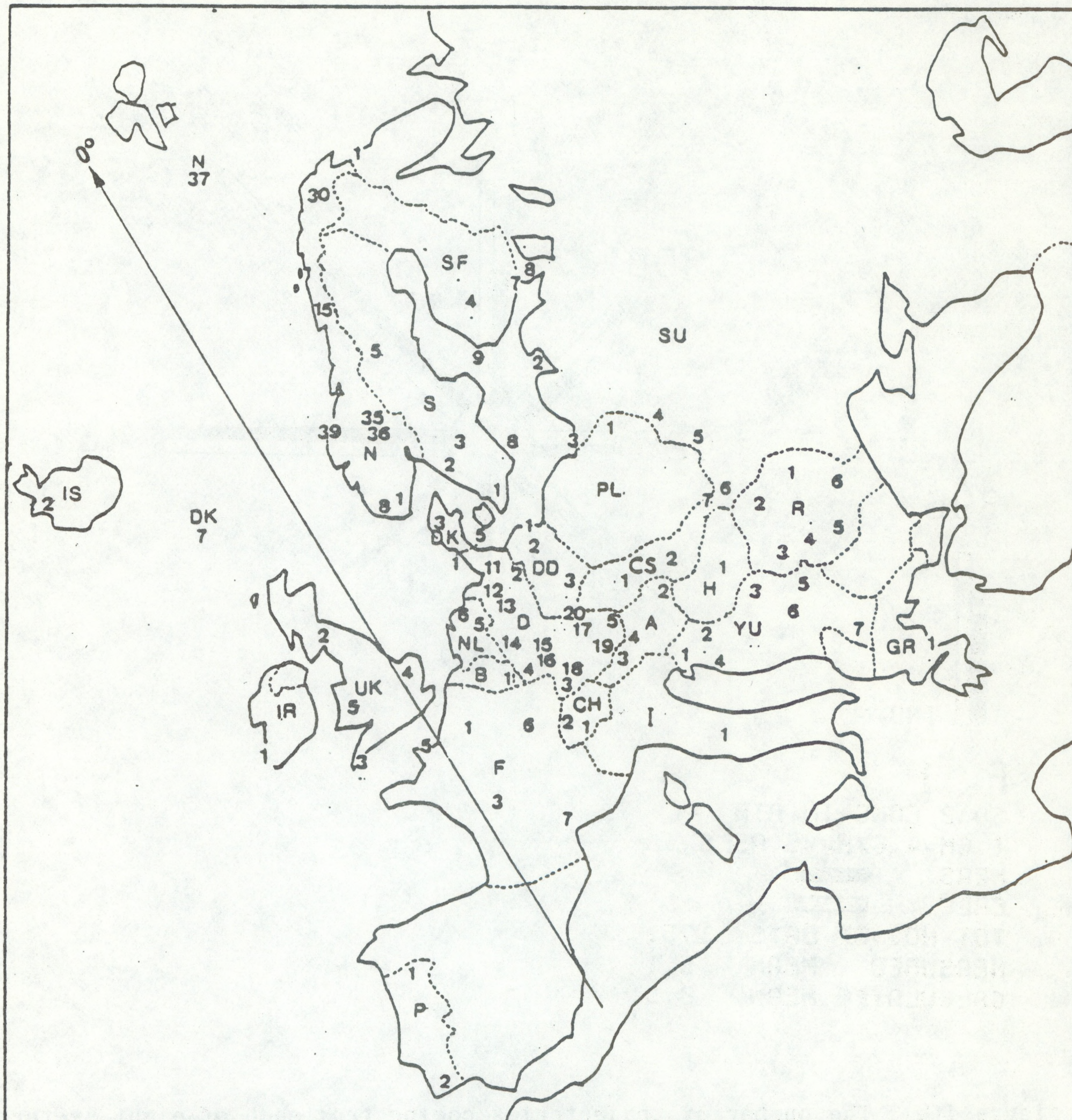

Figure 4(a). Locations of EMEP stations.

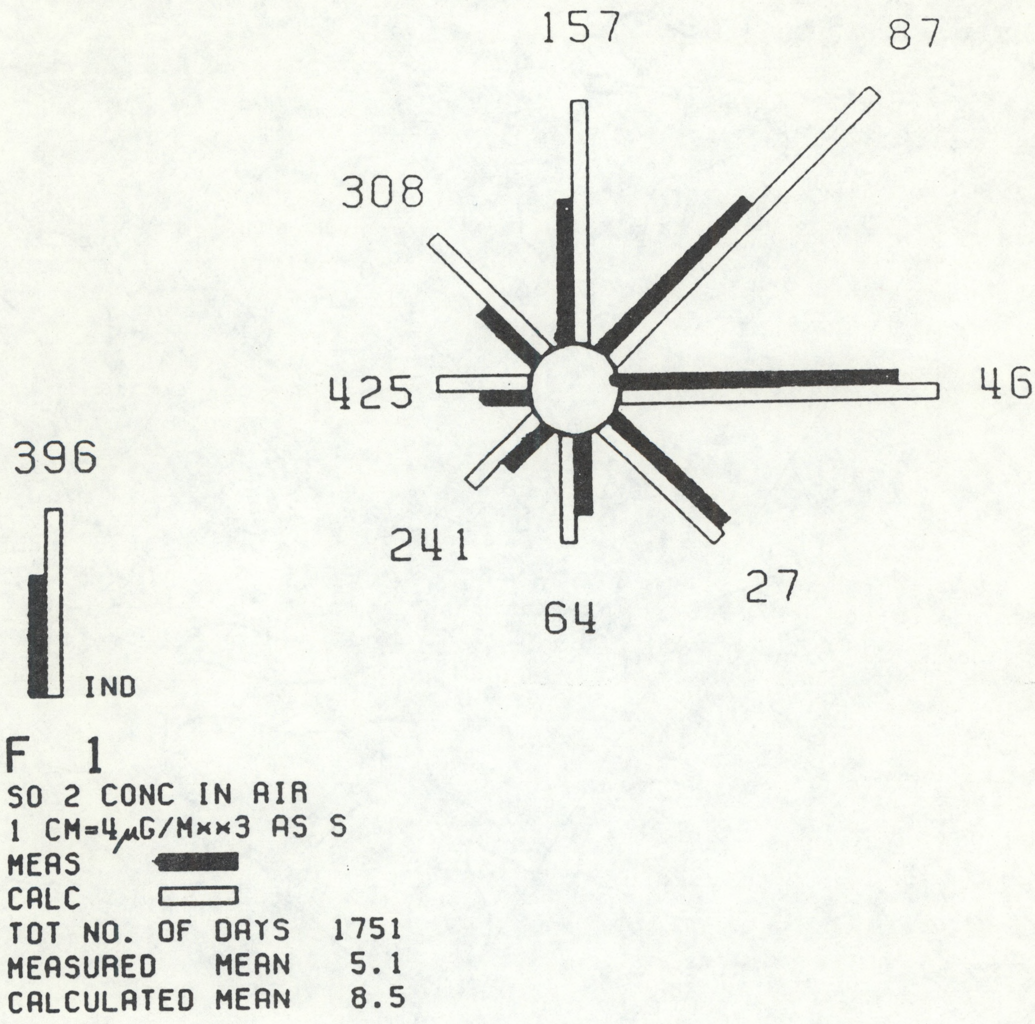

Figure 4(b). The number of trajectories coming from each of eight sectors (numerals), and the measured and calculated SO_2 concentrations for each sector, for station F1. The ninth "sector" marked IND represents the trajectories that were unclassifiable (Lehmhaus et al., 1985).

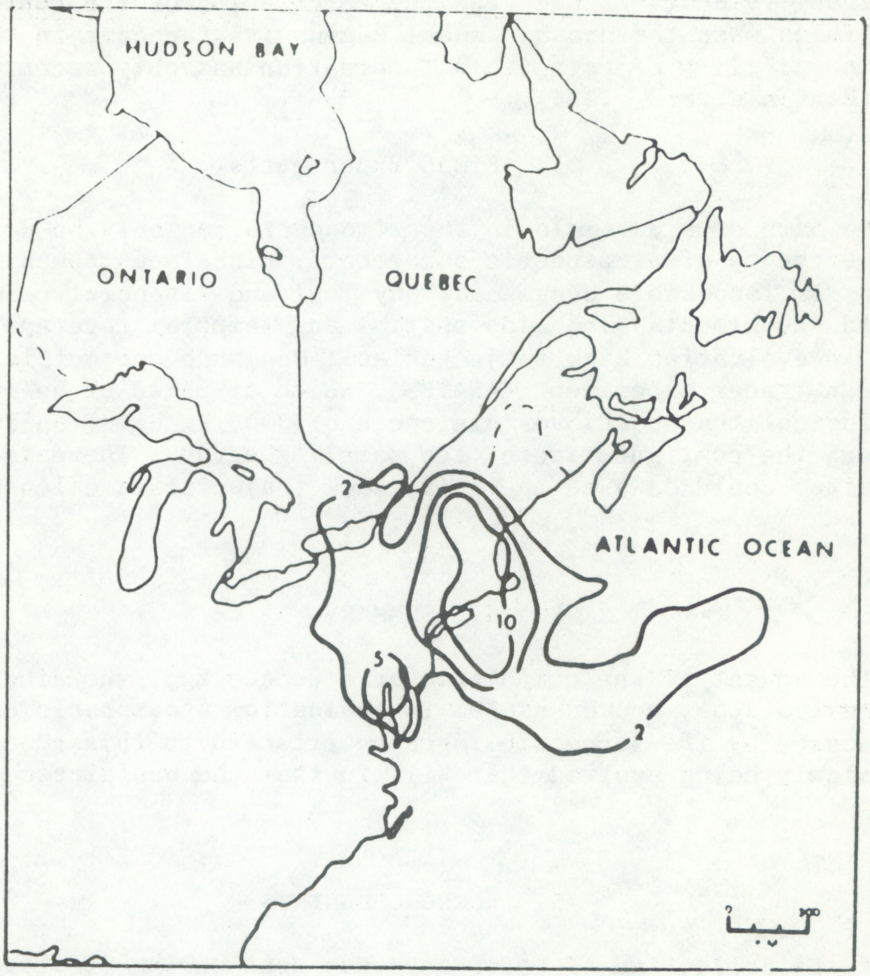

Figure 5. Isopleths of the percentage of times that back trajectories from Hubbard Brook, New Hampshire, crossed grid squares of 50 x 50 km^2 area. Percentages are for the uppermost 10% of the population of sulfate concentrations (Munn et al., 1984).

3.3 Vertical Motion

One of the problems that was discussed earlier was the lack of information on the vertical motion in the trajectory models used. To circumvent the problem, the output of forecast models that produce the vertical velocities is employed. These velocities come from the calculation of the convergence/divergence fields when the dynamic model begins its forecast in three dimensions. The possibility of using this information has only recently been recognized (Martin et al., 1984).

3.4 Field Experiments

The true path of a particle in the atmosphere can only be determined by in-situ measurements of atmospheric parameters, since measurement of all the needed values is impossible because of physical and financial reasons. However, special field experiments with wide spatial and temporal coverage could be useful instead in evaluating back trajectories. One such project is the Across North American Tracer Experiment (ANATEX), which is aimed at an evaluation of the meteorological transport over distances of 3000 km using an inert tracer. Figure 6 shows the configuration of the sampling array. The data collected at any of the sites could be used to verify back trajectories calculated from a given point.

4. SUMMARY

Since the advent of the computer over a decade ago, the single, back-trajectory analysis has proved useful in evaluating atmospheric chemistry data. This is witnessed by the large bibliography attached to this report. New techniques are slowly being evolved that will further the usefulness of this approach.

5. ACKNOWLEDGMENTS

Much of the collection of references was done during my stay at the Centre des Faibles Radioactivites. These references were supplemented, and a more extensive review was presented at the International Symposium on Acidic Precipitation, Muskoka, Canada, in September 1985.

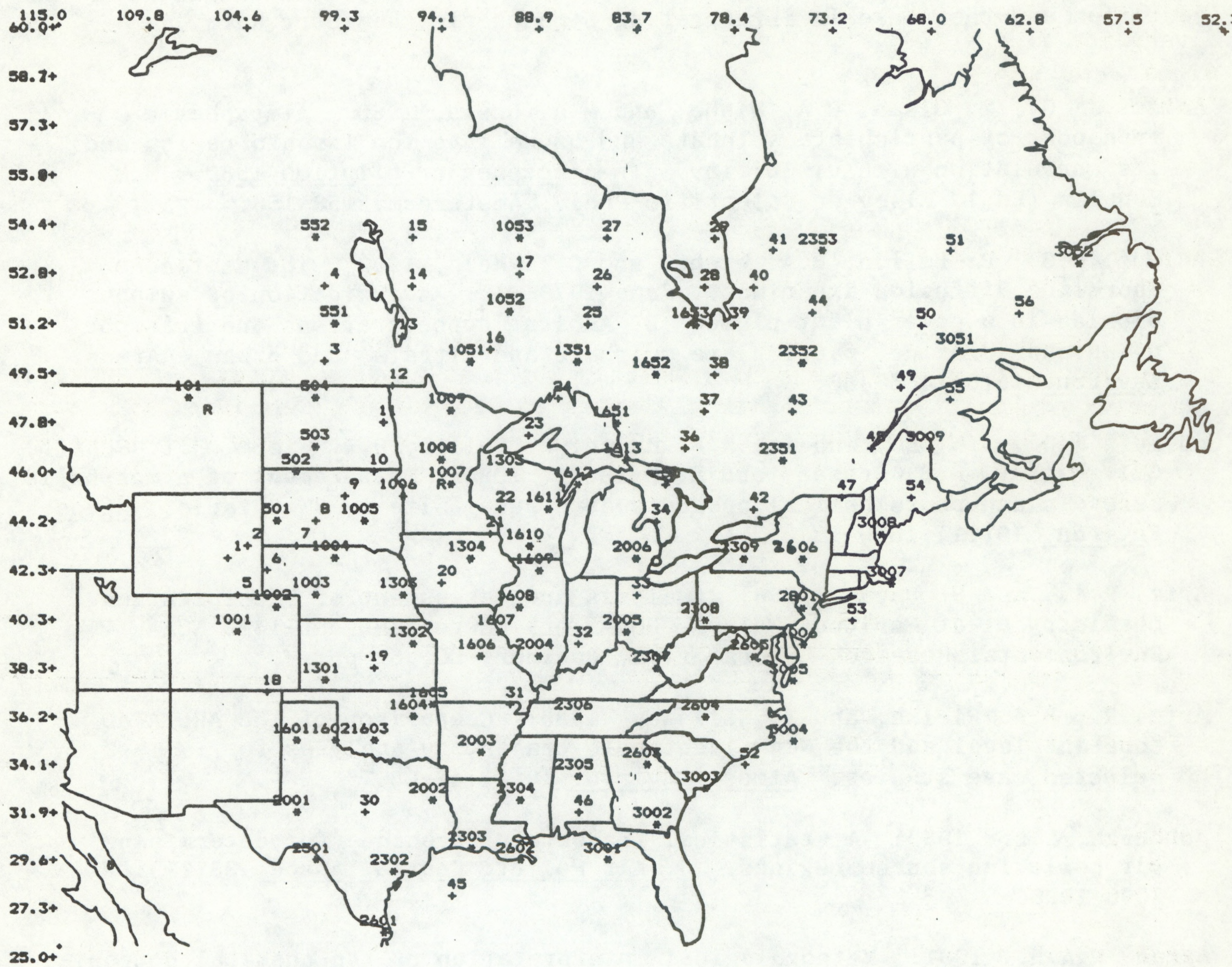

Figure 6. ANATEX source site locations at Glasgow, Montana (GGW), and at St. Cloud, Minnesota (STC), and the ground-level sampling network.

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