MODELING AIR POLLUTION IN THE

TRACKING AND ANALYSIS FRAMEWORK (TAF)

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1. INTRODUCTION

The Tracking and Analysis Framework (TAF) is a set of interactive computer models for integrated assessment of the Acid Rain Provisions (Title IV) of the 1990 Clean Air Act Amendments (Henrion *et al.,* 1997a,b; Sonnenblick and Henrion, 1997). TAF is designed to execute in minutes on a personal computer, thereby making it feasible for a researcher or policy analyst to examine quickly the effects of alternate modeling assumptions or policy scenarios. Because the development of TAF involves researchers in many different disciplines, TAF has been given a modular structure. In most cases, the modules contain reduced-form models that are based on more complete models exercised off-line. The structure of TAF as of December 1996 is shown in Figure 1. Both the Atmospheric Pathways Module (Shannon, 1996a) and the Visibility Module (Shannon, 1996b) produce estimates for regional air pollution variables. In addition, the Soils-Aquatics, Health, and Scenario Benefits Modules utilize the results of regional air pollution modeling as input, but those downstream modules are not addressed here.

As pointed out by Henrion *et al.* (1997a), in developing an integrated assessment model, it is important that module developers are early and explicit in describing their anticipated input needs for their modules and the form of their projected output. If a module as structured would require input information that is not expected to be provided internally or by an upstream module, then at least one of the modules must be modified in order to produce an integrated assessment.

One approach to developing an integrated assessment that can be comprehensive while still being executable in real time on a personal computer is to focus on representative receptor locations rather than on the entire region of interest, and to focus on only certain temporal scales. The Atmospheric Pathways Module is spatially comprehensive, in that spatially integrated concentration and deposition values are calculated for each state and Canadian province. However, the Atmospheric Pathways Module focuses on seasonal and annual source-receptor relationships, rather than on episodic extremes. In the Visibility Module, calculations are made of the seasonal distributions of daily visual impairment, but only at seven selected locations.

Concerns may arise as to whether, in reducing the complexity of models in order to meet the computer memory and execution time requirements of TAF, the models become too simplified and thus do not represent

good science. It is important to establish and maintain the credibility of the modules, and thus of TAF overall, by frequent comparison of module results with observations and with the results of more physically detailed models. To address this concern, the TAF module developers produced module descriptions (on the Internet at *http://www.lumina.com/taflist*) that include numerous comparisons with observations and with more detailed models. In addition, the overall uncertainties in the module should be evaluated, including the effects of uncertainties in inputs from other modules, uncertainties in model physics, and uncertainties from module simplifications; and the effects of that overall uncertainty in the results of the effects and evaluation modules should be examined. The Analytica^{TM} software in which TAF is written has several significant features to address these concerns; the components of a module, including expressions and constants, are conveniently documented with description, units, input requirements, outputs, and references within the on-line version, such that a user can evaluate the appropriateness of the selected form or values (Henrion *et al.,* 1997a). In addition, in Analytica^{TM}, the propagation of uncertainty through the system can be calculated (Sonnenblick and Henrion, 1997). A useful side benefit from the evaluation of uncertainty is guidance for research program managers as to what research questions might be of greatest immediate benefit to improve assessment capabilities.

2. ATMOSPHERIC PATHWAYS MODULE

The reduced-form model in the Atmospheric Pathways Module is a set of linear seasonal source-receptor matrices for eight air concentration and deposition products of SO_x and NO_x emissions: SO_2, SO_4^{2-}, NO_x, and NO_3^-/HNO_3 air concentrations; and wet and dry deposition of S and NO_x-N. The matrices were produced off-line with the Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) model (Shannon, 1981, 1985, 1996a). The memory and execution speed requirements of a desktop integrated assessment are such that the reduced form of a set of source-receptor matrices would likely be adopted from necessity, regardless of what regional model was exercised as a full-form model. Source-receptor matrices have been applied in assessments for decades. The ASTRAP model, in various versions, has also been applied for two decades, so questions may well arise as to whether it is still suitable for assessment today. Briefly, ASTRAP produces seasonal mean two-dimensional horizontal trajectories and wet deposition patterns for a grid of virtual sources covering the emission region of interest, with the trajectories produced from ensemble statistics of individual trajectories calculated at 6-h intervals. The individual trajectories are calculated by using wind and precipitation fields over North America

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that are updated several times per day, and wet removal is a function of the half-power of the precipitation amount. In separate calculations, ASTRAP produces seasonal mean one-dimensional vertical profiles of concentration, plus dry deposition and loss to the free troposphere, for pollutants as a function of effective emission height. The numerical integration uses highly parameterized seasonal and diurnal patterns of dry deposition velocities, vertical stability profiles, and linear chemical transformations (*e.g.*, SO_2 to sulfate). The trajectory and vertical integration statistics are combined with the appropriate seasonal emission inventory, gridded horizontally and vertically, to simulate seasonal mean surface concentrations and deposition totals. We believe that ASTRAP is quite suitable as an off-line full-form atmospheric model for several reasons:

• ASTRAP has been periodically upgraded with improved parameterizations and structure while maintaining its computational efficiency. The version described by Shannon (1996a) has many improvements over the versions described earlier (Shannon, 1981, 1985).

• TAF largely focuses on evaluating effects associated with long-term average concentrations or deposition accumulation over regional scales, which are the spatial and temporal scales of assessment for which ASTRAP was designed.

• Over those scales, the results from ASTRAP compare favorably with observations and with the results of more physically and chemically detailed models (Shannon and Sisterson, 1992; Shannon, 1996a; Shannon *et al.*, 1997).

• Specification of future emission scenarios is necessarily imprecise, and thus some irreducible level of uncertainty exists for atmospheric modeling (Trexler *et al.*, 1996), regardless of the sophistication of the regional model.

Note that the modular form of TAF would allow matrices from another regional model (if similarly defined in terms of source and receptor elements) to be directly substituted in TAF without requiring changes in any other modules, and the assessment community is encouraged to make and test such substitutions.

The use of a source-receptor matrix with different emission vectors involves the assumption of linearity over appropriate temporal and spatial scales. The National Acid Precipitation Assessment Program evaluated the effects of nonlinearity in emission-deposition relationships with the detailed Eulerian model RADM. When episodic simulations were extended over a season or a year by weighting techniques (which in themselves introduce uncertainties), RADM indicated a modest amount of nonlinearity for a 50% rollback in SO_x emissions (simulated deposition reductions of 40% and 44% annually in the region of high emissions for wet and total deposition, respectively [Dennis *et al.*, 1990]). Seasonal departures from linearity tended to be greatest in winter and least in summer. A preliminary analysis of observed regional trends in emissions of SO_2 and precipitation-weighted concentrations (PWCs) of sulfate (Shannon, 1997) indicated that the decrease in sulfate PWCs was *greater* than the decrease in emissions (i.e., the departure from linearity was in the

opposite sense of the nonlinear results of RADM), although the conclusion of the analysis is potentially an artifact of sparse observations at the beginning of the period, possibly contaminated by dry deposition as operators were gaining experience, incomplete inventories of emissions reductions at the end of the period, and climatological variability.

An additional caveat on the use of source-receptor matrices is that the relative horizontal and vertical distribution of emissions within the region represented by a particular source element (*e.g.*, Ohio) is assumed to be constant. Changing the overall emissions from that source effectively scales all sources within the region by the same ratio. For near-term assessment, when the precise location of a change in emissions might be pinpointed (*e.g.*, a plant with emission-control units under construction at the time of the assessment), biases may be associated with the use of source-receptor matrices resolved to the state level. For more distant periods, matrix biases are most likely to be associated with the vertical distribution of emissions, because an emission control policy might be focused on transportation sources (surface emissions) or utility emissions (tall stack emissions). This is an issue more critical for NO_x than for SO_x, because little low-level emission of SO_x is occurring or anticipated. The approach in future versions of TAF will be to have separate source-receptor matrices for near-surface and elevated emissions of NO_x.

A term representing climatological variability (Trexler and Shannon, 1994; Shannon and Trexler, 1995), as estimated from ASTRAP simulations for multiple years of meteorological analyses, is included in the module and is passed through all downstream effects modules, including visibility (Sonnenblick and Henrion, 1997).

The primary limitation in usefulness of the Atmospheric Pathways Module as it currently exists is that additional pollutants need to be included for more comprehensive analyses, particularly in regard to $PM_{2.5}$ and visibility. Large advances in capabilities for rapid integrated assessment would result if simple models for regional-scale ozone could be developed. A promising approach may be a technique in which concentrations of NO_x and VOCs at a receptor are separately estimated with source-receptor matrices, and that mixture is then evaluated as to ozone potential, although going from modeled seasonal mean concentrations of NO_x (already included, but not as NO and NO_2 separately) and VOCs (difficult but perhaps doable) to short-term concentration statistics for ozone in a scientifically credible and useful approach would not be easy.

3. VISIBILITY MODULE

The Visibility Module contains a version of the Visibility Assessment Scoping Model (VASM) (Shannon *et al.*, 1997), which was designed for efficient assessment applications using Monte Carlo methods and thus did not need to be further reduced for TAF. VASM applies Monte Carlo techniques to produce seasonal distributions of daily or hourly visual impairment. The Monte Carlo techniques combine statistics from the Interagency Monitoring of Protected Visual Environments (IMPROVE) network (Malm *et al.*,

1994) of seasonal geometric means and standard deviations of daily concentrations of fine-particle species (sulfate, nitrate, elemental carbon, organic carbon, and dust) and coarse-particle dust, interspecies concentration correlations, relative humidity (RH) climatology, and modeled future concentrations of one or more of the particle species (in TAF, currently only sulfate or nitrate or both). Species not modeled are assumed to maintain their current concentration characteristics. The results from the regional model are applied in VASM in a relative manner; that is, if the model simulations indicate that future concentrations will be 65% of the model simulations for the current emission inventory, the current observed mean is scaled by 65% for future visibility simulations. The sets of short-term concentrations and RH values generated by the Monte Carlo techniques are then applied in optical extinction functions that vary with the concentration of the particle species and RH (for the hygroscopic species such as sulfate) to produce optical extinction calculations; these calculations can be combined with Rayleigh scattering and absorption by NO_2 to produce seasonal distributions of total extinction, b_{ext}, which can be converted to visual-range or deciview distributions. The Visibility Module requires input values of projected atmospheric concentrations of SO_4^{2-} and NO_3^- from the Atmospheric Pathways Module, and produces seasonal and annual distributions of visual range for use in the Scenario Benefits Module.

The RH threshold above which impaired visibility should be considered weather-related is an important and somewhat contentious matter. Undoubtedly, until thick fog forms, the visibility in a polluted humid air mass is worse than it would be with identical meteorology and clean air. Ideally, one would seek to know what the degree of visual impairment would be with and without the concurrent particulate loading. Some RH threshold must be selected to define weather-related impairment; in the analyses of IMPROVE data, the threshold is 90%. In VASM, the Monte Carlo generated realizations of RH are capped at 90%; realizations that would otherwise be higher are reduced to 90%. To match the assumptions of the IMPROVE criteria, such simulations would be discarded from the statistics. In the integrated TAF version, visibility simulations were for noontime conditions, and thus the question became nearly moot because RH values are lowest during the warmest portion of the day. For the VASM version described by Shannon et al. (1997), conditions for the entire diurnal cycle were simulated, and so the treatment of high-RH cases, usually occurring near sunrise, assumed some importance.

The Visibility Module will be improved by incorporating updated and improved extinction curves as a function of RH; the functions can even be made receptor-specific if found useful. It may also be found ultimately useful to make the fraction of total NO_3^-/HNO_3 (the lumped species actually modeled in ASTRAP and thus included in this version of the Atmospheric Pathways module) that is assumed to be in the form of fine-particle ammonium nitrate a function of the sulfate concentration or of the change in the sulfate concentration relative to current conditions. This would be an attempt to account for the lessening competition from sulfate for ammonium as emissions of SO_2 are decreased. The actual changes in TAF to improved formulations for light extinction by sulfate and organic carbon particles as a function of RH would be straightforward. The tricky bit will be reaching a community consensus as to what those functions should be.

The visibility module would be strengthed and few internal changes would be necessary if the atmospheric pathway module included source-receptor matrices for elemental carbon and organic carbon (and if the emissions model projected their emissions). An estimate would also need to be made of the concentrations of those particles, particularly organic carbon, resulting from natural emissions. On the other hand, modeling dust from source to receptor, at least for rural locations, does not seem particularly helpful. Presumably, if the dust is being emitted by natural processes, most of those processes will stay about the same in the future; thus daily distributions derived from Monte Carlo treatment of current dust concentration statistics will be at least as accurate as the results of dust transport modeling.

The Visibility Module could also be improved by increasing the number of locations at which visual impairment is simulated. Although the other module improvements discussed above could be accommodated in the TAF structure fairly easily (knowing what the changes should be is not so simple, of course), computer memory limitations may pose a constraint for the maximum number of visibility receptors. An accompanying paper in this conference (Shannon, 1998) describes how we may seek to extend the spatial coverage of the visibility calculations.

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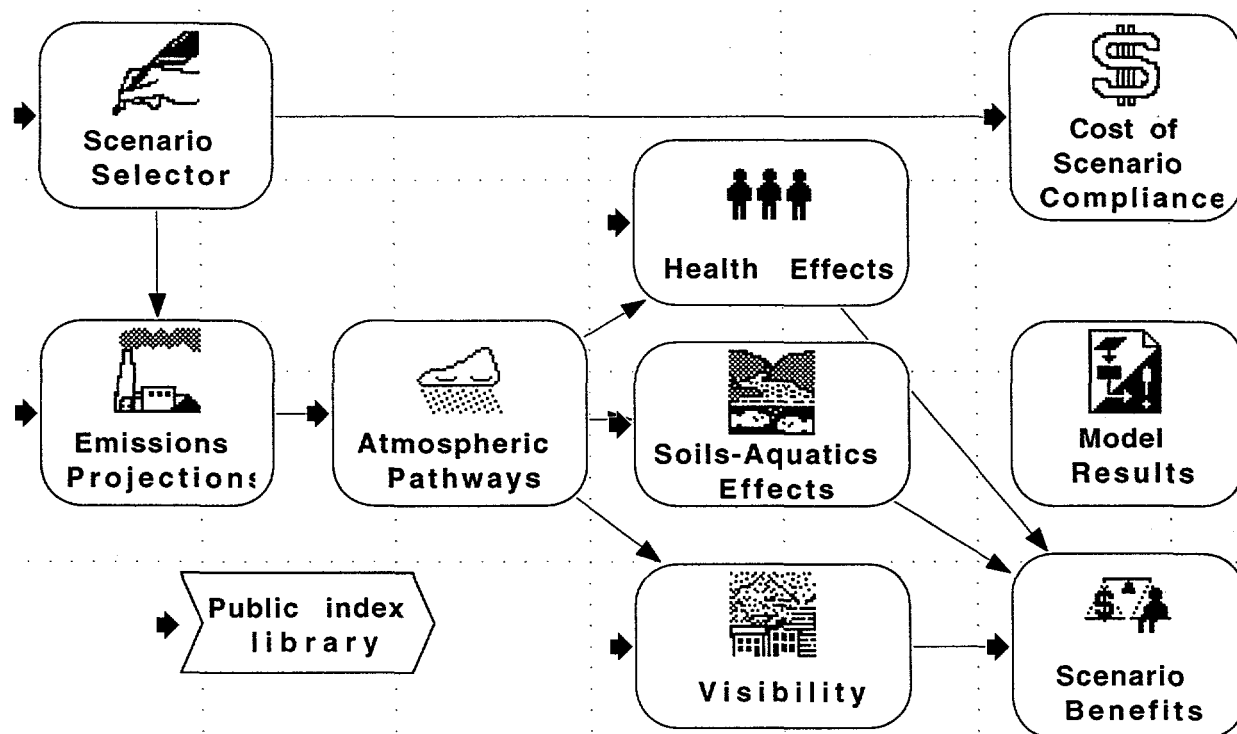
Figure 1: Structure of the Tracking and Analysis Framework as of December 1996