THE USE OF ATMOSPHERIC TRANSPORT PATTERN RECOGNITION TECHNIQUES IN UNDERSTANDING VARIATION IN PRECIPITATION CHEMISTRY

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ABSTRACT  This paper illustrates the utility of pattern recognition as a method for quantifying the relative importance of atmospheric transport as a factor contributing to variability in the chemical composition of precipitation at four different sampling sites, Charlottesville, Virginia; Cape Point, South Africa; Bermuda; and Amsterdam Island. Cluster analysis was used to identify periods of similar transport defined using back trajectories. The resulting patterns determine the relative frequency of precipitation bearing winds arriving from different regions. Significant differences in chemical composition between these transport patterns were identified. Amsterdam Island and Cape Point represent relatively clean sites where composition did not depend on transport. In contrast, at Bermuda and Charlottesville, 20% to 30% of the chemical variability appears to be related to transport. At these sites the influence of dominant source regions were clearly identified.

The purpose of this paper is to illustrate the utility of pattern recognition techniques as tools for interpreting the influence of transport differences on the composition of precipitation. Considerable variation has been observed in the composition of precipitation events measured at individual sites in the Global Precipitation Chemistry Project network (GPCP), the Western Atlantic Ocean Experiment network (WATOX), and the Multi-State Air Pollution Power Production (MAP3S) network. Using precipitation chemistry data collected at two remote GPCP sites (Amsterdam Island and Cape Point, South Africa), one remote WATOX site (Harbor Radio Tower, Bermuda), and an eastern U.S. MAP3S site (Charlottesville, VA), the variable influence of atmospheric transport patterns on the resulting composition has been quantified.

Atmospheric back trajectories have become a standard tool in the interpretation of precipitation chemistry data (Miller, 1987). A common approach to interpreting variability in precipitation composition has been to identify the compass sector from which trajectories arrive at the receptor (Galloway, et al., 1989). This results in the subjective designation of sectors, indicating transport from some general direction (i.e., north, south, east or west). Wind speeds are typically ignored under this approach. The underlying assumption is that by considering differences in transport we may identify the influence of different source regions on the chemical data...
of interest.

A pattern recognition method, like cluster analysis, provides a more objective way of identifying events which share similar transport characteristics. This is a multivariate technique which allows for the consideration of more than one variable such as wind speed and direction. This paper summarizes several studies where cluster analysis was used as a pattern recognition technique to identify periods of similar transport during precipitation events. The purpose of this summary is to illustrate both the powers and limitations of this method.

The following approach was taken at each of these four sites, respectively. One back trajectory was chosen to represent transport during each precipitation event. At the GPCP and WATOX sites, 850 mb isobaric trajectories were calculated using the GAMBIT (Harris, 1982) global model. At the MAP3S site, mixed layer trajectories were calculated using the Heffter (1980) model.

For each data set, the objective of the cluster analysis was to cluster the trajectories into groups representing conditions of similar transport. Trajectory endpoints parameterize wind speed and direction at three hour intervals, going several days back. A hierarchical cluster analysis was performed using these endpoints as cluster variables. The smaller the difference between respective endpoints of two trajectories, the more similar they were. The similarity measure employed was the spatial variance, calculated as the sum of squares of the distance of each trajectory from the cluster's mean trajectory (Ward's Method, Gordon, 1981). The step-wise optimal routine grouped trajectories into clusters until a large percent change in variance resulted, signalling that the last two clusters joined were too dissimilar to warrant their combination. This determined the number of different transport groups identified in the dataset.

A second cluster method was also applied at each site. The iterative technique used randomly selected trajectories as seedpoints for a designated number of clusters, the designated number corresponding to the optimal number of clusters, identified by the hierarchical method. The iterative process joined each trajectory to the closest seedpoint, then calculated a cluster centroid value. These centroids were used as new seedpoints and the clusters were reassigned to the closest center and a new cluster centroid was defined for each of the clusters. This process continued until the iterations converged and cluster centroids no longer changed. This iterative method was effective at identifying outliers in the dataset, trajectories which were unlike any other. When outliers were removed, the process was restarted with a new hierarchical analysis.

This hybrid method of applying both iterative and hierarchical clustering techniques to the data provided a check that the transport patterns identified were, in fact, robust. Results of the two schemes were very similar. One has more confidence in the reality of any group structure indicated when the results of different classification methods agree closely (Gordon, 1981). If transport patterns are truly distinct, any cluster strategy worthy of use should find them.

The first result in these applications was the determination of a flow climatology for each site. The transport clusters illustrate the relative frequency of occurrence of precipitation bearing winds arriving from different regions. Along with the flow climatology, the chemical climatology for each transport pattern was assessed. At each site, the precipitation composition of the resulting clusters was identified. Distributions of per event precipitation amount, ion concentration, and ion deposition were compared between the clusters using nonparametric statistics.

Given the significant marine influence on precipitation chemistry data at the GPCP and WATOX sites, non-seasalt concentrations were calculated
for ions with a significant marine component (Keene, et al. 1986) at these sites.

**Figure 1** Single flow pattern which delivers the largest fraction of sulfate and acidity from January 1977 through December 1985.

At three of the four sites, there was a significant difference in precipitation composition between seasons. In order to address chemical differences related to transport pattern independent of seasonal variability in chemistry, the data for these sites were separated into seasons. In Charlottesville, five cold season and eight warm season transport patterns were identified in the trajectory data. The largest fraction of acid deposition, and the highest sulfate concentrations were associated with relatively low speed transport from the northwest during the warm season. Figure 1 illustrates this transport pattern. These flow conditions delivered roughly 15% of the acid deposition which fell in Charlottesville between 1977 and 1985. It is apparent from this figure that these trajectories crossed industrial source regions in the midwestern states.

By analyzing the variance, between 10% and 25% of the variability in ion concentrations could be related to variations in transport. This left a large portion of the variation within clusters. A significant fraction of this
residual variation (20% to 30%) could be explained by differences in precipitation amount.

On the island of Bermuda, seven flow patterns were identified in each season (Moody and Galloway, 1988). During the cool season it was found that the highest concentrations of non-seasalt sulfate and acidity, and the greatest depositions of these species, occurred with transport from the west and northwest, off the east coast of the United States, thus implicating anthropogenic sources. For comparison, Figure 2 illustrates three of the cool-season transport patterns identified. This figure shows that flow from the south deposited less than 3% of the five year total of non-seasalt sulfate on Bermuda. In the warm season, flow off the coast of the U.S. was less frequent, and the highest concentration and deposition of sulfate occurred with transport from the Bahamas region. This suggests that biogenic sulfur sources may make an important contribution to sulfate deposition and
The frequency of occurrence and NO$_3^-$ deposition associated with different transport patterns for trajectories arriving at Cape Point, South Africa: a) rapid transport from the west, b) relatively low speed transport, with less defined direction.

acidity on Bermuda during the warm season. As with Charlottesville, differences in transport could explain approximately 20% of the variability in sulfate on Bermuda.

At the Cape Point, South Africa site, there was no evidence of significant
seasonal variation in the precipitation chemistry data, so all events were considered together. Five different transport patterns were identified. However, upon comparing the chemistry between these flow patterns, the only constituent which varied with transport was nitrate concentration, as shown in Figure 3. Nitrate was significantly higher during low wind speed conditions and looping trajectories. These low wind speeds may enhance the potential for local sources to contribute to the composition of the precipitation samples.

Precipitation composition on Amsterdam Island did show seasonal variability, with higher concentrations of sulfate and acidity observed in the warm season. In the cool-season, six transport patterns were identified; five were identified in the warm season. In some cases, these flow patterns suggest that the potential exists for material to be transported from South Africa. However, there was no significant difference in the ion concentrations or depositions associated with any of the flow patterns identified.

![Figure 4 Probability distributions of non-seasalt sulfate concentrations for the 3 GPCP sites, and sulfate concentration for the Charlottesville MAP3S site.](image)

It was shown that, at the two most remote sites, differences in atmospheric transport were not very powerful at discerning differences in precipitation composition. However, these two sites (Cape Point, South Africa and Amsterdam Island, in the Central Indian Ocean) had significantly cleaner precipitation to begin with. Figure 4 is a plot of the sulfate distribution for each of the four sites discussed here. It indicates
that precipitation in Charlottesville was most contaminated, and significant contamination was observed on Bermuda. But at the two southern hemisphere remote marine sites, the precipitation was relatively uncontaminated.

At sites where there was significant variability in the composition of precipitation, cluster analysis was a useful method of identifying flow patterns and the contribution they made to ion deposition. At sites where there were only small variations in chemistry, chemical differences between transport patterns were not significant. However, in these cases, the cluster analysis was still useful in identifying the frequency of occurrence of different flow conditions, and the amount of precipitation associated with each pattern.

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