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Project Summary

National Acid Precipitation Assessment Program Emission Inventory Allocation Factors

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The Eulerian Acid Deposition Model being developed for use in the National Acid Precipitation Assessment Program (NAPAP) will require more resolved emissions data than are available in the NAPAP Emissions Inventory. The NAPAP inventory, which separately covers annual emissions from point and countywide area sources, had to be apportioned to reflect hourly emissions with area source emissions assigned to grid squares. Hourly emissions of volatile organic compounds (VOCs) then had to be allocated into photochemical reactivity classes and nitrogen oxide (NO_x) emissions separated into NO and NO_2. This report describes the processes, assumptions, and data sources used in developing the NAPAP temporal, spatial, and species allocation factors. The processing of the NAPAP Emissions Inventory through the Regional Model Data Handling System (RMDHS) and the specifications for a new NAPAP data handling system are also detailed.

This Project Summary was developed by EPA's Air and Energy Engineering Research 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 most extensive use of the NAPAP Emissions Inventory will be to support the Eulerian Acid Deposition Model currently under development. The NAPAP inventory, compiled using EPA's Emission Inventory System (EIS), contains annual emissions from point and area sources. Area sources are compiled on a county total basis while point source data are compiled for individual sources. Emission totals in the NAPAP inventory for VOCs and NO_x actually represent composites of various individual species. To support the Eulerian model, further temporal, spatial, and species resolution is required.

The RMDHS was used to resolve the NAPAP inventory for use as an Eulerian model input tape. RMDHS calculated hourly emission totals of NO_x, SO_2, SO_4, NH_3, and VOCs, allocated VOCs and NO_x into photochemical reactivity classes, separated out major point sources, and assigned minor point sources and area sources to grid cells. The major inputs that enabled RMDHS to generate the Eulerian modeler's tape from the NAPAP annual emission inventory were temporal, spatial, and pollutant species allocation factors, whose development is described below.

Temporal Allocation Factor Development

RMDHS apportioned the NAPAP annual emissions totals into hourly totals for a typical summer weekday by applying the NAPAP temporal allocation factors, a series of fractional multipliers, to the EIS emission file. First, a seasonal fraction is applied to determine quarterly emissions for the summer season. Next, a daily fraction is applied which apportions the seasonal total to a daily total for a "typical" weekday:

$$\text{daily fraction} = \frac{1}{(13 \text{ weeks/season})(\text{number of operating days/week})}$$

Similarly, hourly totals are calculated by multiplying the daily totals by one of 24 hourly fractions representing an entire diurnal pattern. For example, if all of a plant's emissions occur during an 8 a.m. to 5 p.m. workday, the hourly fraction for each of these hours would be:

$$\text{hourly fraction} = \frac{1}{9 \text{ operating hours/day}} = 0.111$$

The hourly fraction for the 15 hours of nonoperation would, of course, be zero.

RMDHS can generate default temporal factors based on operating rates contained in EIS point source records or uniform emissions distributions for area sources if no patterns are supplied. Therefore, primary emphasis was placed on developing temporal factors for the 54 NAPAP area source categories. Since the temporal distribution of emissions most often directly reflects the temporal patterns of the activities that cause the emissions, related categories were grouped together.

GCA developed temporal factors based on literature and data sources published by the U.S. Department of Energy, Department of Transportation, Civil Aeronautics Board, National Weather Service, and Bureau of the Census. Also examined were previously compiled regional scale inventories such as the Northeast Corridor Regional Modeling Project (NECRMP), Regional Air Pollution Study (RAPS), and the Sulfate Regional Experiment (SURE), and inventories developed by several states in support of their State Implementation Plans (SIPs).

Since the NAPAP study area spans four time zones, temporal factors were standardized to reflect Greenwich Mean Time (GMT) by creating four separate, time-zone-specific temporal factor files, each with local time adjusted to reflect GMT, and processing the EIS data accordingly. Thus, hourly emissions in the Eulerian model input tape reflect GMT.

Spatial Allocation Factors

Spatial allocation factors were developed to apportion NAPAP area source emissions from counties to individual grid cells. The NAPAP grid system consists of 37,440 grid cells (156 rows, 240 columns) approximately 20 x 20 km, extending from 65° to 125° West longitude and from 25° to 51° North latitude.

Each spatial allocation factor assigns a portion of a particular county's area source emissions to a specific grid cell. Generally, since the actual subcounty distribution of area source emissions is unknown, emissions are assumed to be distributed according to the known distribution of some surrogate indicator (e.g., population).

The objective in NAPAP was to develop as many surrogate values as possible for each county to allow maximum flexibility in assigning county level area source emissions to specific grid cells. The surrogate indicators used in NAPAP include housing and population counts, total land area, and 10 land use classifications. Once the distribution of the surrogate indicators was known, county level area source emissions were spatially distributed by matching area source emission categories to the most appropriate surrogate indicator.

Housing and population surrogates were derived from the 1980 Census by assigning housing units and population counts to grid cells based on the latitude and longitude of the centroid of each enumeration district. Land use surrogates were derived using Landsat land use percentages for each grid cell and grid/county relationships in the algorithm:

$$SPAFCT_{CSi} = \frac{(A_{Ci})(A_{Si})}{\sum_{i}^{n}(A_{Ci})(A_{Si})}$$

where: $SPAFCT_{CSi}$ = The spatial allocation factor for county C, land use type S, and grid i

A_{Ci} = The portion of county C that falls within grid i

A_{Si} = The portion of grid i with land use type S

n = The total number of grids covering county C

The final step in defining spatial allocation factors was development of the surrogate factor selection file, which assigns each of the 54 NAPAP area source categories to the most appropriate surrogate indicator.

Species Allocation Factors

The NAPAP Emissions Inventory includes annual emission rates for NO_x and VOCs. The Eulerian Acid Deposition Model requires disaggregation of VOC emissions into photochemical reactivity classes and separation of NO_x into NO and NO_2. There are numerous possible VOC speciation schemes based on different modeling chemistries. To provide the flexibility of developing and testing a number of reactivity schemes in NAPAP, it was decided to provide a general species listing for NAPAP point and area source classes, which in turn could be adapted to fit any particular modeling requirements. This objective was achieved by coding a set of "species profiles," each of which provides a typical list of VOCs for a given process. Each specie is defined by its Storage and Retrieval of Aerometric Data (SAROAD) code, molecular weight, and weight percent of total VOC emissions.

A separate SCC Index File was created to link the emission inventory emission classes (referenced by Source Classification Code/SCC) to the most appropriate species profile. Finally, a photochemical class assignments file assigned each VOC specie (referenced by SAROAD code) to the appropriate reactivity class. This approach was taken to provide flexibility in establishing SCC-profile-reactive class relationships.

RMDHS Processing

The allocation factors and emissions data developed for the NAPAP study were processed into a modeler's tape using the Regional Model Data Handling System (RMDHS). RMDHS, developed in 1981, is a package of four major programs which was used to preprocess NECRMP data into input format of the Regional Oxidant Model (ROM). The basic functions of RMDHS include the calculation of projected emission rates, disaggregation of NO_x and VOCs into component species, calculation of hourly emission rates for all pollutant species, and the spatial allocation of ground level point sources and area sources. Figure 1 summarizes the operation of the major components of RMDHS.

The Eulerian Acid Deposition Model to be used in NAPAP requires input data similar to that used in the ROM; thus, RMDHS required relatively minor modifications to ready it for use in NAPAP. These changes primarily reflect the increased size of the study area, and different target source categories and pollutants than those used in NECRMP.

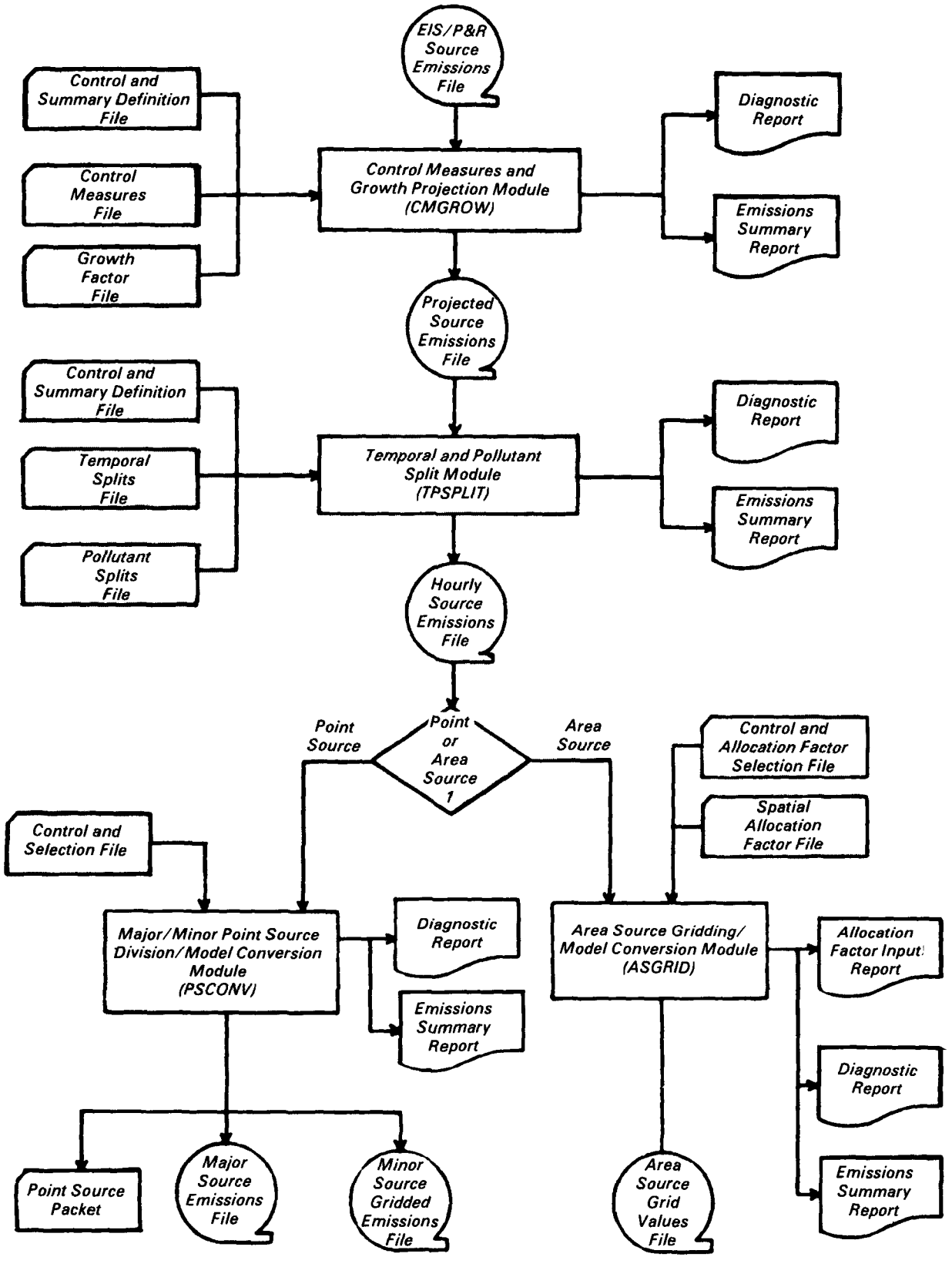


Figure 1. *General data flow plan for the Regional Model Data Handling System.*

Specifically, in order to meet the interim (FY-84) NAPAP deliverable requirements, the system was required to accommodate:

- SO_x resolved to SO_2 and SO_4;
- 48-state geographic domain;
- NH_3; and
- Four separate time zones resolved to Greenwich Mean Time.

Several programs in the RMDHS were modified to satisfy these requirements. Further changes were performed by Engineering-Science (E-S), including compression of the NAPAP master file to lower data processing costs, and the disaggregation of the master file based on time zone boundaries.

The output of RMDHS to be used as input to an Eulerian model consists of a major source emissions file, a minor source gridded emissions file, and an area source grid values file. These three files were output separately for each of the four time zone specific areas in the NAPAP study scope; some of the time zone specific output data were merged as appropriate.

NAPAP Emissions Inventory Data Handling System Design Specifications

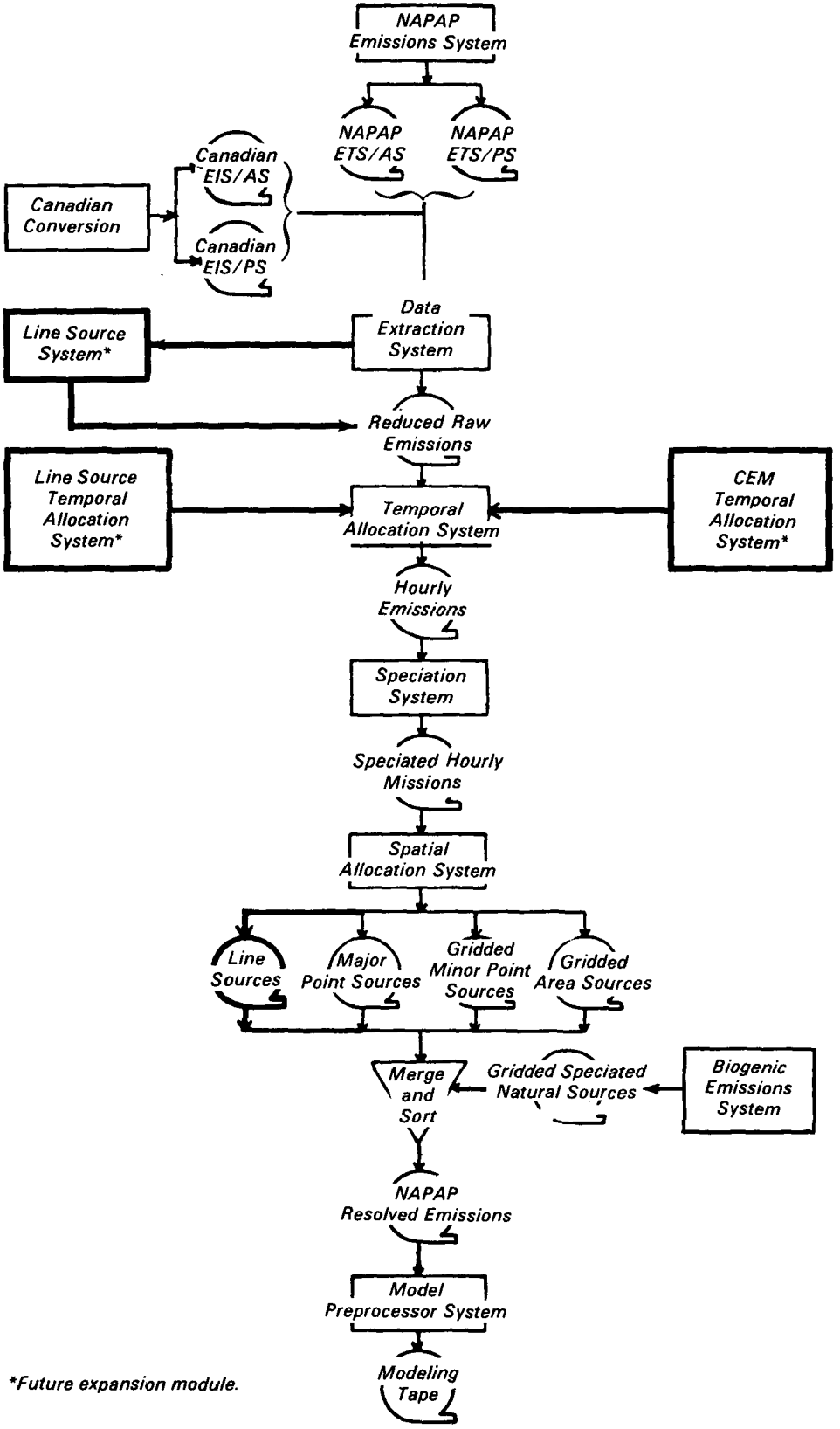
As described above, a modified version of the Regional Model Data Handling System (RMDHS) was used to create an interim (FY-84) 1980 NAPAP inventory Eulerian model input tape. GCA also assessed the feasibility of substantially modifying RMDHS to address the more comprehensive FY-85 deliverable, which would include:

- Significantly more VOC species resolution (CB/X chemistry classes);
- Addition of HCl, HF (and possibly V and Mn) as new pollutants;
- Derivation of alkaline dust from TSP;
- TSP resolved to particle size classes;
- Additional Area Source categories;
- Incorporation of Canadian data; and
- Incorporation of Natural Sources data.

As a result of the investigation, GCA concluded that the modifications required to RMDHS would be major, and that the modified system would be very expensive to operate. Therefore, we believe that further changes to RMDHS would not be the most effective course of action for EPA to undertake. Instead, we recommend that EPA consider development of a new, more suitable system that would incorporate sufficient flexibility to address not only changes specific to NAPAP, but would also be easily adaptable for other similar regional scale undertakings, such as the Regional Particulate Modeling (RPM) Study and the Northeast Regional Oxidant Study (NEROS). This system should be structured in a highly modular fashion with the inherent flexibility needed to address regional undertakings incorporated in all aspects of the design.

The NAPAP emission data preprocessing system, or the Flexible Regional Emissions Data System (FREDS), will consist of a number of independent subsystems used to extract pertinent emissions data from EIS/PS and EIS/AS records, resolve them temporally and spatially, and resolve composite emissions to individual species. It includes capabilities to incorporate natural (biogenic) emissions with man-made sources data into the temporal, spatial, and species resolution process. It will also incorporate sufficient flexibility to allow needed future enhancements. Currently envisioned future improvements include better handling of line source emissions and incorporating continuous emissions monitoring (CEM) data. The relationships of the various 1985 and future subsystems are shown in Figure 2.

Each of the above subsystems of FREDS will exist as an independent module. All software will be developed using state-of-the-art modular (structured) programming techniques and will reflect maximum flexibility to easily accommodate future enhancements and modifications. It is currently envisioned that the FREDS system will be developed on the NCC IBM generally using EPA software development standards.



*Future expansion module.

Figure 2. *Relationship of major modules of the Flexible Regional Emissions Data System (FREDS).*

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The complete report, entitled "National Acid Precipitation Assessment Program Emission Inventory Allocation Factors," (Order No. PB 86-104 247/AS; Cost: $16.95, subject to change) will be available only from:
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