United States
Environmental Protection
Agency

Air and Energy Engineering
Research Laboratory
Research Triangle Park NC 27711

Research and Development

EPA/600/S7-87/025 Feb. 1988

EPA

Project Summary

Flexible Regional Emissions Data System (FREDS) Documentation for the 1980 NAPAP Emissions Inventory

Lysa G. Lebowitz and Andrew S. Ackerman

The report documents the development of the Flexible Regional Emissions Data System (FREDS) for the 1980 NAPAP Emissions Inventory. FREDS extracts emissions data, pertinent modeling parameters (e.g., stack height, exhaust gas temperature), and source identification information and applies appropriate temporal, spatial, and pollutant species allocation factors to derive a gridded, speciated, and temporally resolved emissions file suitable as input to regional-scale atmospheric simulation models (e.g., Regional Acid Deposition Model, Regional Oxidant Model). FREDS consists of five main modules which are used to apply allocation factors to the annual emissions data, plus peripheral software used to ensure the quality of and maintain the allocation factor files. Separate programs are used to process point and area sources. The five main modules are the Model Data Extraction Module, the Temporal Allocation Module, the Speciation Module, the Spatial Allocation Module, and the Model Input Preprocessor. The modules can be implemented in a logical sequence or independently of the others. In addition, FREDS has been designed in a modular fashion, facilitating future modifications to the system. FREDS and associated peripheral software are written in the language of the Statistical Analysis System (SAS) and are installed on EPA's National Computer Center's IBM 3090.

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 coordiantes eight 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 sources thought to be important in acid deposition processes. To fulfill its stated objective and to support other related NAPAP research, the Task Group on Emissions and Controls has generated a number of major emissions data bases using 1980 as the base year.

Processing of the 1980 NAPAP Emissions Inventories required the design of an emissions data handling system—the Flexible Regional Emissions Data System (FREDS). The primary focus of these inventories is the fulfillment of the emissions data requirements for development and testing of the Eulerian Regional Acid Deposition Model (RADM). In addition, emissions data are also used to support applications of the Regional Oxidant Model (ROM).

To support development and testing of these models, the 1980 Annual Inventory (Version 5.0) was resolved temporally, spatially, and by component species using FREDS. An Eulerian modeling emissions inventory (Version 5.2) and an oxidant modeling emissions inventory (Version 5.3) were created. The temporal, spatial, and species resolution of the emisisons data bases are summarized in Table 1. Annual emissions were allocated to 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 were spatially resolved to modeling grid cells; TSP emissions were assigned to alkalinity classes; NO_x emissions were split into NO and NO_2 constituents; and THC emissions were apportioned into as many as 28 photochemical reactivity classes.

To create the 1980 NAPAP Modeling Emissions Inventories, FREDS requires input files of temporal, spatial, and pollutant species allocation factors. The development of these factors is documented in separate reports. FREDS was also used to generate a SAS version of the 5.0 NAPAP Emissions Inventory for incorporation into the Acid Deposition Data Network (ADDNET).

FREDS Overview

FREDS is a software system designed to produce an emissions inventory suitable for input to regional acid deposition models. FREDS extracts emissions data, pertinent modeling parameters (e.g., stack height, exhaust gas temperature), and source identification information from EIS Master File records or preprocessed SAS files and applies appropriate temporal, spatial, and pollutant species allocation factors to derive a gridded, speciated, and temporally resolved emissions file suitable as input to a regional scale atmospheric simulation model. FREDS for the 1980 NAPAP Emissions Inventory consists of five main modules which are used to apply allocation factors to the annual emissions data, plus peripheral software used to quality assure and maintain the allocation factor files. Separate programs are used to process point and area sources. The five primary modules are the Model Data Extraction Module (MDEM), the Temporal Allocation Module (TAM), the Speciation Module (SM), the Spatial Allocation Module (SAM), and the Model Input Preprocessor (MIP). For final processing, the SAS formatted MIP output is converted to EBCDIC characters. An overview of FREDS modules is presented in Figure 1. Each module can be implemented in a logical sequence or independently of the others. To maximize flexibility, FREDS allows user definition of up to 15 pollutant emissions and their identities (referenced by Storage and Retrieval of Aerometric Data (SAROAD) pollutant code), the temporal scenario, spatial grid origin and grid cell size, and the number and relationship of pollutant subspecies. Grid definition is specified in a user generated Spatial Allocation Module Control Options File. To speciate emissions for various chemcial mechanisms or pollutant subclasses, the user inputs the requested classes using files containing the desired speciation factors. In addition, FREDS has been designed in a modular fashion, facilitating future modifications to the system. FREDS and associated peripheral software are written in the command language of the Statistical Analysis System (SAS) and are installed on the National Computer Center's IBM 3090.

Conclusion

FREDS software provides a versatile and powerful computer program to allocate emission inventory data into various levels of spatial, temporal, and species resolution. The system was used

Table 1. *1980 NAPAP Emissions Inventory Coverage*

	Annual Emissions Inventory Version 5.0	*Eulerian Model Emissions Inventory Version 5.2*	*Oxidant Model Emissions Inventory Version 5.3*
Temporal resolution	*Annual/seasonal*	*Hourly emissions values for typical weekday, Saturday, and Sunday for all four seasons*	
Geographic domain and resolution	*48 contiguous states and Canada; area sources at the county level*	*48 states and Canada; separate major point source file with minor point sources and area sources assigned to 20 x 20 km grid cells*	
Anthropogenic point sources	*Stationary sources emitting 100 or more tons of criteria pollutants in 1980*		
Anthropogenic area sources	*Stationary sources emitting less than 100 tons of criteria pollutants in 1980 and area sources*		
Pollutants	*SO_2, SO_4, TSP, Pb, CO, HCl, HF, NO_x, NH_3, VOC, total hydrocarbons (THC)*	*SO_2, SO_4, TSP (Ca, Mg, K, Na), Pb, CO, HCl, HF, NO, NO_2, NH_3, VOC, THC (methane, ethane, ethylene, propane, propylene, N-butane, 1,2-butane, isobutene, trans-2-butene, pentane, isopentane, 2,3-dimethylbutane, other alkenes, other alkanes, formic acid, acetic acid, other organic acids, formaldehyde, acetaldehyde, propionaldehyde, acetone, other ketones, other aldehydes, xylene, benzene, toluene, ethylbenzene, other aromatics)*	*SO_2, SO_4, TSP (Ca, Mg, K, Na), Pb, CO, HCl, HF, NO, NO_2, NH_3, VOC, THC, (methane, paraffins, ethylene, olefins, formaldehyde, other aldehydes, toluene, xylene, isoprene, nonreactives)*

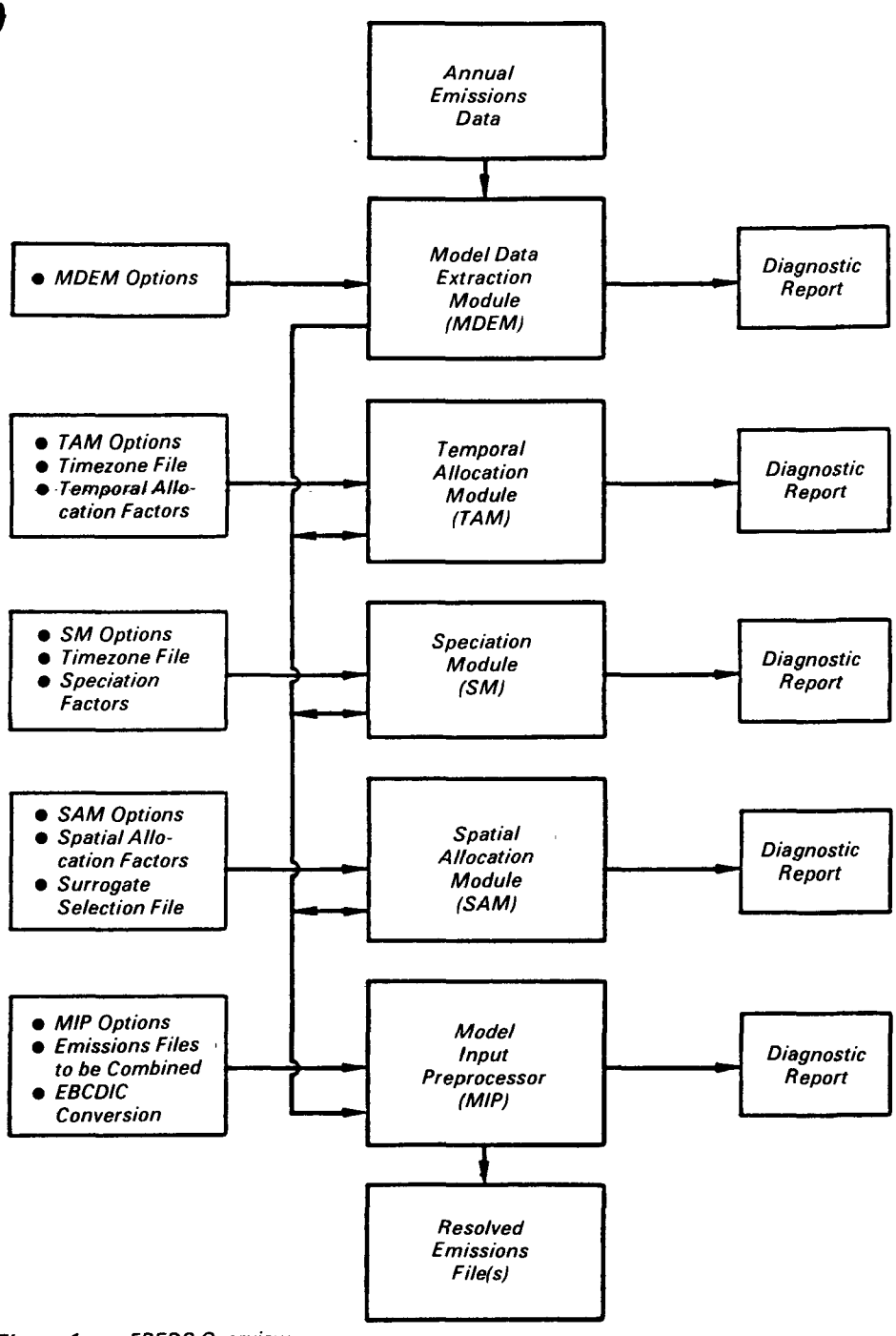

Figure 1. *FREDS Overview.*

successfully in a first of a kind application to process the 1980 NAPAP Emissions Inventory into data bases to support the requirements of acid deposition and photochemical oxidant atmospheric models. The documentation of the program in accordance with EPA's automatic data processing standards ensures that it will be a useful tool for future applications.

L. G. Lebowitz and A. S. Ackerman are with Alliance Technologies Corporation, Bedford, MA 01730.
***J. David Mobley** is the EPA Project Officer (see below).*
The complete report, entitled "Flexible Regional Emissions Data System for the 1980 NAPAP Emissions Inventory," consists of the following:
Document (Order No. PB 88-129 499/AS; Cost: $38.95, subject to change)
Software Location Factor Files (Order No. PB 88-129 481/AS; Cost $800.00 [document listed above is included in the price of the software], subject to change)
The above will be available only from:
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650
The EPA Project Officer can be contacted at:
Air and Energy Engineering Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

United States
Environmental Protection
Agency

Center for Environmental Research
Information
Cincinnati OH 45268

Official Business
Penalty for Private Use $300

EPA/600/S7-87/025