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# Project Summary

# Adaptation of the Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) Model to the EPA VAX Computer-- Modifications and Testing

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**We modified the original 1985 IBM-3033 version of the Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) model to create the ASTRAP-EPA version for applications on the EPA VAX-8600 computer using existing EPA preprocessed meteorological and emissions data files. The cumulative effect of the model modifications was assessed by comparing the quarterly 1980 calculations of sulfur wet deposition of both versions with screened measurements. The seasonal correlation coefficients and standard errors of each model version are insignificantly different at the 0.05 level, demonstrating that the two model versions indeed produce similar results. In general, the improvements in model design only slightly enhance model performance.**

**Sensitivity of ASTRAP-EPA calculations of sulfur wet deposition was also assessed for several model assumptions and values of model parameters. ASTRAP-EPA model predictions are most sensitive to three parameters -- the model time step, the truncation of trajectories near the border of wind-data-void regions, and the temporal aggregation of ensemble trajectory statistics. The maximum quarterly predictions of sulfur wet deposition, across southwestern Pennsylvania and northern West Virginia, decrease by as much as 30% when either the model time step changes from 3 hours to 6 hours, or when trajectories are not truncated, or when trajectory statistics are not temporally aggregated.**

***This Project Summary was developed by EPA's Atmospheric Research and Exposure Assessment Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).***

## Introduction

The Advanced Statistical Regional Air Pollution (ASTRAP) model developed by the Argonne National Laboratory calculates long-term mean air concentrations and deposition amounts of oxides of sulfur and nitrogen and quantifies the linear relationships between emissions from virtual sources and ambient concentrations at receptors across North America. Since the model uses trajectory statistics to parameterize atmospheric transport and diffusion, model applications are restricted to time periods of a month or more. These long-term source-receptor relationships have been used by the Agency in identifying prime emission control regions and assessing emission reduction strategies for the acidic precipitation program.

The 1985 version of the ASTRAP model code was obtained and adapted to the EPA VAX-8600 computer to improve our understanding of the model capabilities, to assess the effects of modeling approaches and assumptions on the results, and for possible applications as a screening model for regional sulfate and fine particle concentrations and regional visibility. During this process, the code was modified to create a model version named ASTRAP-EPA, which uses existing EPA meteorological data files and provides the user the

flexibility of redefining default model parameters.

In the final report, we: (1) summarize the attributes and assumptions of the ASTRAP model, (2) document the modifications to adapt the model to the EPA VAX-8600 computer, (3) assess the effects of the modifications by intercomparing 1980 quarterly predictions of both versions with measurements, and (4) assess the model sensitivity to input parameters and model assumptions.

## Attributes of the ASTRAP Model

The ASTRAP model simulates the transport, dispersion, and deposition of oxides of sulfur and nitrogen across North America with a resolution of one-third that of the National Meteorological Center (NMC) grid, or 127 km at 60° N latitude. Since dry and wet deposition rates and linear chemical transformation rates are specified in the model code, only aggregated emission rates and gridded wind velocities and precipitation amounts are required for model applications. Model output consists of long-term mean air concentrations and deposition amounts at receptor points; linear source-receptor relationships are quantified via a postprocessor. Because of the statistical nature of the model, applications of this model are not recommended for periods less than one month.

The modeling approach of ASTRAP is unique. Rather than directly simulating processes for the pollutants emitted from all point and area sources in the modeling domain, the model simply:

(1) Computes for each of 123 virtual sources (at the center of groups of 9 cells) the coordinates of the ensemble mean positions, standard deviations, and spatial correlations of 6-h trajectory endpoints for puffs released at 6-h intervals and tracked for periods of 7 days, and

(2) Constructs bivariant normal density functions that describe the spatial distribution of mass for the ensemble of equal-age trajectory endpoints.

Separate sets of statistics are compiled for airborne pollutant plumes and wet deposition events. With the transport and diffusion statistics, the prescribed dry deposition velocities, an emissions field, and the scavenging algorithm, dry and wet deposition fields can also be generated. Using these density functions greatly reduces computational time, thereby making multi-year applications of this model feasible, since subprogram VERT must be applied only once per season and subprogram HORZ only once per season of each modeled year. Further, for ascertaining the effects of emission control strategies, the reapplication of these two subprograms is not necessary.

A potential limitation of the ASTRAP model relates to its calculation of transport near the model domain border and regions where wind data are non-existent (e.g., the Atlantic Ocean and Gulf of Mexico). Statistics for ensemble trajectories can be biased when some trajectory segments extend beyond the region where wind data are available. That is, trajectory segments with endpoints east of the Atlantic Coast are not considered in the statistical computations, thereby placing more emphasis on those remaining trajectory segments, which normally pertain to lighter winds. As a result, the simulated transport of an ensemble of puffs (especially for sources along the East Coast) would be based on fewer meteorological cases; thus, a sudden change in the ensemble trajectory direction and/or speed would result. The model assumes that any bias in the ensemble trajectory statistics would not significantly effect the simulations of air concentrations and wet and dry deposition amounts.

## Differences Between ASTRAP and ASTRAP-EPA

In 1988, a copy of the 1985 IBM-3033 code of the ASTRAP model was modified by EPA and renamed ASTRAP-EPA to accomplish the following four tasks:

(1) Adapt the code for applications on the VAX-8600 computer.

(2) Adapt the model to accept EPA-preprocessed meteorological and emissions data files as input.

(3) Adjust some of the modeling approaches without substantially increasing the computational requirements.

(4) Create a versatile model, one that affords the less-experienced user options for the values of such model parameters as size and location of modeling domain, model time steps without necessitating code recompilations.

The most obvious difference between the two versions of the model is the model grid configurations. ASTRAP uses two fixed NMC grids (with a polar stereographic projection aligned along 80° W longitude and true at 60° N latitude): A 17-by-19 grid with a spacing of approximately 380 km for wind data and a 51-by-45 grid with a spacing one-third that of the first grid for precipitation and emissions data and model calculations of concentrations and depositions. In contrast, ASTRAP-EPA uses a single latitude-longitude grid for both input data and model calculations and affords the user the opportunity to easily redefine the grid resolution and geographical domain in subroutine PARAMETER statements. The reason for converting to the latitude-longitude grid, which has a resolution similar to that of the 51-by-45 ASTRAP grid (i.e., approximately 120 km), was to accommodate the EPA emissions and meteorological preprocessors.

ASTRAP was designed for use by the original model developer with most parameterization rates and options internal to the code. Therefore, an ASTRAP user is required to modify and recompile the model code when a change in a single model parameter is desired, rather than merely redefining the value of a model parameter read from an input file. ASTRAP-EPA, on the other hand, provides the user the following options:

(1) Read a preprocessed sulfate emissions grid or default to the original ASTRAP fixed percentages of $SO_2$ emission rates.

(2) Select a subset of the emissions grid for any model application, or, as before, use the emissions data for all virtual sources.

(3) Redefine many preprocessor and model parameters, such as the dimensions of the model domain, grid resolution, and model time step, without necessitating source code recompilations.

(4) Apply the model for multiple months or seasons or, as before, apply the model for only one month or season per model execution.

(5) Specify any set of weights for use in computing a puff transport vector from boundary-layer-wind-profile data.

(6) Construct source-receptor relationships or just grids of mean air concentrations and deposition amounts.

## Intercomparisons of Predictions and Model Performances

For each quarter of 1980, ASTRAP and ASTRAP-EPA predictions of sulfur wet deposition were intercompared at 32 to 37 sites across eastern North America. Based on the locations and magnitudes of the maximum quarterly predictions, the two model versions produce similar results.

Both model versions anchor the maximum quarterly predictions of sulfur wet deposition across the Upper Ohio River Valley (i.e., northern West Virginia, eastern Ohio, western Pennsylvania, and southwestern New York). Further, the magnitudes of the greatest quarterly predictions are very similar:

4 to 5 kg S/ha in the Winter quarter,

5 to 6 kg S/ha in the Spring quarter,

5 to 9 kg S/ha in the Summer quarter, and

2 to 4 kg S/ha in the Autumn quarter.

However, the quarterly mean predictions for ASTRAP-EPA generally are lower than those for ASTRAP; 22% to 36% less for all quarters except the Winter quarter when the ASTRAP-EPA mean is 13% greater. Because of the relatively few sites across the large modeling domain, we are not able to determine whether these dissimilarities are significant; that is, given the spacing between sites, a slight shift in the quarterly ASTRAP patterns of the predictions could account for much of the differences. Therefore, based on this aspect of the comparison, one cannot state that the two model versions vastly differ.

The purpose of the intercomparison of model performances is to determine whether the two model versions are substantially different from each other. The correlations of both sets of predictions with measurements are similar in that the correlation coefficients do not significantly differ from each other at the 0.05 level of statistical significance (Table 1). Further, the correlations for both sets show the best agreement with the measurements in the Spring and Summer quarters, when 25% to 45% of the variance is explained, and the worst for the other two quarters when only 5% to 15% of the variance is explained.

The S.E.'s are virtually identical for both the Spring and the Summer quarters; a slight improvement is noted in the ASTRAP-EPA performance for these two quarters. In contrast, the S.E.'s for the other two quarters differ by 40% from those for ASTRAP-EPA, exceeding those for ASTRAP in the Winter quarter and vice versa for the Autumn quarter. However, S.E.'s for each quarter do not significantly differ from each other at the 0.01 level.

## ASTRAP-EPA Sensitivity Analyses

The sensitivity of ASTRAP-EPA calculations of sulfur wet deposition to some of the model parameters and assumptions of both ASTRAP and ASTRAP-EPA (Table 2) are assessed in the final report. Rather than assessing model sensitivity at each of the nearly 2,300 receptor cells, calculations are only intercompared at receptor cells along a 2,000-km band stretching from central Alabama to southern Quebec.

Temporally aggregating the ensemble trajectory statistics tends to decrease the sulfur wet deposition predictions across the two high emission regions -- by -40% to -48% near the Alabama-Georgia border and -14% to -35% near the Pennsylvania-West Virginia border, depending on the season. However, elsewhere predictions are virtually identical. Thus, the aggregation appears to smooth the gradients of sulfur wet deposition near regions of significant emissions.

With few exceptions, the doubling of the time step decreases the sulfur wet deposition predictions. The most significant changes occur near the two high emissions regions; as great as -26% along the Alabama-Georgia segment and -31% near the Pennsylvania-West Virginia segment, depending on the season. Across the New York segment, the summer predictions actually increase slightly (by less than 4%), while for the other quarters, the predictions decrease by as much as 18%.

*Table 1. Comparison of Performance Measures of Both Model Versions for the Prediction of 1980 Quarterly Sulfur Wet Deposition at the ISDME Sites*

| | | Correlation Coefficient | | Standard Error | | |
|---|---|---|---|---|---|---|
| Quarter | Number of sites | ASTRAP | ASTRAP -EPA | ASTRAP | ASTRAP -EPA | % Difference |
| Winter | 32 | 0.38 | 0.24 | 1.24 | 1.77 | +42 |
| Spring | 37 | 0.52 | 0.61 | 1.16 | 1.11 | - 4 |
| Summer | 37 | 0.67 | 0.61 | 1.73 | 1.63 | - 6 |
| Autumn | 35 | 0.38 | 0.38 | 1.26 | 0.76 | -40 |

*Table 2. Parameter Values and Assumptions That Were Modified for the Sensitivity Analyses*

| Parameter/Assumptions | Parameter values |
|---|---|
| Temporal aggregation for ensemble trajectory statistics | Original [b]<br>None |
| Model time step | 3 hours [b]<br>6 hours |
| Weighting scheme for mass transport vector[a] | (1L + 1U)/2 [b]<br>(2L + 1U)/3<br>(1L + 2U)/3<br>1L<br>1U |
| Trajectory truncations at borders of data-void regions | Truncation [b]<br>Extrapolation |
| Initial vertical distribution of emissions | Low Layer Only<br>Upper Layer Only<br>Mid and Upper Layers [b]<br>All 3 Layers |
| Number of virtual sources | 443 [b]<br>117 |
| Primary sulfate emissions | 5% of $SO_2$<br>Actual [b] |

[a] For this investigation, the transport vector is either a weighted average of the surface (the low-level, L) and the 850- mb (the upper-level, U) wind velocities or is identical to one or the other.
[b] ASTRAP-EPA base-case conditions.

ASTRAP computes its transport vectors using equally weighted means of the lowest 2 (Autumn and Winter), or 3 (Spring and Summer), 500-meter-layer wind velocities. Since it preprocesses wind data differently, the ASTRAP-EPA transport vectors were computed via a different method--weighted means of the wind velocities at the surface and 850-mb level (the latter approximating 1500 meters). This analysis explored the effects on the winter calculations from the five sets of weights in Table 2, ranging from one extreme (the surface wind vector, 1L) to the other (the 850-mb wind vector, 1U). For this series of applications, the area and point source emissions were injected into layers 3 and 5, respectively (200-300 m and 400-600 m, respectively).

Compared to the base case predictions, ASTRAP-EPA predictions south of New York increase with increasing weights of the surface wind velocities and decrease with increasing weights of the 850-mb wind velocities. For the extreme cases, increases of 80% across Alabama and decreases of 40% across Georgia occur for the 1L and 1U cases, respectively. This relationship reflects the lower transport speeds at the surface, compared to those at the 850-mb level, and the resultant extension of the residence time of the pollutant mass over each receptor point. In contrast, the predictions north of Pennsylvania are less than those of the base case for all four alternative sets of weights, by as much as 27% for the low-level wind vector (1L). Also across this region, predictions decreased less than 10% for the other sets of weights. It appears that for the 1L and 2L1U cases, the additional sulfur removal across West Virginia and Pennsylvania makes less mass available for wet deposition along the northeastern segment of the band. Consequently, for these two cases, the spatial gradient is markedly enhanced along the West Virginia-New York segment.

As expected, when trajectories are extrapolated, sulfur wet deposition predictions indeed decrease everywhere along the band from 8% to 23%, averaging 16%. The largest decreases occur across Quebec and northern New York. When summer trajectories are extrapolated rather than truncated, the predictions tend to decrease by as much as 20% across the Southeast and Quebec, but actually increase by as much as 22% across West Virginia. The increase could be caused by returning trajectories from the Atlantic Ocean. Therefore, when trajectories are truncated, as they are in ASTRAP, the predictions of sulfur wet deposition generally would be biased on the high side. The magnitude of this bias is expected to be highest for those receptor cells along the Atlantic coast with significant sulfur sources (e.g., New York City).

The sensitivity analysis of the initial vertical distribution of emissions shows the greatest differences from the base case predictions result when all the emissions are injected into Layer 5. For this initial distribution, predictions increase virtually everywhere along the band by 15% to 25% in summer and 5% to 10% in winter. The increases resulting from the even initial distribution are half that of the Layer 5 predictions. Predictions decrease when the emissions are injected into Layer 1 (10% to 15% in summer and 5% to 10% in winter). For all model applications, the predictions are most sensitive across New York and Quebec.

The sensitivity of ASTRAP-EPA to the manner in which sulfate emissions are defined is slight. Along the entire band, the predictions from the ASTRAP approach are less than those of ASTRAP-EPA by no more than 5%.

## Conclusions and Recommendations

During the process of adapting the ASTRAP model to the EPA VAX-8600 computer, the model design was modified to utilize existing EPA meteorological and emission files and to provide the user more flexibility in changing parameterization rates. As a means of assessing the cumulative effects of these changes on model predictions, the sulfur wet deposition calculations from both model versions were compared to measurements. Although a slight improvement in model performance is observed in this performance assessment, the differences in the correlation coefficients and standard errors are not statistically significant at the 0.05 level. That is, based on the model performance assessments, the ASTRAP-EPA results are very similar to those of ASTRAP.

The ASTRAP-EPA sensitivity analyses demonstrate that the predictions of sulfur wet deposition along the band of receptors stretching from Alabama to Quebec are sensitive to several user-specified parameters. When only one parameter is changed for each model application, some quarterly predictions of sulfur wet deposition decrease from base case values by as much as 30% when either the model time step is doubled from 3 hours, or when the trajectory statistics are not temporally aggregated, or when trajectories are not truncated at the borders of wind-data-void regions. The most significant decreases along the band typically occur in the regions where annual sulfur wet deposition is relatively high (i.e., across Alabama, western Pennsylvania and West Virginia).

One should apply this model with caution until we can recommend values of these and other model parameters after ASTRAP-EPA is evaluated in 1992 with the ACID-MODES data base. The 1988 and 1989 ACID-MODES data will, for the first time, enable us to assess the performance of regional air pollution models for more than one modeled parameter, providing a more rigorous evaluation and a better understanding of model behavior. Therefore, we recommend that the performance of ASTRAP-EPA be assessed using all pertinent data from this field study. Although the relationships between sulfur emissions and regional visibility are not well defined, statistical comparisons of modeled and observed spatial patterns of sulfate air concentrations will provide insight to the predictive capability of the model.

***Terry L. Clark**, also the EPA Project Officer (see below), and Dale H. Coventry are with the National Oceanic and Atmospheric Administration of the U.S. Department of Commerce on assignment to the Atmospheric Research and Exposure Assessment Laboratory, Research Triangle Park, NC 27711.*

*The complete report, entitled "Adaptation of the Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) Model to the EPA VAX Computer -- Modifications and Testing," (Order No. PB91-127 720/AS; Cost: $15.00, subject to change) will be available only from:*

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