



Project Summary

Flexible Regional Emissions Data System (FREDS) Documentation for the 1985 NAPAP Emissions Inventory

Lysa G. Modica, Daniel R. Dulleba, Robert A. Walters, and John E. Langstaff

The Flexible Regional Emissions Data System (FREDS) is a modular software system that takes the NAPAP annual point and area source emissions inventories and derives a resolved emissions data base suitable for input to atmospheric pollution simulation models, such as the Regional Acid Deposition Model (RADM). The primary functions of FREDS are to resolve annual emissions to hourly values, to apportion county-level area source emissions to grid cells, and to perform speciation of selected pollutants into user-defined species classes. FREDS consists of seven primary modules written in SAS* and Fortran which perform the tasks of extraction of desired data from the annual inventories, temporal and spatial allocation, speciation, conversion to modeling format and quality control of the flow of data through the system. The order in which the allocation and speciation modules are to be executed is flexible, and not all of these modules must be executed, allowing for different applications and desired formats. The user can specify the parameters of execution and define the allocation and speciation both geographically and by source type by means of control options files and allocation factor files. FREDS was first designed and used to process the 1980 NAPAP emissions inventories, and has been significantly

enhanced for processing the 1985 NAPAP emissions inventories. The flexible design of FREDS ensures that it will be a useful system for processing other emissions inventories for modeling applications.

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).

Background

The National Acid Precipitation Assessment Program (NAPAP) was established by Congress in 1980 to coordinate and expand research on problems posed by acid deposition in and around the U.S. The program is managed through the Interagency Task Force on Acid Precipitation which currently coordinates seven task groups having specific technical responsibilities. The Task Group on Emissions and Controls is charged with development of comprehensive and accurate inventories of emissions from anthropogenic sources thought to be important in acid deposition processes. To fulfill its objective and to support other related NAPAP research, the Task Group on Emissions and Controls is generating a number of major emissions data bases using 1980 and 1985 as base years.

The primary focus of the NAPAP inventories is the fulfillment of the emissions data requirements for application of the Eulerian Regional Acid Deposition Model (RADM). In addition, emissions data are used to support applications of other regional models including the Regional Oxidant Model (ROM). To support development and testing of these models, the 1985 NAPAP annual inventory must be resolved temporally, spatially, and by component species. The temporal, spatial, and species resolution of the annual and resolved emissions data bases are summarized in Table 1. For RADM, annual emissions are required at the hourly level for a typical weekday, Saturday, and Sunday in each season (12 temporal scenarios); county-level area sources and major and minor point sources must be spatially resolved to modeling grid cells; TSP emissions are assigned to species and size classes; NO_x emissions are split into NO₂ and HO₂ constituents; and VOC emissions are apportioned into approximately 30 photochemical reactivity classes. The Flexible Regional Emissions Data System (FREDS) was created to meet these needs.

FREDS was originally developed for the processing of the 1980 NAPAP Emissions Inventory. To meet the needs of the 1985 inventory, several significant enhancements to the FREDS software were undertaken. Some of these changes were necessary to accommodate new and/or expanded data requirements, particularly in the area of hydrocarbon and particulate speciation; other modifications and additions were identified as desirable as a result of experience with the 1980 inventory. These enhancements ensure that FREDS will continue to be a valuable tool for future applications.

The primary objectives of this effort are to document the FREDS software used to process the 1985 NAPAP Annual Emissions Inventory and to provide the user with the necessary specifications for execution of FREDS modules. Input/output formats are also supplied for all files based on the order of module execution for RADM modeling inventory development.

FREDS Overview

FREDS is a modular software system that extracts pertinent modeling parameters from annual emissions inventories and applies spatial, temporal, and pollutant species allocation factors in order to create a resolved emissions inventory suitable for use as model input

to Eulerian regional models. Written in SAS and Fortran, FREDS consists of seven primary subsystems:

- The *Hydrocarbon Preprocessor* (HCPREP) is used to interconvert between total hydrocarbons (THC) and nonmethane volatile organic compounds (VOC), providing a consistent basis for hydrocarbon emissions estimates. It also compensates for the lack of aldehydes in AP-42 emission factors calculated using flame ionization detection (FID).
- The *Model Data Extraction Module* (MDEM) reads an annual point or area source emissions file, condenses it by retaining only pertinent modeling parameters, and produces a file suitable for processing through the rest of FREDS. MDEM can also produce industry-specific subfiles, and separate "major" and "minor" point sources if specified by the user.
- The *Temporal Allocation Module* (TAM) accepts a FREDS-compatible file as input, and applies seasonal, daily, and hourly allocation factors to annual emissions records. For point sources, TAM can construct these factors from NEDS operating rate data if a profile is not provided for the source. TAM also offsets all temporal data to Greenwich Mean Time (GMT).
- The *Speciation Module* (SM) accepts SAS-formatted emissions files and merges them with hydrocarbon and NO_x speciation factors generated by the Pollutant Splits System (PSPLIT) and/or factors in a Speciation Factor File, such as particulate alkalinity and size classes. Users may, by manipulating the input files, speciate any of the annual pollutants into as many as 32 classes.
- The *Spatial Allocation Module* (SAM) matches and merges area source emissions with spatial allocation factors, enabling the emissions to be assigned to modeling grid cells. Point sources are assigned to grids based on latitude/longitude or UTM coordinates, while area source emissions are apportioned on a county basis to grids according to known distributions of surrogate spatial indicators.
- The *Model Input Preprocessor* (MIP) combines the resolved emissions files, sorts the resulting data set, and produces a point or point or area source modeler's tape in either SAS or EBCDIC format. For point sources, the MIP output consists of an emissions file with allocation factors assigned to each source. Due to space considerations, area source MIP output is a

gridded, hourly emission file for one user-specified temporal scenario.

- The *Quality Control Module* (QCM) accepts FREDS-compatible files at any stage of processing and compares national, state, and source category emissions totals to baseline emissions totals input to FREDS, supplementing the diagnostic checks carried out within the other modules. QCM also ensures that the point source temporal allocation fractions sum to unity within user-specified tolerances.

Figure 1 is a simplified diagram of FREDS processing for the 1985 NAPAP Emissions Inventory, illustrating the interrelationship of the various major components. National Emissions Data System (NEDS) data provide the basis for the NAPAP point and area source emissions estimates for criteria pollutants; emissions data for noncriteria pollutants were developed by EPA's Air and Energy Engineering Research Laboratory (AEERL). Hydrocarbon emissions are adjusted to a consistent basis using HCPREP; the resulting files represent the NAPAP Annual Inventory. Resolution of emissions is provided in the three allocation modules (SM, SAM, and TAM); these can be run in any order but must be preceded by MDEM, and MIP must be the last module executed. Output data sets from any module can be routed through QCM to ensure that emissions totals are not being altered during the resolution process. While the primary function of FREDS is to fulfill the data requirements for RADM development and testing, the design of the system allows sufficient flexibility for a variety of applications. FREDS allows user definition of the pollutants to be processed and the user can readily vary temporal factor data, the extent and origin of the spatial grid and the grid cell size, and the number and relationship of pollutant sub-species. Each module also utilizes a control options file to pass job parameters to the program, which can be adapted to suit individual data needs.

Report Organization

The documentation of FREDS is structured in accordance with EPA's automated data processing standard and consists of:

- Introduction
- System Charts
- Detailed Program Description
- Input/Output Format Description
- Control Statements
- Operating Instructions
- Environment

Table 1. 1985 NAPAP Emissions Inventory Coverage.

	<i>Annual Emissions Inventory</i>	<i>Regional Modeling Emissions Inventory</i>
<i>Anthropogenic point sources</i>	<i>Stationary sources emitting greater than or equal to 100 tons of criteria pollutants in 1985</i>	
<i>Anthropogenic area sources</i>	<i>County-level area sources and stationary sources emitting less than 100 tons of criteria pollutants in 1985</i>	
<i>Natural area sources</i>	<i>Emissions of sulfur compounds, nitrogen compounds, hydrocarbon species and ammonia from biogenic and geophysical processes; TSP from natural sources</i>	
<i>Geographic domain</i>	<i>The 48 contiguous states and part of Canada</i>	
<i>Pollutants</i>	<i>SO₂, SO₄, CO, TSP, HCl, HF, NO_x, NH₃, VOC, THC</i>	<i>SO₂, SO₄, CO, TSP (reactive Ca, Mg, K, Na: 0-2.5 μm, 2.5-10 μm, and total; TSP: 0-2.5, 2.5-6, and 6-10 μm), HCl, HF, NO, NO₂, NH₃, VOC, THC, 30 VOC species classes</i>
<i>Temporal resolution</i>	<i>Annual</i>	<i>Hourly emissions values for typical weekday, Saturday, and Sunday for all four seasons</i>
<i>Spatial resolution</i>	<i>Point source locations specified by latitude and longitude; area sources at the county level</i>	<i>Point and area sources assigned to grid cells 1/6° latitude by 1/4° longitude (approximately 20 × 20 km)</i>

- Example Speciation Module Run and Description

● Conclusion

FREDS software provides versatile and powerful computer programs to allocate emission inventory data into various levels of spatial, temporal, and species resolution. The system was used successfully in a first of a kind application to process the 1980 NAPAP Emissions Inventory to support the specific requirements of acid deposition and photochemical oxidant atmospheric models. For use with the 1985 NAPAP emissions data base, several enhancements and modifications were implemented to allow for new and expanded data requirements, to improve processing efficiency, and to provide higher quality output data. The successful completion of these modifications will facilitate the processing of the 1985 NAPAP Emissions Inventory in a timely and cost-effective manner while maintaining maximum flexibility for specialized applications.

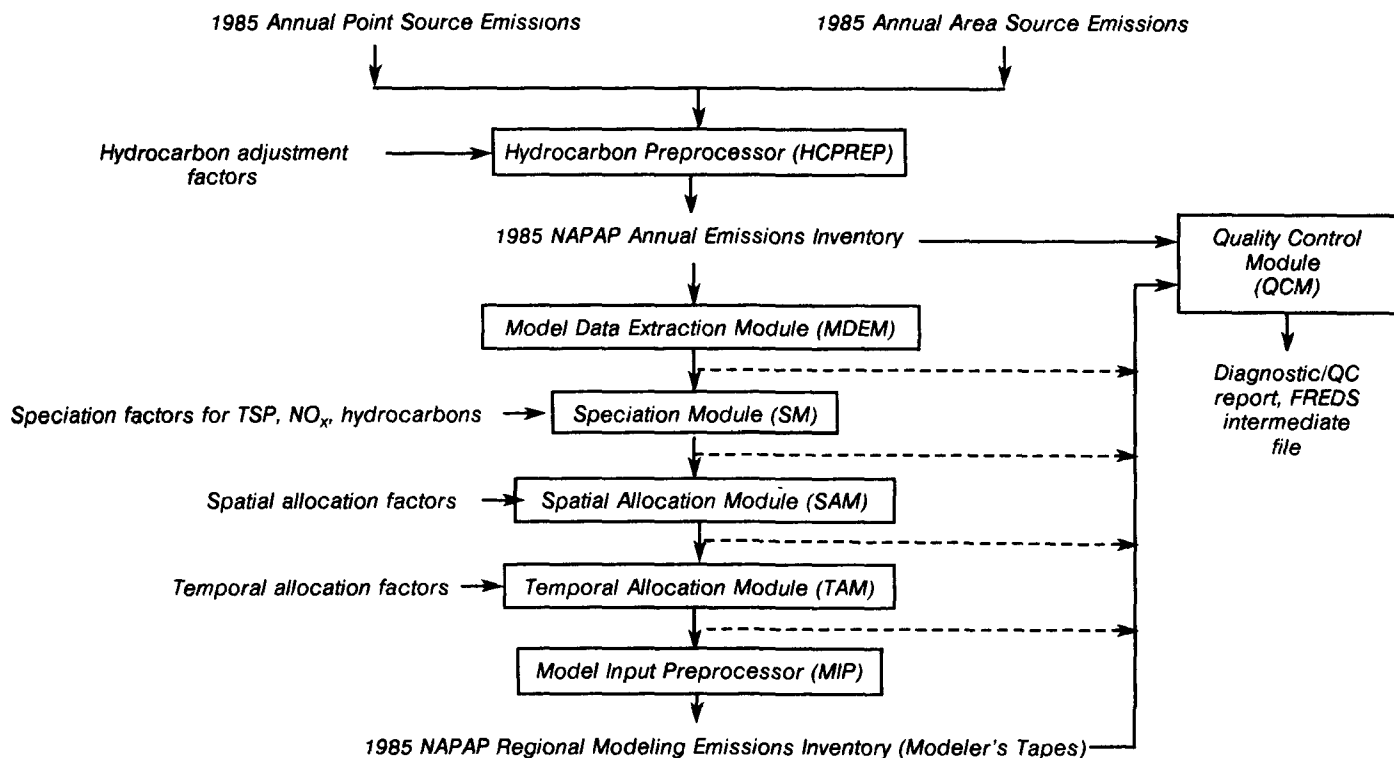


Figure 1. Simplified diagram of FREDS processing.

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Robert C. Lagemann is the EPA Project Officer (see below).

The complete report consists of tape and paper copy, entitled "Flexible Regional Emissions Data System (FREDS) Documentation for the 1985 NAPAP Emissions Inventory."

Paper Copy (Order No. PB 89-198 816/AS; Cost: \$42.95)

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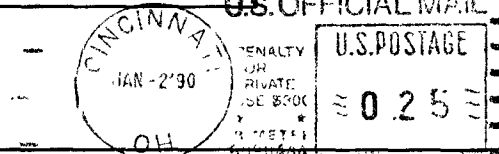
The above documents will be available only from: (costs subject to change)

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