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DEVELOPMENT OF MESOSCALE AIR QUALITY SIMULATION MODELS

VOLUME 5. USER'S GUIDE TO THE MESOFILE POSTPROCESSING PACKAGE

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TABLE OF CONTENTS

	Page
LIST OF ILLUSTRATIONS	vii
LIST OF TABLES	ix
1. INTRODUCTION	1
1.1 Background	1
1.2 Overview of MESOFILE	3
1.3 Direct-Access Disk Storage System	7
2. DETAILED MESOFILE DESCRIPTION	9
2.1 MESOFILE Overview	9
2.2 MESOFILE Components	11
2.2.1 Subroutine ECHO	11
2.2.2 Subroutine DEFN	13
2.2.3 Subroutine FIND	19
2.2.4 Subroutine SEEK	21
2.2.5 Subroutine AVRG	23
2.2.6 Subroutine ADD1	25
2.2.7 Subroutine ADD2	28
2.2.8 Subroutine STAT	30
2.3 Sample Card Inputs for Some Useful MESOFILE Applications	42
3. MESOPLOT DESCRIPTION	45
4. PLOTVEC DESCRIPTION	53
5. BACKUP01 AND ZERO50 DESCRIPTION	57
REFERENCES	
ABSTRACT	

LIST OF ILLUSTRATIONS

Figure		Page
1-1	Integrated Mesoscale Modeling System	2
1-2	File Management and Analysis (MESOFILE)	4
1-3	Examples of MESOFILE Graphical Displays	6
2-1	Sample ECHO Output--File 13 (Library File)	12
2-2	Sample ECHO Output--Partial Contents of File 15 (NAMELIST File)	14
2-3	Schematic Illustration of the Averaging Process	26
2-4	Sample of Statistical Output	33
2-5	Grid Subsets Used in the Statistical Calculations	36
2-6	Flow Chart of Subroutine STAT	37
3-1	Sample MESOPLOT Contour Plots	46
4-1	Sample PLOTVEC Vector and Contour Plots	54

LIST OF TABLES

Table		Page
1-1	Components of the MESOFILE File Management Package	5
1-2	Logical Unit File Structure	8
2-1	Form of MESOFILE Card Inputs and Subroutine Identifiers	10
2-2	Card Inputs to Subroutine ECHO	16
2-3	Card Inputs to Subroutine DEFN	18
2-4	Card Inputs to Subroutine FIND	20
2-5	Card Inputs to Subroutine SEEK	22
2-6	Card Inputs to Subroutine AVRG	24
2-7	Card Inputs to the Line Printer Plotting Routine	27
2-8	Card Inputs to Subroutine ADD1	29
2-9	Card Inputs to Subroutine ADD2	31
2-10	Statistical Measures Calculated by Subroutine STAT	34
2-11	Card Inputs to Subroutine STAT	40
3-1	Card Inputs to MESOPLOT--'SAME' NAMELIST	49
3-2	Card Inputs to MESOPLOT--'DIFF' NAMELIST	50
3-3	Card Inputs to MESOPLOT--'DATE' NAMELIST	51
4-1	Card Inputs to PLOTVEC--'SAME' NAMELIST	55
4-2	Card Inputs to PLOTVEC--"DIFF' NAMELIST	56

1. INTRODUCTION

1.1 Background

As a result of the national commitment to the greatly expanded use of indigenous coal reserves to meet growing energy generation demands, several regions of the country (and in particular the Four Corners region of the southwestern United States) will see increased region-wide development of coal-fired steam electric power plants, and/or coal gasification and oil shale recovery facilities. As mandated by federal statutes and regulations reflecting the strong nationwide support for environmental protection, additional fossil-fuel based energy resource development (ERD) will only be permitted where consistent with the maintenance of human health, welfare, and environmental quality. Suitable MESOSCALE air quality modeling tools are needed to assess the impacts of different energy development scenarios on regional air quality. To meet this need in the public interest, the National Oceanic and Atmospheric Administration (NOAA) has sponsored a study by Environmental Research & Technology, Inc. (ERT) to develop, compare, evaluate, and exercise a number of alternative approaches to regional-scale ambient air quality modeling in the Four Corners area, with the objective to provide a suite of air quality simulation models that are both technically sound and computationally practical for assessing regional-scale impacts of energy development scenarios, specifically in the Four Corners area, and more generally as well.

Three different regional-scale air quality transport-diffusion models have been developed to address various features of point-source plume dispersion of the mesoscale--e.g., dispersion at ranges of 100 to 1,000 kilometers (km) . These models are described, compared and documented in companion volumes 1-4 in this series of documents entitled "Development of Mesoscale Air Quality Simulation Models" (Bass et al. 1979; Benkley and Bass 1979a, b, and c; Morris et al. 1979).

The three models are:

- MESOPLUME, a variable-trajectory Gaussian "plume-segment" model;
- MESOPUFF, a variable-trajectory Gaussian "puff" superposition model; and
- MESOGRID, an Eulerian grid model based on the method of moments.

The three models share, where possible, the identical modules for plume rise, plume decay and deposition, plume growth with distance or travel time, and treatment of plume fumigation by entrainment within the growing mixed layer.

To facilitate exact comparisons of these regional-scale dispersion models for specified sets of model parameters and meteorological conditions, an efficient, easy-to-use "mesoscale modeling system" has been designed. This system, schematically depicted in Figure 1-1, is a fully integrated set of independent components comprising meteorological preprocessing, transport-diffusion, and post-processing functions.

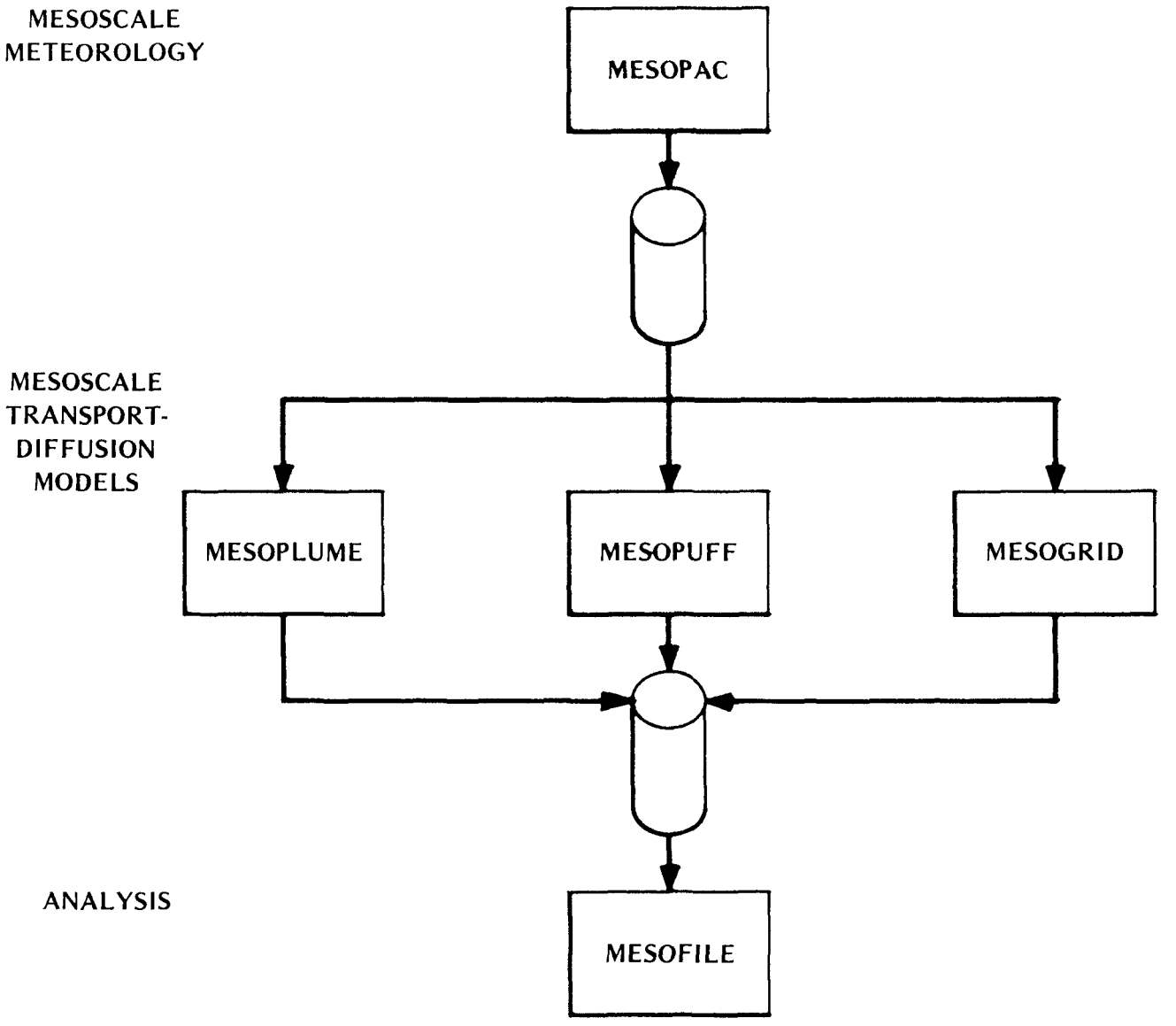

Figure 1-1 Integrated MESOSCALE Modeling System

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The mesoscale meteorology preprocessor, called MESOPAC, provides the necessary meteorological input for any of the three mesoscale transport-diffusion models (MESOPLUME, MESOPUFF, or MESOGRID). Each of these models in turn identically communicates its results to the postprocessing system, MESOFILE, responsible for file management, display, and statistical analysis of all model output fields. This document describes and illustrates the use of the MESOFILE system and suggests other areas of application that go well beyond the uses put to MESOFILE in the present contractual effort.

1.2 Overview of MESOFILE

The MESOscale FILE management and analysis system (MESOFILE) shown in Figure 1-2, is a flexible post-processing package, designed especially for interface with the regional-scale models. It consists of file management, file merging and manipulation, statistical analysis, and graphical display components (see Table 1-1). The file management package records, catalogues, and archives all the relevant output from the MESOPUFF, MESOPLUME, and MESOGRID regional scale diffusion models. The concentration field output of any of the mesoscale diffusion models can be routed to either the line printer or to direct-access disk storage for subsequent processing.

The direct-access storage system allows for automatic storage and cataloging of all the output data fields from the diffusion models through the file management subroutine (FILMAN). Subroutine FILMAN will produce, for each run for which output has been requested for disposal to disk, a record of the date of the run, the run characteristics, the disk file location it assigns automatically to all the concentration data output, and the values of all the input parameters for the run. The MESOFILE program allows this information to be retrieved for all the previous runs made on a particular set of disk files.

In addition, the MESOFILE user can arbitrarily specify the time averaging interval for the model concentration fields to allow statistical analyses to be defined over any multiple of the basic (hourly) time step. Computer core resource limitations require that the diffusion models operate only with a limited number of sources within a given run (ten sources for the plume and puff models; fifty sources for the grid model). MESOFILE can be used to sum the concentration fields obtained from separate runs made with subsets of the total source inventory to obtain an assessment of the impact of the full source inventory. Two-dimensional fields of mean winds, mixing heights, Pasquill-Gifford-Turner (PGT) stability classes, as well as ambient air concentrations can be coutour plotted with the MESOPLOT and PLOTVEC programs (see Sections 3 and 4). Figure 1-3 illustrates some of the kinds of graphical displays produced by the MESOPLOT and PLOTVEC routines.

BACKUP01 and ZERO50 are additional file management programs that are useful in operating the file management system. Because the location of the output of each model run is recorded by the file management system, an abnormally terminated run must be erased from the run log before more model runs can be made. This is accomplished

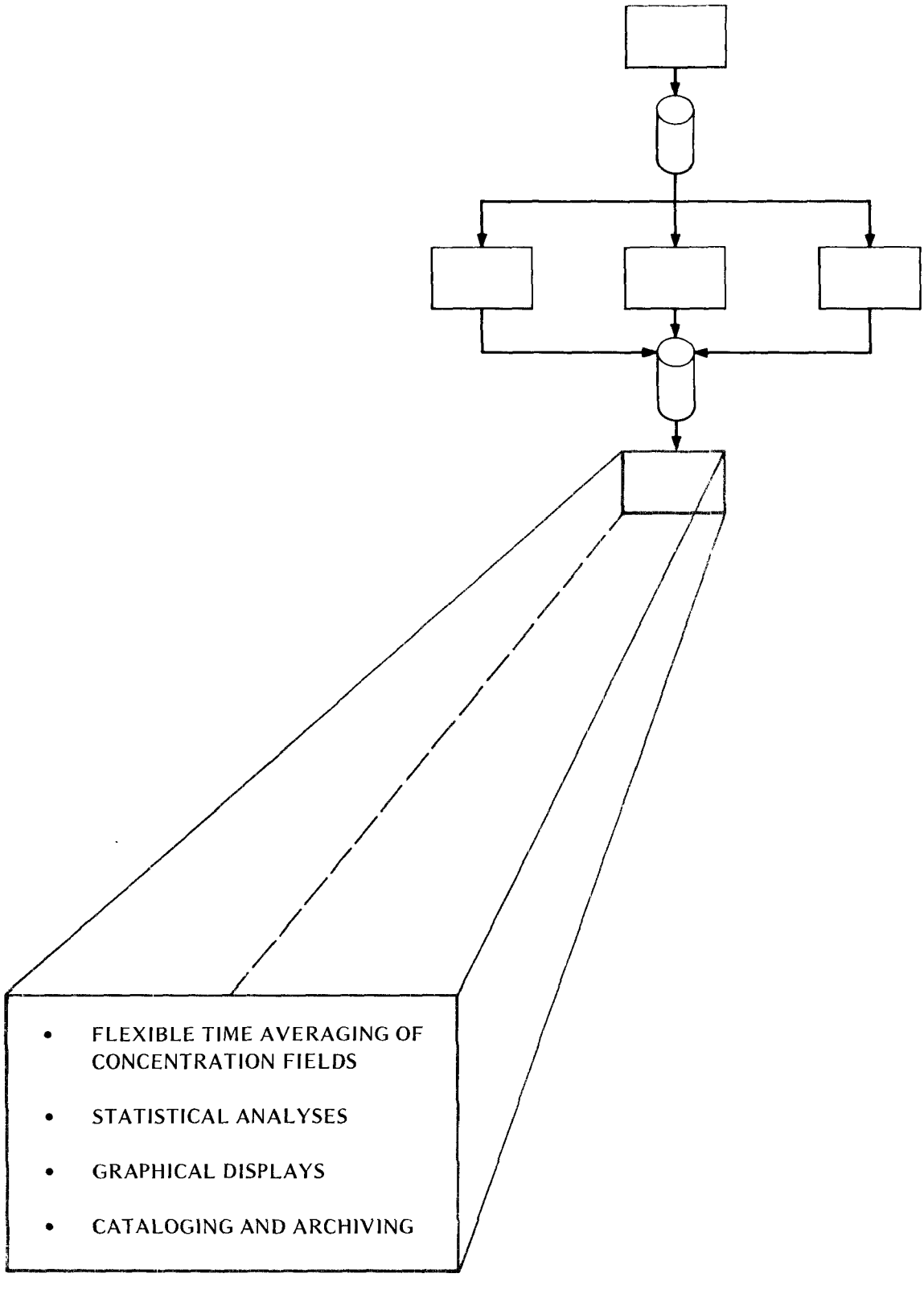

Figure 1-2 File Management and Analysis (MESOFILE)

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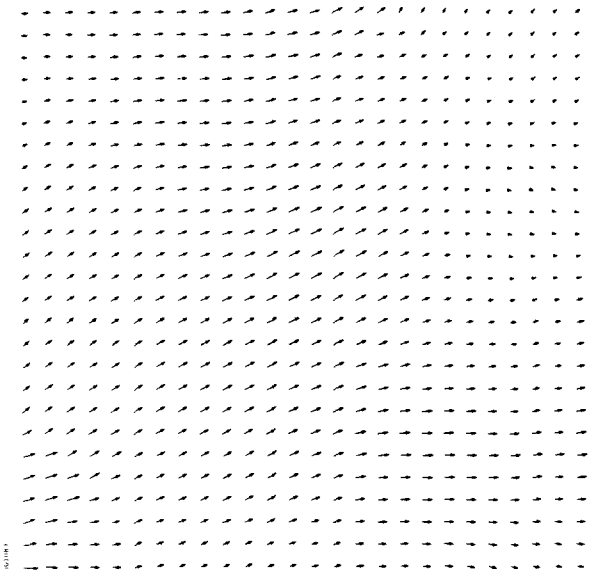
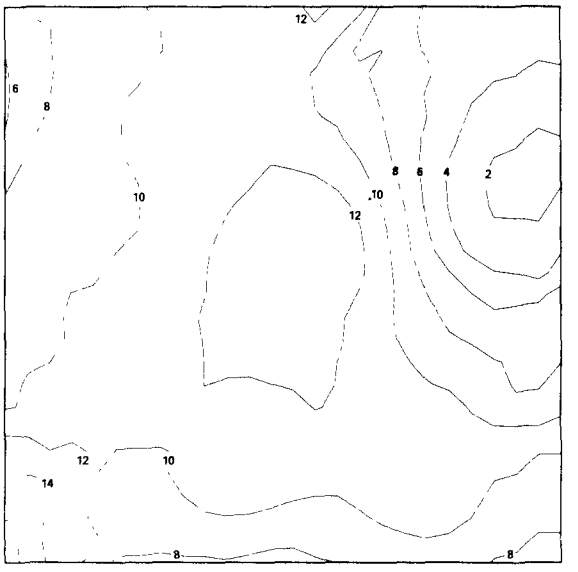
TABLE 1-1

COMPONENTS OF THE MESOFILE FILE MANAGEMENT PACKAGE

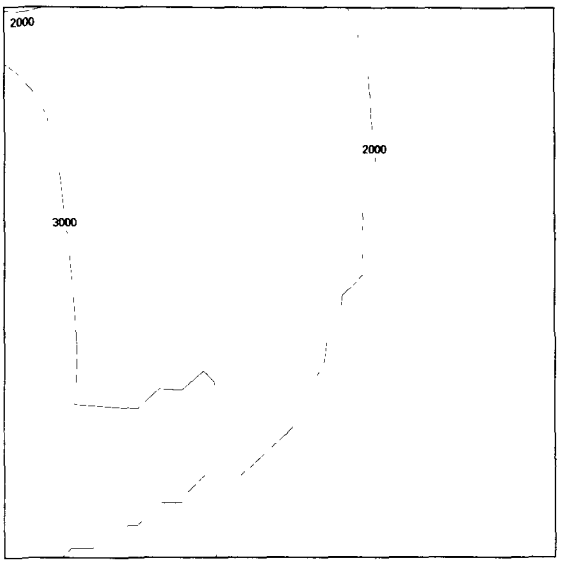
Name	Purpose
FILMAN (subroutine resident in the meso-scale diffusion models)	records and catalogues model output and run log data
MESOFILE	performs file merging and manipulation operation and statistical analysis; prints run data recorded on disk by subroutine FILMAN
MESOPLOT	produces line printer and Calcomp contour plots of concentration, mixing height, and Pasquill-Gifford-Turner stability fields
PLOTVEC	produces Calcomp vector plots of the MESOPAC wind field output and Calcomp and line printer plots of the corresponding isotach fields
BACKUP01	decrements the file pointer to remove the last model run from the run log stored on disk (removes a 'bad' run from the system)
ZERO50	reinitializes the file pointer to remove all previous model runs from the run log stored on disk



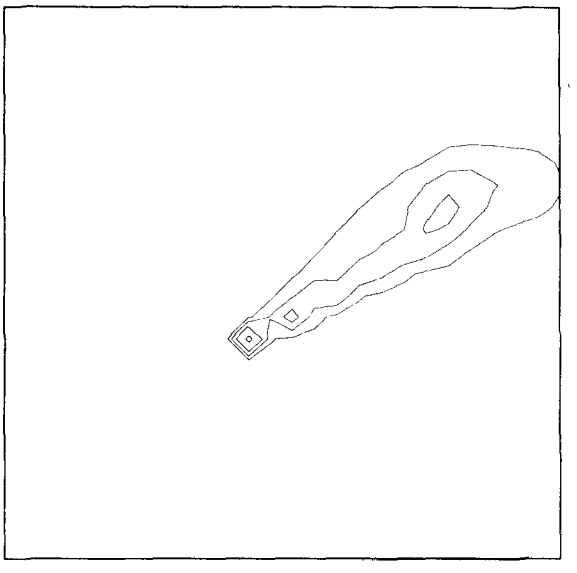
Wind Vectors



Wind Isotachs (m/s)



Mixing Height Field



Concentration Isopleths ($\mu g/m^3$)

Figure 1-3 Examples of MESOFILE Graphical Displays

by the BACKUP01 program (see Section 5). The direct access disk files are currently sized to accommodate up to 25 model runs. After the disk files are full, the model output may be spooled to tape, and the run log can be reinitialized allowing this disk space to be reused for up to 25 additional model runs. The ZERO50 program is used for this purpose (also see Section 5). It should be emphasized that when a run log has been altered, either by BACKUP01 or ZERO50, the concentration output data stored on the direct access disk files corresponding to the run or runs removed from the run log are no longer accessible by the file management system.

1.3 Direct-Access Disk Storage System

The direct-access disk storage system used by the mesoscale modeling package has the logical unit file structure shown in Table 1-2. Direct-access Files 13, 15, 21, 22, 23, and 24 are used by the diffusion models; File 25 is used by the MESOFILE post-processor. The file characteristics (see Table 1-2) are currently fixed within the diffusion models and MESOFILE package by Fortran "Define File" statements in the code and may require specific modification for adaptation to the user's host system.

Library File 13 contains a single-record description for each model run and is sized to accommodate a maximum of 25 independent model runs. A printout of the library file can be produced by MESOFILE's ECHO subroutine (see Section 2.2.1).

NAMELIST File 15 contains a one-record detailed description of the parameters used for each model run. Each record in this file contains a duplicate of the corresponding File 13 record for the run and the NAMELIST parameters used to make the run.

Concentration Files 21 and 22 contain the SO_2 and $SO_4^{=}$ gridded concentration fields for each model output time step. An identifying header record (identical to the format used for File 15) precedes the concentration fields. Files 21 and 22 are sized to accommodate a maximum of 1,800 records each; therefore, for example, the results of 10 independent model simulations, each of 179-hour duration with hourly output, will fit exactly within the 1,800 records allotted. The run number and pointer files (23 and 24), which are transparent to the user, preserve information between runs necessary to maintain proper archival sequencing of run outputs.

TABLE 1-2

LOGICAL UNIT FILE STRUCTURE

Device Logical Unit Number	File Name	Record Structure
13	Library	25 records, 14 words/record
15	NAMELIST	25 records, 800 words/record
21	SO_2 Concentration	1,800 records, 1,610 words/record
22	$SO_4^{=}$ Concentration	1,800 records, 1,610 words/record
23	Run Number	1 record, 2 words
24	Pointer	1 record, 4 words
25	MESOFILE Output	100 records, 1,610 words/record

2. DETAILED MESOFILE DESCRIPTION

2.1 MESOFILE Overview

The MESOFILE program consists of a set of modular subroutines that the user explicitly invokes by card (or card-image) inputs to construct the desired sequence of post-processing operations. The modular nature of MESOFILE provides powerful flexibility. It is possible to perform a wide variety of post-processing operations in a sequence specifically designed to meet the user's particular needs. These features of modularity and flexibility, however, require a greater degree of user interface than a simple "black box" post-processing program. The MESOFILE card inputs required for the most common applications of the program are presented as examples in Section 2.3.

The main program of MESOFILE reads the user's card inputs and calls the appropriate subroutines. There are eight subroutines available to perform a variety of file management and post-processing functions. Other second-level subroutines, transparent to the user, are invoked as appropriate by the user-called subroutines. Table 2-1 contains a description of the basic form of the card inputs to MESOFILE, as well as a list of the subroutines and their functions that are available to the user. Each subroutine requested by the user (with subroutine identifier cards) is called, in order, as it appears in the inputs. There are, however, some restrictions on the order in which subroutines may be called. For example, the pollutant of interest must be specified before the concentration data can be located; therefore, the subroutine identified in Table 2-1 as belonging to calling order Group A must precede those in Group B. Likewise, because data must be located before they can be processed, the subroutines in Group B must be called before the subroutines in Group C. At the end of the run, subroutine DECODE is automatically called as part of the normal termination of MESOFILE. DECODE gives a useful summary of all the subroutines called, the values of the input parameters, the input/output options, and the locations (record numbers) of the MESOFILE disk output (on File 25) for this MESOFILE run.

As indicated in Table 2-1, following a title card and the subroutine identifier card is the NAMELIST card containing the necessary input data. In FORTRAN NAMELIST formatted inputs, the first character of each input record must be a blank, followed by an & and the NAMELIST name. The input data, separated by commas, must appear between the NAMELIST name and an &END. All the NAMELIST names in MESOFILE are either "SAME" (in subroutines called by the user via subroutine identifier cards) or "DIFF (in the line printer plotting subroutines).

The following section contains a detailed description of the functions, the required inputs, and the output options of each MESOFILE subroutine. Annotated sample inputs follow each subroutine description to demonstrate each of the options available to the user. Sample inputs for the most common applications of MESOFILE are presented in Section 2.3.

TABLE 2-1

FORM OF MESOFILE CARD INPUTS AND SUBROUTINE IDENTIFIERS

MESOFILE CARD INPUTS

- TITLE CARD

  Up to 64 characters (columns 1-64) (followed by one set of cards as specified below for each subroutine requested by the user)

- SUBROUTINE IDENTIFIER CARD

  Contains 4-letter subroutine identifier (in Columns 1-4)

- NAMELIST INPUT CARD #1

  Read by the subroutine called

- NAMELIST INPUT CARD #2

  Read by the line printer plotting routine (needed only if line printer plots are produced and contour levels other than the default contour levels are used).

SUBROUTINE IDENTIFIER	CALLING ORDER GROUP	SUBROUTINE FUNCTION (Also see detailed subroutine descriptions - Section 2.2
• ECHO		Access and Prints File Management Data
• DEFN	A	Defines Pollutant, Grid Size, and Routes Output
• FIND	B	Locates First Order Model Output
• SEEK	B	Locates Higher Order MESOFILE Output
• AVRG	C	Averages Arrays
• ADD1	C	Sums Arrays "Vertically"
• ADD2	C	Sums Arrays "Horizontally"
• STAT	C	Calculates Statistics

2.2 MESOFILE Components

2.2.1 Subroutine ECHO

Each time a run is made of MESOPLUME, MESOPUFF, or MESOGRID in which output of concentration data to disk is requested, the file management subroutine FILMAN (contained in each of the models) stores the following information in Library File 13:

- run number,
- date of the run,
- date of the simulated period,
- number of output concentration arrays,
- averaging time,
- save frequency,
- record numbers of the output fields, and
- indicator signifying whether the run terminated normally.

The values of all the NAMELIST input parameters used in the run are stored in NAMELIST File 15. The system keeps a log of every model run made and records the values of all the input parameters used in each run. The only exception is that model runs having no disk output requested do not call the FILMAN subroutine; these runs are not included in the run log and NAMELIST files. The data stored in Files 13 and 15 are retrieved by subroutine ECHO, which will output the entire contents of either file on request. A sample echo of the File 13 library is shown in Figure 2-1. The following parameters are used to describe each model run.

- INUMB - the model run number that is automatically assigned by the direct access disk output subroutine (FILMAN).
- DATFLD - the date (day, month, year) of execution of the model (<u>not</u> the day (or days) simulated).
- MODEL - the mesoscale dispersion model run.
- YR/DAY/HR - the starting year, Julian day, and hour of the simulated period. (Note that the first gridded concentration field is not output until ISAVEF * DTIME hours of simulation time have elapsed, where DTIME is the basic time step of the model in hours and ISAVEF is the concentration array disk output frequency, in terms of DTIME.
- NGRIDS - the total number of concentration arrays output to disk for each pollutant during the model simulation (NGRIDS = NADVTS/ISAVEF, where NADVTS is the length of the simulation in terms of the basic time step, DTIME).
- AVG - the concentration array averaging frequency in hours.
- SAVE - the concentration array disk output frequency, in hours.
- ISAFE - the direct access disk file record number of the duplicate File 15 NAMELIST information.

INUMB	DATFLD	MODEL	YR/DAY/HR	NGRIDS	IAVG	ISAVEF	ISAFE	IBEGIN	ISTOP	ICHECK
1	14 FEB 1979	MESOGRID	78/165/ 0	120	1	1	1	2	121	1
2	14 FEB 1979	MESOGRID	78/165/ 0	120	1	1	122	123	242	1
3	15 FEB 1979	MESOGRID	78/165/ 0	120	1	1	243	244	363	1
4	15 FEB 1979	MESOGRID	78/165/ 0	120	1	1	364	365	484	1
5	16 FEB 1979	MESOPLUM	78/165/ 0	3	24	24	485	486	488	1
6	16 FEB 1979	MESOPUFF	78/165/ 0	3	24	24	489	490	492	1
7	16 FEB 1979	MESOGRID	78/165/ 0	3	24	24	493	494	496	1
8	19 FEB 1979	MESOPUFF	78/165/ 0	120	1	1	497	498	617	1
9	19 FEB 1979	MESOPUFF	78/165/ 0	120	1	1	618	619	738	1
10	8 MAR 1979	MESOPLUM	78/165/ 0	5	24	24	739	740	744	1
11	8 MAR 1979	MESOPLUM	78/165/ 0	5	24	24	745	746	750	1
12	8 MAR 1979	MESOPLUM	78/165/ 0	5	24	24	751	752	756	1
13	8 MAR 1979	MESOPLUM	78/165/ 0	5	24	24	757	758	762	1

Figure 2-1 Sample ECHO Output-File 13 (Library File)

- IBEGIN - the direct access disk file record number of the first of the NGRIDS number of concentration arrays output to File 21 (for SO_2) and File 22 (for $SO_4^=$).
- ISTOP - the direct access disk file record number of the last of the NGRIDS number of concentration arrays output to File 21 (for SO_2) and File 22 (for $SO_4^=$).
- ICHECK - the run termination status indication; ICHECK = 1 indicates the model simulation run terminated normally; ICHECK = 0 indicates it terminated abnormally.

Because the file management system records the location of the output of each run, an abnormally terminated run must be erased from the library file before subsequent model runs to be stored on disk are made (see BACKUP01, Section 5). The disk space occupied by this "bad" output is released for reuse by running the BACKUP01 program.

Figure 2-2 displays the contents of NAMELIST File 15 as output by subroutine ECHO. In this example, thirteen sets of namelist parameters--one set for each model run--are stored in File 15. (The user cannot specify which NAMELIST set is desired; the entire contents of File 15 is printed if NFILE = 15). Table 2-2 summarizes the card input options. The following are sample card inputs.

- Sample Input--Example 1A

```
TITLE CARD
ECHO
 &SAME NFILE=13,&END
```

- Sample Input--Example 1B

```
TITLE CARD
ECHO
 &SAME NFILE=13,&END
ECHO
 &SAME NFILE=15,&END
```

The number of the file to be dumped appears between the NAMELIST name (&SAME) and an &END. The call to subroutine ECHO in Example 1A will produce a listing of the run library; in Example 1B, a listing of both the run library and the NAMELIST parameters for each run will be produced.

2.2.2 Subroutine DEFN

Subroutine DEFN allows the user to specify for a particular MESOFILE run:

- the concentration grid size,
- the pollutant of interest (SO_2 or $SO_4^=$), and
- the starting record of the disk output on the MESOFILE disk file (File 25).

```
INUMB    DATFLD        MODEL      YR/DAY/HR     NGRIDS      IAVG      ISAVEF     ISAFE     IBEGIN     ISTOP     ICHECK
-------------------------------------------------------------------------------------------------------------------------
  8   19 FEB 1979     MESOPUFF    78/165/ 0       120         1          1         497        498       617         1

*************************************************************************************************************************

&MODEL
LPLUME=F,LPUFF=T,LGRID=F,LPAC=F
&END
&CONTR
DTIME=  1.00000000    ,MTFREN=          1,IAVG=          1,NADVTS=        120
&END
&GRID
IELMET=          26,JELMET=          26,DELTMT=  40000.0000    ,IASTAR=          1,IASTOP=         26,JASTAR=          1,JASTOP=
        26,ISASTR=          1,JSASTR=          1,ISASTP=         26,JSASTP=         26,MESHDN=          1
&END
&SIGMA
AY=  .329999983    ,  .220000029    ,  .170000017    ,  .120000005    ,  .860000253E-01,  .570000000E-01,BY= -.100000024    ,
 -.100000024    , -.100000024    , -.100000024    , -.100000024    , -.100000024    ,AZ=  .479999930E-03,  .630000234E-01,
  .100000024    ,  .329999983    ,  .410000026    ,  .319999993    ,BZ=  1.10000038    ,  .899999738E-01, -.899999738E-01,
 -.420000017    , -.529999971    , -.579999983
&END
&METD
METSRT=    7816500,METCOD=       1003,LSENSE=F
&END
&PUFF1
NPUFTS=  125714704,NSAMAD=          4,LVARSA=F,MAXSAM=        100
&END
&PUFF2
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&END
&REMOV
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  .0             ,  .0
&END
&OUTPT
LECHO=T,LPRINT=T,IPRINF=         24,LEXACT=F,LSAVE=T,ISAVEF=          1
&END
&SOURC
NSOURC=          1,STAKHT=  236.000000    ,  .0             ,  .0             ,  .0             ,  .0             ,  .0             ,
  .0             ,  .0             ,  .0             ,  .0             ,XXSTAK=  8.80000019    ,  .0             ,  .0             ,
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  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,  1.00000000    ,
```

Figure 2-2 Sample ECHO Output-Partial Contents of File 15 (NAMELIST File)

```
1.00000000 , 1.00000000 , 1.00000000 , 1.00000000 , 1.00000000 , 1.00000000 , 1.00000000 ,
```

TABLE 2-2

CARD INPUTS TO SUBROUTINE ECHO

SUBROUTINE ECHO

NAMELIST TITLE - SAME

Parameter	Type	Definition	Default
NFILE	INTEGER	Logical unit number of the file to be printed (NFILE = 13 for library lines; NFILE = 15 the NAMELIST parameters).	13

The concentration array size, IMAX * JMAX, (see Table 2-3), must, of course, be the same as the array size specified in the mesoscale model run used to generate the concentration data. The default values for the concentration array size in MESOFILE are the same as the default values in the MESOPLUME, MESOPUFF, and MESOGRID models, i.e., 26 x 26. Most of the model runs generate both SO_2 and $SO_4^=$ concentration data; MESOFILE, however, operates on only one pollutant at a time, assumed to be SO_2 unless the user specifies $SO_4^=$.

All MESOFILE disk output (concentration fields, difference fields, etc.) is written to the MESOFILE output File 25. Each output field requires one record of disk space on File 25. The user must specify the record where the disk output is to start for a particular MESOFILE run. The first output array is written at this record; the second output array is written at the next record, etc. Each time an array is written to disk, the disk file pointer is incremented by one. A particular MESOFILE run, for example, may write n concentration arrays on Records 1 through n; the user may wish to save this output, and, on a subsequent MESOFILE run, the output may be directed to begin at record n+1.

The starting record number for MESOFILE disk output is not supplied with a default value; this prevents accidental overwriting of previously stored data. The user must specify this parameter if the MESOFILE run is to generate any disk output. The concentration array size and pollutant are used in block data; subroutine DEFN must therefore be called only if:

- any disk output is generated in the MESOFILE run,
- the concentration array size is different from the default 26 x 26, or
- the pollutant of interest is not SO_2.

Table 2-3 contains a description of the card inputs to subroutine DEFN. The following are sample card inputs.

- Sample Input--Example 2A

```
TITLE CARD
DEFN
 &SAME IMAX=40,JMAX=40,IOUT=1,&END
```

- Sample Input--Example 2B

```
TITLE CARD
DEFN
 &SAME IPOL=2,IOUT=20,&END
```

The call to subroutine DEFN in Example 2A sets the concentration array size to 40 x 40. The disk file output pointer, IOUT, is given a value of 1. Any disk output that may be generated later in the MESOFILE run, therefore, will start on Record 1 of File 25. In Example 2B, $SO_4^=$ is specified as the pollutant of interest. The disk output of this MESOFILE run will begin on Record 20. The concentration array size is assumed (by default) to be 26 x 26.

TABLE 2-3

CARD INPUTS TO SUBROUTINE DEFN

SUBROUTINE DEFN

NAMELIST TITLE - SAME

Parameter	Type	Definition	Default
IPOL	INTEGER	Pollutant (for SO_2, IPOL = 1; for $SO_4^=$, IPOL = 2).	1
IMAX	INTEGER	Number of elements of the concentration array in the X direction ($\leq$40).	26
JMAX	INTEGER	Number of elements of the concentration array in the Y direction ($\leq$40).	26
IOUT	INTEGER	Record number of File 25 at which MESOFILE disk output is to start.	-

2.2.3 Subroutine FIND

FILMAN, the file management subroutine incorporated in each of the mesoscale air quality simulation models, dynamically allocates available disk records (on previously created disk Files 21 and 22) to store SO_2 and $SO_4^{=}$ concentration fields, and records the location of these fields in the Library File (File 13). These cataloging and archiving operations are automatically controlled by FILMAN as long as sufficient disk space was originally allocated when disk Files 21 and 22 were created. The concentration fields for any previous MESOPLUME, MESOPUFF, or MESOGRID run are located (and therefore can be accessed by other MESOFILE subroutines) with a call to subroutine FIND.

Subroutine FIND performs the following sequence of operations:

- reads user inputs (see Table 2-4) to identify the model output to be located:
  - model run number;
  - starting hour, day, and year of data; and
  - number of concentration fields;
- determines disk file record numbers of requested concentration data by reading Library File (File 13);
- checks data of first concentration array to verify that the proper arrays have been located; and
- defines the requested set of concentration arrays as runstream number n, where n = 1 (first call of FIND/SEEK), n = 2 (second call of FIND/SEEK), etc.

Each call to subroutine FIND defines a runstream (i.e., one or a group of concentration fields) that can be accessed by other MESOFILE subroutines. A runstream number is a sequential internal reference number associated with a group of concentration arrays located by subroutine FIND or SEEK and is used to identify these arrays in other MESOFILE subroutines. FIND is one of two runstream defining subroutines (subroutine SEEK is the other). The first set of concentration fields located by FIND (or SEEK) is referred to as Runstream 1, the second set of concentration fields defines Runstream 2, etc; concentration array runstream numbers should not be confused with model run numbers INUMB.

Because subroutine FIND is used to locate the output of any previously run model, it must be called before an attempt is made to process these data subsequently with any of MESOFILE's data processing subroutines. Before any MESOFILE data processing subroutines of MESOFILE are called, subroutines FIND and SEEK must be used to locate all the model output. The following are sample card inputs.

- Sample Input--Example 3

```
TITLE CARD
FIND
 &SAME INUMB=4,IYEAR=78,IDAY=166,IHOUR=1,IGRIDS=24,&END
FIND
 &SAME INUMB=4,IYEAR=78,IDAY=165,IHOUR=1,IGRIDS=120,&END
FIND
 &SAME INUMB=8,IYEAR=78,IDAY=165,IHOUR=1,IGRIDS=120,&END
```

TABLE 2-4

CARD INPUTS TO SUBROUTINE FIND

SUBROUTINE FIND

NAMELIST TITLE - SAME

Parameter	Type	Definition	Default
INUMB	INTEGER	Run number of the air quality model run.	-
IHOUR	INTEGER	Ending hour of the first concentration array of interest.	-
IDAY	INTEGER	Day number of the first concentration array of interest.	-
IYEAR	INTEGER	Year of the first concentration array of interest.	-
IGRIDS	INTEGER	Number of concentration arrays.	-

In Example 3, the run number identified as INUMB = 4 is a MESOGRID run starting at Hour 0, Day 165, Year 78 (refer back to Figure 2-1). Because each of the models output their concentration arrays at the conclusion of a time step, the first concentration array recorded is for Hour 1 on Day 165. The first sample input above specifies Runstream 1 as consisting of 24 hourly concentration arrays, starting at Hour 1, Day 166 and ending at Hour 0, Day 167. The second call to subroutine FIND defines Runstream 2 as the set of concentration arrays output from Run Number 4, starting at Hour 1, Day 165, through Hour 0, Day 170, (i.e., starting time plus 120 hours). Runstream Number 3 is specified as the output from the MESOPUFF model (Run Number 8) for the same 120-hour time period.

2.2.4 Subroutine SEEK

Each set of data to be accessed by the data processing subroutines of MESOFILE must be located and assigned a runstream number. The SO_2 and $SO_4^=$ concentration data, output directly by the models to disk Files 21 and 22, are referred to as "first" order data fields and are located by calls to subroutine FIND. MESOFILE, however, has the ability to process first order data and output the resultant fields (e.g., averaged concentration fields, summed concentration fields, or several types of concentration difference fields), to disk File 25 for storage and further processing. These derived fields, which have undergone at least one level of MESOFILE processing, are referred to as "higher" order data fields. The user wishing to reference higher order data must supply the location (File 25 record number) of the data to MESOFILE by a call to subroutine SEEK.

Subroutine SEEK performs the following operations:

- reads user inputs to identify the MESOFILE output of interest:
  - NSTART and
  - NSTOP and
- defines the requested set of data fields as runstream number n, where n = 1 (first call of FIND/SEEK), n = 2 (second call of FIND/SEEK), etc.

The card input requirements of subroutine SEEK are described in Table 2-5. The following are sample card inputs.

- Sample Input--Example 4

```
TITLE CARD
FIND
 &SAME INUMB=4,IYEAR=78,IDAY=166,IHOUR=1,IGRIDS=24,&END
SEEK
 &SAME NSTART=12,NSTOP=12,&END
SEEK
 &SAME NSTART=10,NSTOP=23,&END
```

As in the previous example, Runstream Number 1 is defined as a set of 24 hourly, first order concentration arrays. Runstreams 2

TABLE 2-5

CARD INPUTS TO SUBROUTINE SEEK

SUBROUTINE SEEK

NAMELIST TITLE - SAME

Parameter	Type	Definition	Default
NSTART	INTEGER	Starting disk record number on File 25 of the output of interest.	-
NSTOP	INTEGER	Ending disk record number on File 25 of the output of interest.	-

and 3, however, are composed of higher order data fields. The second runstream consists of a single data field (record 12 on file 25), whereas Runstream 3 is defined to be the 14 data arrays contained in records 10 through 23.

2.2.5 Subroutine AVRG

Subroutine AVRG calculates time averages of first order or higher order concentration data. This subroutine performs the following operations:

- initializes NAMELIST SAME parameters to default values,
- reads user inputs,
- calculates number of arrays in the runstream specified by the user and determines a repetition factor, IREPF,
- for each array in the runstream, reads array and if requested, prints the input array and sums arrays,
- after AVETM arrays have been read and summed, divides by AVETM to obtain average, and performs linear scaling calculation, and
- if requested, writes averaged array to disk (File 25), writes averaged array on line printer, and plots averaged array.

The user has the option of printing, plotting, or writing the averaged arrays to disk File 25. The user specifies the runstream number of the data set to be averaged and the averaging frequency (in terms of arrays), so that the appropriate block averages will be computed. A background concentration factor or a concentration multiplicative scaling factor may be included in the calculations as well (see Table 2-6). Each averaged array may be adjusted by the form:

$$\bar{C}_{ADJ} = a * \bar{C} + b.$$

The location of all MESOFILE disk output (File 25) is controlled by the IOUT variable of subroutine DEFN. The first output grid is written on record IOUT of file 25, the next grid is written on record IOUT + 1, etc. The user specifies the location where the disk output is to start; the disk file pointer is incremented each time a grid is written to disk. The following are sample card inputs.

- Sample Input--Example 5

```
TITLE CARD
DEFN
 &SAME IOUT=50,&END
FIND
 &SAME INUMB=4,IYEAR=78,IDAY=167,IHOUR=0,IGRIDS=12,&END
SEEK
 &SAME NSTART=1,NSTOP=30,&END
AVRG
 &SAME IRUN=1,AVETM=3,DISK=1,PLOT=1,NEWV=1,APE=1,&END
```

TABLE 2-6

CARD INPUTS TO SUBROUTINE AVRG

SUBROUTINE AVRG

NAMELIST TITLE - SAME

Parameter	Type	Definition	Default
IRUN	INTEGER	Runstream number.	-
AVETM	INTEGER	Averaging time (in terms of number of arrays).	-
PRINT	INTEGER	Line printer output control variable. PRINT = 1--averaged concentration arrays are printed; PRINT = 0--averaged concentration arrays are not printed.	1
DISK	INTEGER	Disk output control variable. DISK = 1--average concentration arrays are written on disk; DISK = 0--averaged concentration arrays are not written on disk.	0
PLOT	INTEGER	Line printer plotting control variable. PLOT = 1--plots are produced; PLOT = 0--plots are not produced.	0
NEWV	INTEGER	Plotter contour values control variable--also see Table 2-7. NEWV = 1--user input contour values (if NEWV = 1, user must insert a DIFF NAMELIST card with the apprropiate contour information); NEWV = 0--default contour values.	0
APE	INTEGER	Controls echo of input (unaveraged) fields. APE = 1--input fields are printed; APE = 0--input fields are not printed.	0
a,b	REAL	Adjustment factors for the averaged concentration field. a--multiplicative factor, b--additive factor, of the form, $\overline{C}_{adj} = a * \overline{C} + b.$	a = 1. b = 0.

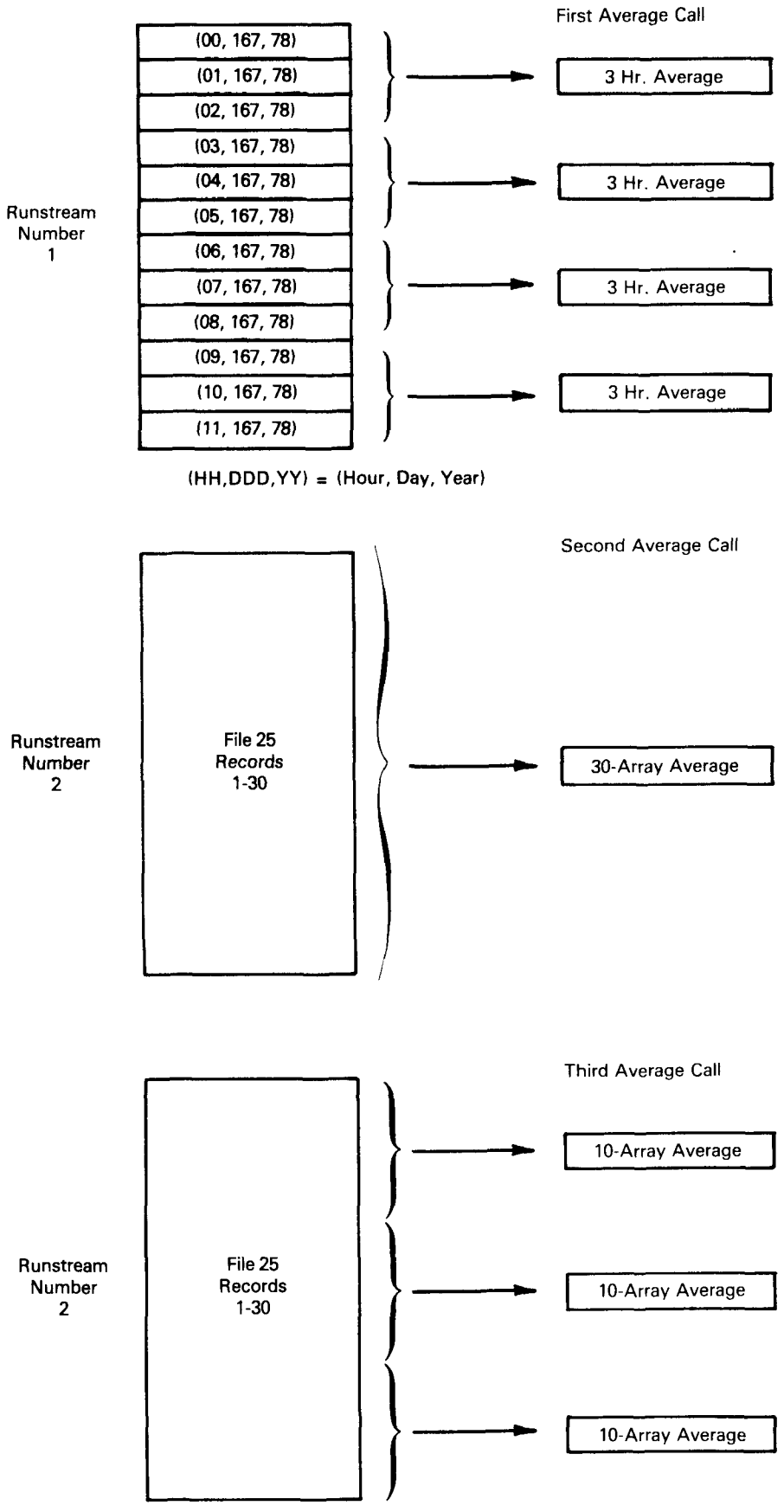
```
 &DIFF N=5,THR=-1.E-10,0.1E-6,1.E-6,10.E-6,100.E-6,20*0.0,&END
AVRG
 &SAME IRUN=2,AVETM=30,PRINT=0,DISK=1,PLOT=1,&END
AVRG
 &SAME IRUN=2,AVETM=10,PRINT=0,DISK=1,PLOT=1,&END
```

The call to subroutine DEFN sets the disk output pointer IOUT to 50. The averaged concentration arrays written to disk, therefore, will occupy records 50 through 50 + n on File 25, where n is the number of arrays output to disk. Subroutine FIND is called to define a 12-array runstream consisting of hourly concentration fields, as illustrated schematically in Figure 2-3. Runstream Number 2 is defined as the higher order data on records 1-30 of File 25. The first call to subroutine AVRG averages the data defined by Runstream 1 into four 3-hour averaged arrays (again see Figure 2-3). The maximum output available to the user is requested. The hourly concentration input fields and the averaged fields are printed. The averaged fields are also plotted (with user input contour levels) and written to disk (on records 50-53). The second call to subroutine AVRG results in one 30-array average from the data in Runstream 2. Only two output options are invoked: line printer plots and disk output. The disk output is routed to Record 54 because the previous AVRG call put arrays into Records 50 to 53. The contour levels of the line printer plot will be the same as in the previous AVRG call; when new contour levels are defined (as in the first AVRG call), the plotting routine will continue to use them until other contour levels are redefined in a DIFF NAMELIST (see Table 2-7). All the parameters in NAMELIST SAME that have default values are reset to their default values each time the subroutine is called. The third AVRG call uses Runstream Number 2 data to calculate three 10-array averages. The output options are the same as with the second AVRG call, and the disk output is stored on Records 55 to 57 of File 25.

2.2.6 Subroutine ADD1

Subroutines ADD1 is used to sum all the arrays in a runstream to yield a simple summed output array. That is,

$$(C_{sum})_{ij} = \sum_{k=1}^{N} C_{ij}^{k}$$



7901346

Figure 2-3 Schematic Illustration of the Averaging Process

TABLE 2-7

CARD INPUTS TO THE LINE PRINTER PLOTTING ROUTINE

NAMELIST TITLE - DIFF

(included only for line printer plots with user input contour levels)

Parameter	Type	Definition	Default
N	INTEGER	Number of contour levels (must be 25)	9
THR(25)	REAL ARRAY	Contour values*	$-1.\times 10^{-10}$ 0.1×10^{-6} 0.5×10^{-6} 1.0×10^{-6} 2.0×10^{-6} 5.0×10^{-6} 10.0×10^{-6} 25.0×10^{-6} 50.0×10^{-6}

*The first element of THR should be less than the minimum value of the field being plotted.

where $(C_{sum})_{ij}$ is the (i,j) element of the summed array, and (C^k_{ij}) is the (i,j) element of the kth array in the consisting of N arrays (k = 1...N). The output options include an echo of the input arrays, line printer gridded output, line printer plots, and disk output and are the same as those in subroutine AVRG. The adjustment factors a and b for the summed concentration field are also available (see Table 2-8). Each call to subroutine ADD1 will initialize the output array to zero before adding to it sequentially the concentration arrays of the specified runstream, unless the INIT variable is set to zero in the ADD1 input NAMELIST. With INIT = 0, a cumulative sum can be calculated with successive ADD1 calls.

The following are sample card inputs.

- Sample Input--Example 6

```
TITLE CARD
DEFN
 &SAME IOUT=50,&END
SEEK
 &SAME NSTART=1,NSTOP=6,&END
SEEK
 &SAME NSTART=20,NSTOP=22,&END
ADD1
 &SAME IRUN=1,DISK=1,&END
ADD1
 &SAME IRUN=2,INIT=0,DISK=1,&END
```

The call to subroutine DEFN requests that the disk output of this MESOFILE run begin at record 50 on disk File 25. Two runstreams are defined: a six array runstream (Number 1) and a three array runstream (Number 2). The first call to ADD1 sums the data in Runstream Number 1 (Records 1 to 6) and prints the result on the line printer and record 50. The second ADD1 call, because INIT = 0, adds the array in Runstream Number 2 to the summed array calculated in the first ADD1 call, and the result is also written on disk (Record 51) and on the line printer.

2.2.7 Subroutine ADD2

Subroutine ADD2 calculates "horizontal" sums of the arrays in two runstreams. That is,

$$D^k_{ij} = A^k_{ij} + B^k_{ij}$$

where the summation extends over all k = 1...N arrays in runstreams A and B, and D is the resultant runstream. Two runstream numbers must therefore be supplied to subroutine ADD2 as input, and both runstreams must contain the same number of concentration arrays. The other NAMELIST inputs are the same as the subroutine ADD1 inputs (see

TABLE 2-8

CARD INPUTS TO SUBROUTINE ADD1

Description of Inputs to Subroutine ADD1

NAMELIST TITLE - SAME

Parameter	Type	Definition	Default
IRUN	INTEGER	Runstream number.	-
INIT	INTEGER	Determines whether the summing array is initialized to zero; INIT = 1--array initialized to zero; INIT = 0--array is not initialized.	1
PRINT	INTEGER	Line printer output control variable. PRINT = 1--summed array is printed; PRINT = 0--summed array is not printed.	1
DISK	INTEGER	Disk output control variable. DISK = 1--summed array is written on disk; DISK = 0--summed array is not written on disk.	0
PLOT	INTEGER	Line printer plotting control variable. PLOT = 1--plots are produced; PLOT = 0--plots are not produced.	0
NEWV	INTEGER	Plotter contour values control variable (also see Table 2-7). NEWV = 1--user input contour values (if NEWV = 1, user must insert a DIFF NAMELIST card with the appropriate contour information); NEWV = 0--default contour values.	0
APE	INTEGER	Controls echo of input fields. APE = 1--input fields are printed; APE = 0--input fields are not printed.	0
a, b	REAL	Adjustment factors for the summed concentration field, a--multiplicative factor, b--additive factor, of the form, $C_{adj} = a * C + b$.	a = 1. b = 0.

Table 2-9 for a complete description of the ADD2 input parameters). The following are sample card inputs.

- Sample Input--Example 7

```
TITLE CARD
DEFN
 &SAME IOUT=50,&END
FIND
 &SAME INUMB=4,IYEAR=78,IDAY=165,IHOUR=1,IGRIDS=6,&END
FIND
 &SAME INUMB=3,IYEAR=78,IDAY=165,IHOUR=1,IGRIDS=6,&END
ADD2
 &SAME IRUN1=1,IRUN2=2,DISK=1,PLOT=1,&END
```

The call to subroutine DEFN requests that disk output start on record 50 of disk File 25. Six output files of two MESOGRID runs (see Figure 2-1) are defined as Runstreams 1 and 2 with the calls to subroutine FIND. The arrays of each runstream are added together, printed, written to disk, and plotted with the default contour levels. The "horizontal" summary process with the two 6-array runstreams results in an output runstream of 6 arrays.

2.2.8 Subroutine STAT

Subroutine STAT is designed to produce quantitative as well as qualitative measures of the point-by-point and bulk differences between two concentration fields--a 'base' field and a 'test' or 'perturbed' field. The base concentration fields are reference fields resulting from a particular model run specified by the user. The test concentration fields can be any other model output generated with some test parameter of the model varied; for example, the emission inventory, deposition velocity, decay rate, time step, or even the mesoscale model used, may be varied and the results defined as the test concentration fields.

When the user has defined a base case and test case concentration field (or set of fields), line printer plots or gridded tables of the following fields may be produced:

- the base field, identified as BF,
- the test field, identified as TF,
- the difference field, identified as DF = $C_B - C_T$,
- the fractional difference field identified as FDF = $\frac{C_B - C_T}{C_B}$, and
- the weighted difference field identified as WDF = $\frac{C_B - C_T}{\overline{C}_B}$

where C_B is the base field concentration at a particular grid point, C_T is the test field concentration at that point, and C_B is defined below.

TABLE 2-9

CARD INPUTS TO SUBROUTINE ADD2

SUBROUTINE ADD2

NAMELIST TITLE - SAME

Parameter	Type	Definition	Default
IRUN1	INTEGER	Runstream Number 1.	-
IRUN2	INTEGER	Runstream Number 2.	-
PRINT	INTEGER	Line printer output control variable. PRINT = 1 - summed arrays are printed; PRINT = 0 - summed arrays are not printed.	1
DISK	INTEGER	Disk output control variable. DISK = 1--summed arrays are written on disk; DISK = 0 - summed arrays are not written on disk.	0
PLOT	INTEGER	Line printer plotting control variable. PLOT = 1--plots are produced; PLOT = 0--plots are not produced.	0
NEWV	INTEGER	Plotter contour values control variable. NEWV = 1--user input contour values (if NEWV = 1, user must insert a DIFF NAMELIST card with the appropriate contour information--see Table 2-7); NEWV = 0--default contour values.	0
APE	INTEGER	Controls echo of input fields. APE = 1--input fields are printed; APE = 0--input fields are not printed.	0
a, b	REAL	Adjustment factors for the summed concentration fields, a--multiplicative factor b--additive factor of the form, $C_{adj} = a * C + b$.	a = 1. b = 0.

The fractional difference field FDF can be calculated only for grid points with nonzero base field concentrations, but because the FDF is most meaningful in comparing base case and test case plumes which overlap exactly or nearly exactly, the FDF is calculated only for those points in the intersection of the two plumes (that is $C_B = 0$ and $C_T = 0$)

The WDF is the difference field weighted by the average base plume concentration (C_B).

$$\overline{C}_B = \frac{\sum_{n=1}^{N} (C_B)_n}{N}$$

where N includes only those points in the base field plume (defined as the set of points in the base field with nonzero concentrations).

In addition to line printer plots of the DF, FDF, and WDF, subroutine STAT has the ability to write these fields to the MESOFILE direct access disk output file (File 25), so that Calcomp plots may be generated for these fields.

Variation of the test parameter can substantially change the nature of the concentration distribution in the base and test plumes; these differences in turn determine which of the difference field representations is appropriate for a particular analysis. The FDF field is useful in determining the relative spatial location of the base and test plumes and differences in the concentration distribution, and should be used when the effect of the input parameter does not change the gross spatial distribution of the plume. The WDF allows the differences in concentration to be weighted by a constant factor.

Subroutine STAT also generates a set of quantitative (statistical) measures of the differences in the base case and test case concentration fields. Whereas the graphical output is optional, the statistical output is always produced. Figure 2-4 is a sample of the statistical output. The statistics calculated and the subsets of the grid over which the calculations are performed are contained in Table 2-10 and Figure 2-5. Clearly, the most meaningful statistic for a given base case-test case comparison depends heavily on the nature of the test parameter varied and must be determined by the user.

Figure 2-6 is a flowchart of subroutine STAT. The input variables are defined in Table 2-11. It is assumed that the statistics for multiarray runstreams are to be calculated on an array-by-array basis; the variable BYONE, therefore, has a default value of 1. It is possible, however, to logically concatenate successive arrays in a particular runstream by specifying BYONE = 0. For example, consider base case and test case runstreams consisting of three 24-hour averages. If BYONE = 1, array-by-array statistics (i.e., 3 sets of statistics, one set for each 24-hour averaged array) will be produced; BYONE = 0 will result in only one set of statistics over the entire 72-hour period.

It is possible to write DF, FDF, or WDF to the MESOFILE direct access disk output file (File 25), although only one of these fields can be written on a particular call to STAT.

```
THE FOLLOWING RECORDS WERE USED AS THE BASE FIELD:
FIRST RECORD =     46      LAST RECORD =     46

THE FOLLOWING RECORDS WERE USED AS THE PERTURBED FIELD:
FIRST RECORD =     51      LAST RECORD =     51


STATISTICS FOR THE SET OF ALL GRID POINTS:


AVERAGE BASE FIELD VALUE (AVEB) =  0.15684E-06
AVERAGE PERTURBED FIELD VALUE (AVEP) =  0.16300E-06
AVERAGE DEVIATION (AD) = -0.61647E-08
AVERAGE ABSOLUTE DEVIATION (AAD) =  0.52787E-07
MAXIMUM LOCAL DEVIATION (XMLD) =  0.91118E-05
DIFFERENCE OF MAXIMA (DLM) B-P = -0.21656E-05
FRACTIONAL DIFFERENCE OF MAXIMA (FDLM) B-P = -0.26802E+00
MAXIMUM BASE FIELD VALUE (XMBF) =  0.80800E-05
MAXIMUM PERTURBED FIELD VALUE (XMPF) =  0.10246E-04


STATISTICS FOR THE SET OF POINTS WITHIN THE UNION OF THE TWO PLUMES:

AVERAGE DEVIATION (AD1) = -0.11512E-07
AVERAGE ABSOLUTE DEVIATION (AAD1) =  0.98574E-07
CORRELATION COEFFICIENT (RBA) =  0.79


STATISTICS FOR THE SET OF POINTS WITHIN THE INTERSECTION OF THE TWO PLUMES:

AVERAGE DEVIATION (AD0) = -0.54887E-08
AVERAGE ABSOLUTE DEVIATION (AAD0) =  0.97060E-07
AVERAGE FRACTIONAL DEVIATION (AFD0) = -0.33695E+00
AVERAGE ABSOLUTE FRACTIONAL DEVIATION (AAFD0) =  0.61030E+00
MAXIMUM ABSOLUTE FRACTIONAL DEVIATION (XMLFD0) =  0.25661E+02


PLUME CHARACTERISTICS


TOTAL NUMBER OF GRID POINTS =      676
NUMBER OF GRID POINTS CONTAINED IN THE INTERSECTION OF THE BASE AND PERTURBED PLUMES =      344
NUMBER OF NON-ZERO CONCENTRATIONS (BASE OR PERTURBED) =      362
NUMBER OF GRID POINTS IN THE BASE PLUME =      350
NUMBER OF GRID POINTS IN THE PERTURBED PLUME =      356
AVERAGE BASE PLUME VALUE (AVEB0) =  0.30292E-06
AVERAGE PERTURBED PLUME VALUE (AVEP0) =  0.30952E-06
FRACTIONAL DEVIATION OF THE MEANS (FDM) = -0.21788E-01
```

Figure 2-4 Sample of Statistical Output

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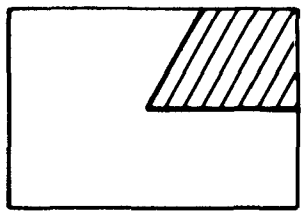
TABLE 2-10

STATISTICAL MEASURES CALCULATED BY SUBROUTINE STAT

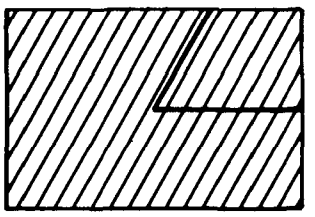
	Variable Name	Grid Points Included
1. Mean base plume concentration, $\overline{C}_B$	AVEBO	BP
2. Mean test (perturbed) plume concentration, C_T	AVEPO	TP
3. Mean base field concentration	AVEB	BF
4. Mean test field concentration	AVEP	TF
5. Average deviation, C_B-C_T	AD AD1 AD0	BFTF BTU BTI
6. Average absolute deviation, C_B-C_T	AAD AAD1 AAD0	BFTF BTU BTI
7. Maximum local deviation, MAX $\{C_B-C_T\}$	XMLD	BFTF
8. Maximum base field value, MAX $\{C_B\}$	XMBF	BF
9. Maximum test field value, MAX $\{C_T\}$	XMPF	TF
10. Difference of maxima, MAX $\{C_B\}$ - MAX $\{C_T\}$	DLM	DFTF
11. Fractional difference of maxima, $\frac{\text{MAX}\{C_B\} - \text{MAX}\{C_T\}}{\text{MAX } C_B}$	FDLM	BFTF
12. Correlation coefficient, $\frac{\overline{C_B C_T} - \overline{C}_B\,\overline{C}_T}{\left[\overline{C_B^2} - (\overline{C}_B)^2\right]\left[\overline{C_T^2} - (\overline{C}_T)^2\right]}$	RBA	BTU

TABLE 2-10 (Continued)

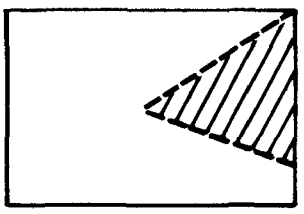
13. Average fractional deviation, $\overline{\left\{\frac{C_B - C_T}{C_B}\right\}}$	AFDO	BTI
14. Average absolute fractional deviation $\overline{\frac{\lvert C_B - C_T \rvert}{C_B}}$	AAFDO	BTI
15. Maximum absolute fractional deviation, $\mathrm{MAX}\left\{\frac{\lvert C_B - C_T \rvert}{C_B}\right\}$	XMLFDO	BTI
16. Fractional deviation of the means $\frac{\overline{C}_B - \overline{C}_T}{\overline{C}_B}$	FDM	$\overline{X}_B$-BP $\overline{X}_T$ - TP



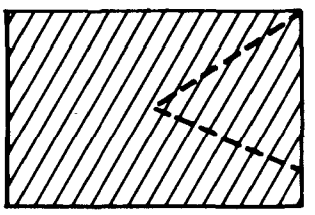
(BP) BASE PLUME ONLY



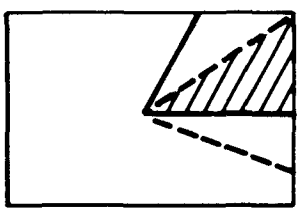
(BF) ENTIRE BASE FIELD GRID



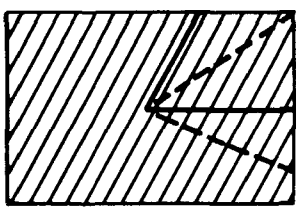
(TP) TEST PLUME ONLY



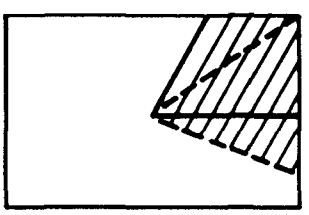
(TF) ENTIRE TEST FIELD GRID



(BTI) BASE - TEST PLUME INTERSECTION



(BFTF) BASE FIELD - TEST FIELD UNION



(BTU) BASE - TEST PLUME UNION

Figure 2-5 Grid Subsets Used in the Statistical Calculations

7904297

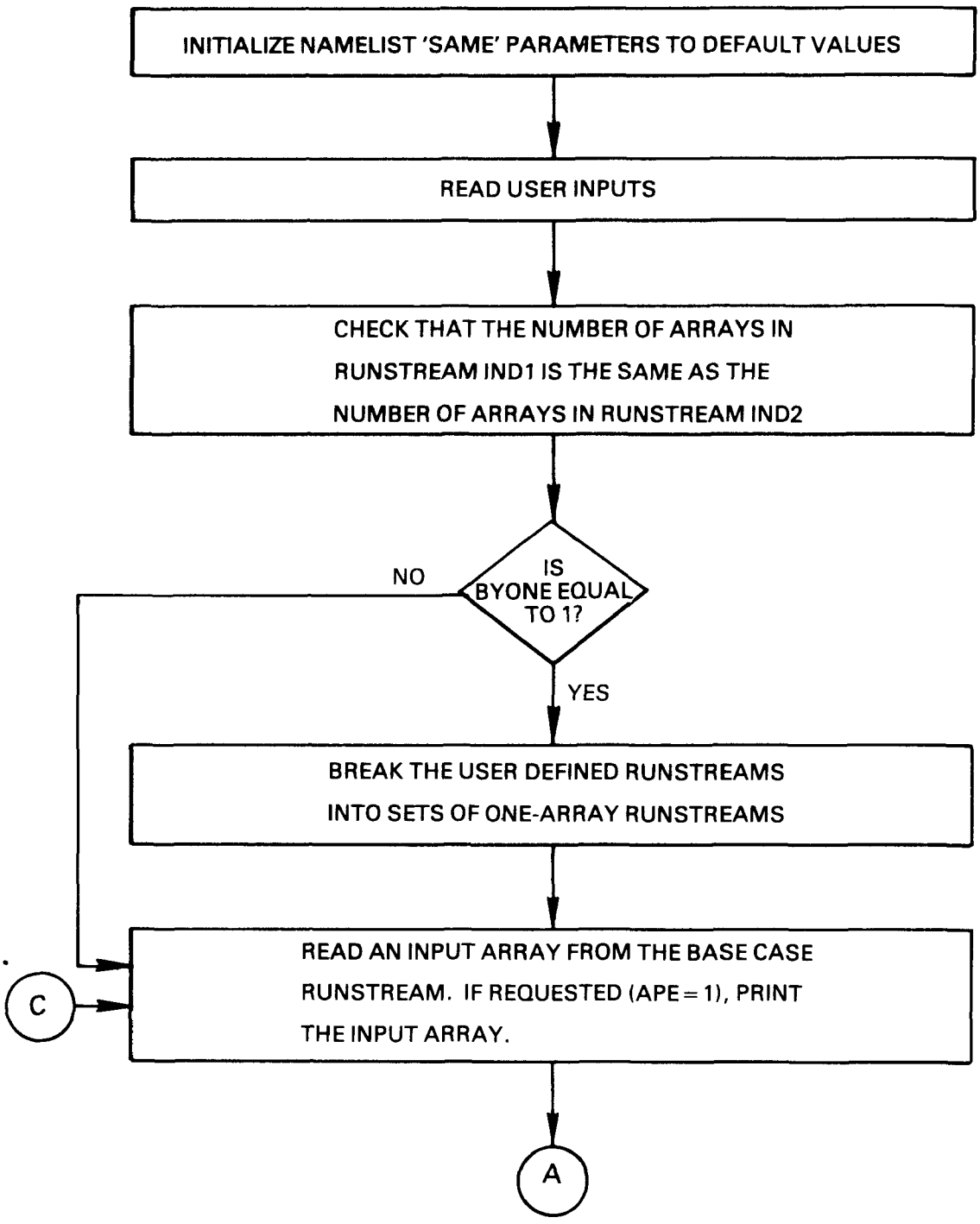


Figure 2-6 Flow Chart of Subroutine STAT

7904296

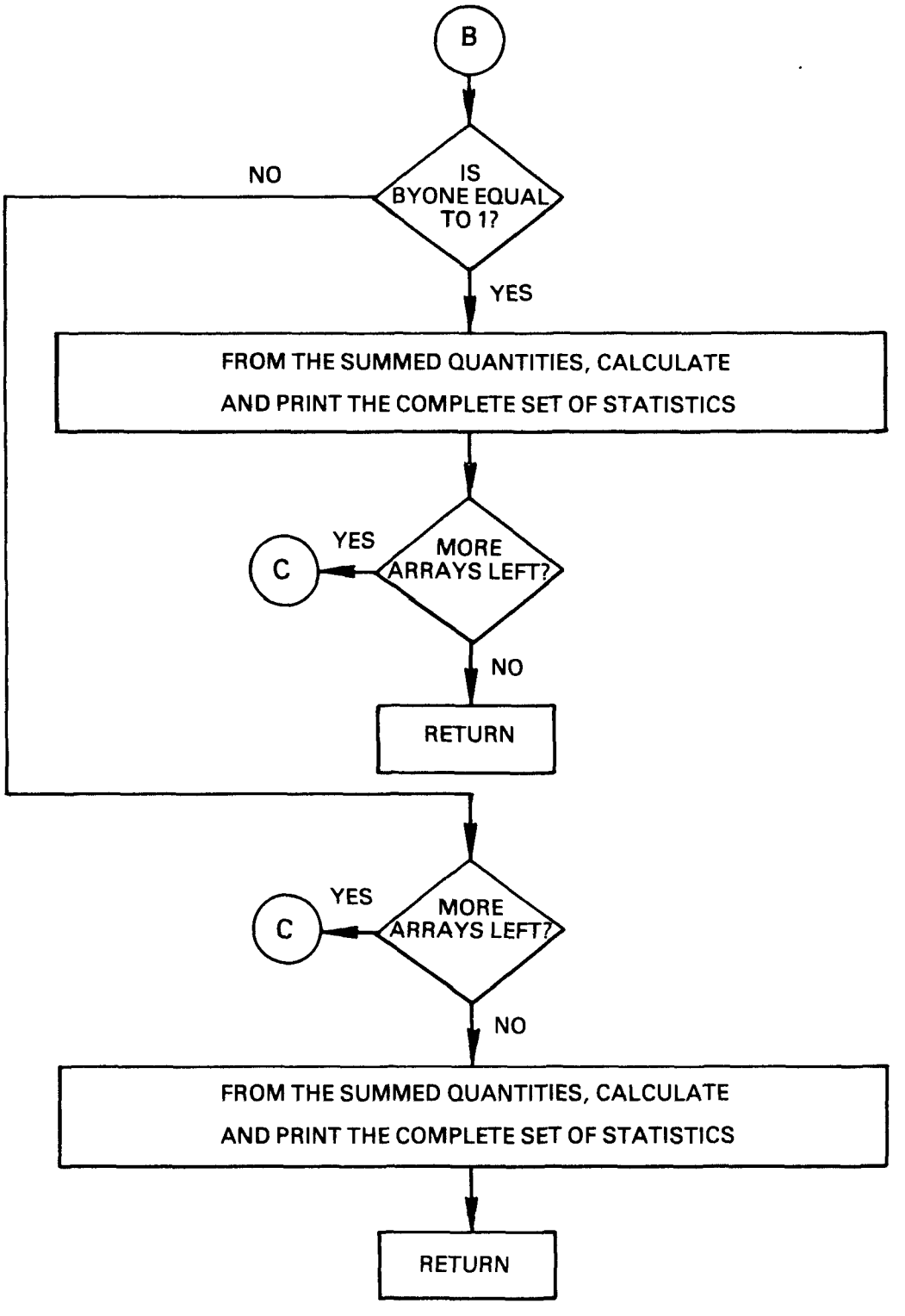


Figure 2-6 Continued

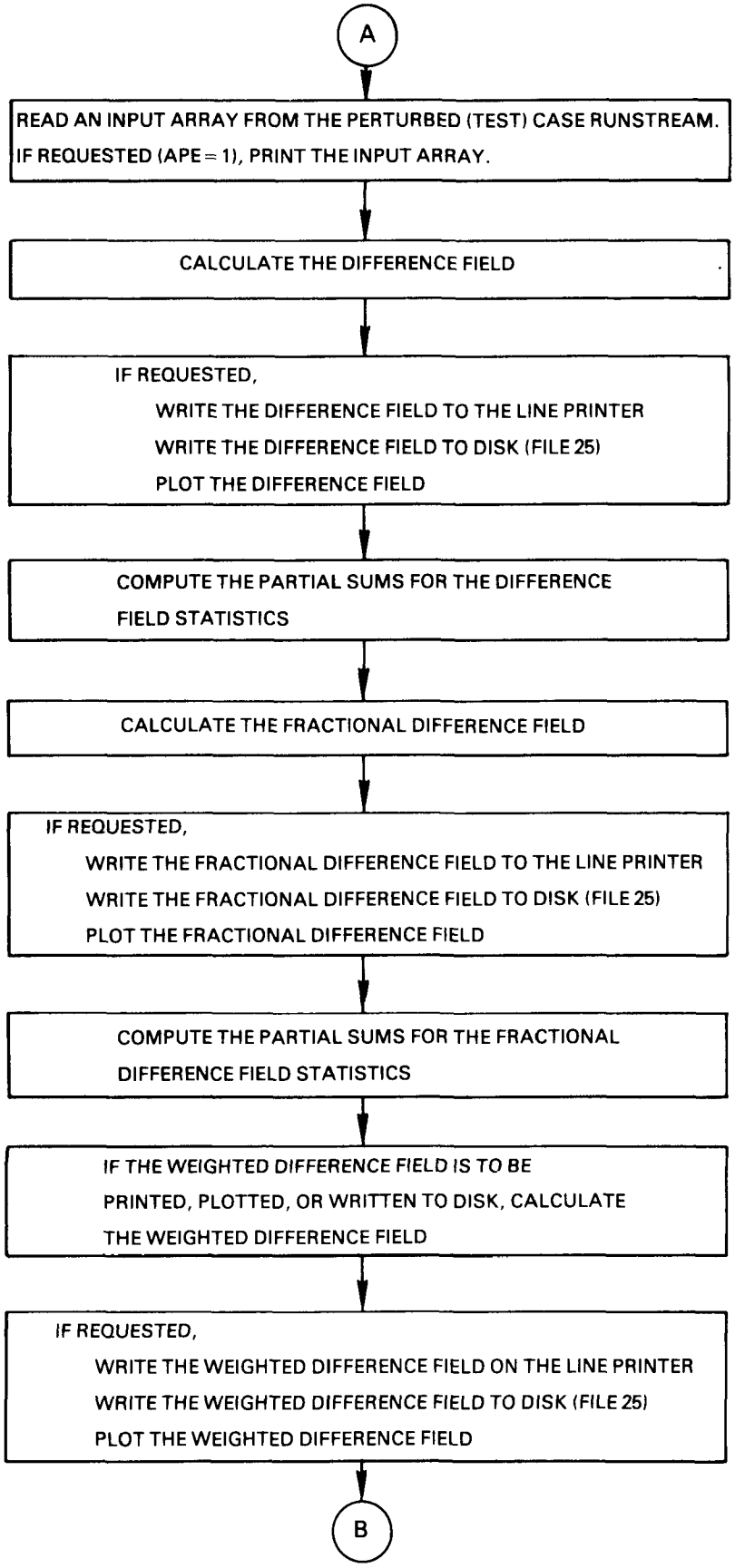


Figure 2-6 Continued

TABLE 2-11

CARD INPUTS TO SUBROUTINE STAT

SUBROUTINE STAT

NAMELIST TITLE - SAME

Parameter	Type	Definition	Default
IND1	INTEGER	Base case runstream number.	-
IND2	INTEGER	Perturbed (test) case runstream number.	-
BYONE	INTEGER	Determines whether multi-array runstreams are to be treated as one concatenated data set (producing one set of statistics) or as a group of one-array runstreams (producing a set of statistics for each array pair) BYONE = 1--array by-array statistics; BYONE = 0--collective statistics.	1
PRINTD	INTEGER	Line printer output control variable for the difference fields. PRINTD = 1--difference fields are printed; PRINTD = 0--difference fields are not printed.	0
DISKD	INTEGER	Disk output control variable for the output fields. DISKD = 1--difference fields are written on disk; DISKD = 0--difference fields are not written on disk.	0
PLOTD	INTEGER	Line printer plotting control variable for the difference fields. PLOTD = 1--plots are produced; PLOTD = 0--plots are not produced.	0
NEWVD	INTEGER	Plotter contour values control variable (also see Table 2-7). NEWVD = 1--user input contour values (if NEWV = 1, user must insert a DIFF NAMELIST card with the appropriate contour information) NEWVD = 0--default input contour values.	0
PRINTF	INTEGER	Same as PRINTD, except for the fractional difference fields.	0

TABLE 2-11 (Continued)

DISKF	INTEGER	Same as DISKD, except for the fractional difference fields.	0
PLOTF	INTEGER	Same as PLOTD, except for the fractional difference fields.	0
NEWVF	INTEGER	Same as NEWVD, except for the fractional difference fields.	0
PRINTW	INTEGER	Same as PRINTD, except for the weighted difference fields.	0
DISKW	INTEGER	Same as DISKD, except for the weighted difference fields.	0
PLOTW	INTEGER	Same as PLOTD, except for the weighted difference fields.	0
NEWVW	INTEGER	Same as NEWVD, except for the weighted difference fields.	0
APE	INTEGER	Controls echo of input fields. APE = 1--input fields are printed; APE = 0--input fields are not printed.	0

The following are sample card inputs.

- Sample Input--Example 8

```
TITLE CARD
DEFN
 &SAME IOUT=50,&END
SEEK
 &SAME NSTART=9,NSTOP=12,&END
SEEK
 &SAME NSTART=19,NSTOP=22,&END
SEEK
 &SAME NSTART=28,NSTOP=32,&END
STAT
 &SAME IND1=1,IND2=2,DISKD=1,PLOTD=1,NEWVD=1,&END
 &DIFF THR=-100.E-6,-5.E-6,-1.E-6,-.5E-6,-1.E-15,0,1.E-15,
 E.5-6,1.E-6,5.E-6,15*0.0,N=10,&END
STAT
 &SAME IND1=1,IND2=3,DISKD=1,PLOTD=1,&END
```

In this example, the call to subroutine DEFN requests that the disk output of this MESOFILE run start at Record 50 of disk File 25. Three runstreams are defined by calls to subroutines SEEK, each consisting of four arrays. The first call to STAT results in four sets of statistics; each array of Runstream 1 is compared to the corresponding array of Runstream 2. The fields associated with the runstream identified with IND1 are defined to be the base case fields; IND2 defines the test case fields. The difference fields are plotted with the user-specified contour levels in the DIFF NAMELIST, and they are written to disk File 25 (on Records 50 to 53). The second call to STAT will produce statistics comparing the arrays in Runstream 1 (base case) to the arrays in Runstream 3 (test case). The difference fields are plotted with the same contour levels as in the previous STAT call; when new contour levels are defined (in the DIFF NAMELIST), they become the "default" contour levels for subsequent calls to the plotting routine. The difference fields are written to disk File 25 on Records 54 to 57.

2.3 Sample Card Inputs for Some Useful MESOFILE Applications

- Print Library File 13

```
TITLE CARD
ECHO
 &SAME NFILE=13,&END
```

- Print Library File 13 and NAMELIST File 15

```
TITLE CARD
ECHO
 &SAME NFILE=13,&END
ECHO
 &SAME NFILE=15,&END
```

- Calculate 24-hour SO_2 averages from hourly output of two model runs; write results on disk

```
TITLE CARD
DEFN
 &SAME IOUT=1,&END
FIND
 &SAME INUMB=1,IYEAR=78,IDAY=165,IHOUR=1,IGRIDS=120,&END
FIND
 &SAME INUMB=2,IYEAR=78,IDAY=165,IHOUR=1,IGRIDS=120,&END
AVRG
 &SAME IRUN=1,AVETM=24,DISK=1,&END
AVRG
 &SAME IRUN=2,AVETM=24,DISK=1,&END
```

- Perform statistical analysis of the 24-hour average concentrations calculated for two model runs in example above

```
TITLE CARD
SEEK
 &SAME NSTART=1,NSTOP=5,&END
SEEK
 &SAME NSTART=6,NSTOP=10,&END
STAT
 &SAME IND1=1,IND2=2,&END
```

- Calculate and plot "horizontal" sums of the hourly SO_2 output of two model runs (useful for runs made with different subsets of the entire source inventory; the resulting horizontal sum is a superposition of the concentration fields reflecting the effects of the sources modeled in two runs)

```
TITLE CARD
DEFN
 &SAME IOUT=11,&END
FIND
 &SAME INUMB=3,IYEAR=78,IDAY=165,IHOUR=1,IGRIDS=24,&END
FIND
 &SAME INUMB=4,IYEAR=78,IDAY=165,IHOUR=1,IGRIDS=24,&END
ADD2
 &SAME IRUN1=1,IRUN2=2,PRINT=0,PLOT=1,&END
```

- Transfer a set of 3 hourly concentration fields from the SO_2 concentration File (21) to the MESOFILE output File (25) (useful if the hourly concentration fields are to be plotted with the Calcomp plotting routine MESOPLOT (see Section 3).

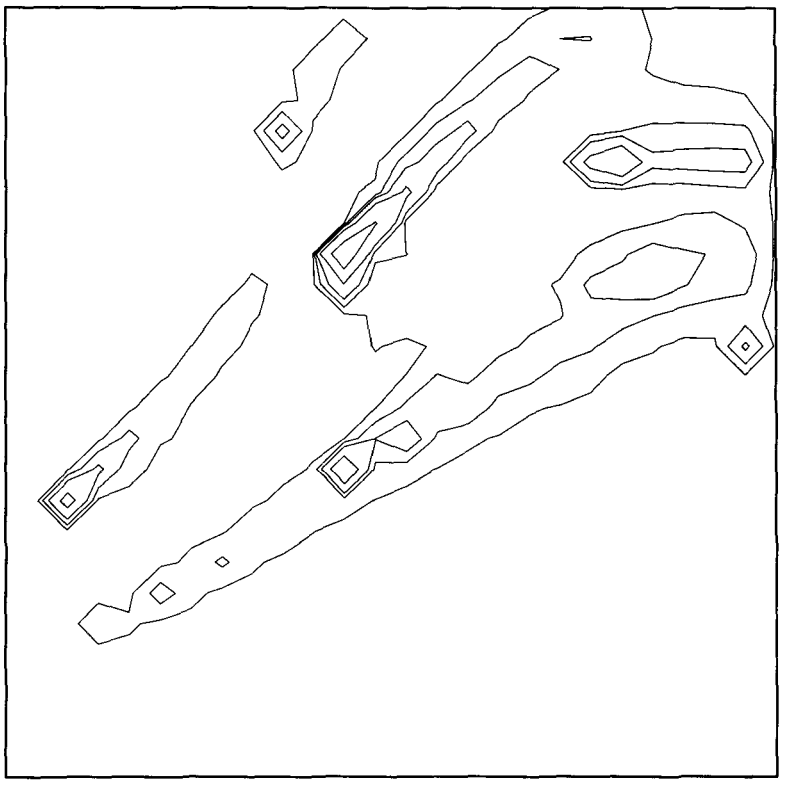
```
TITLE CARD
DEFN
 &SAME IOUT=35,&END
FIND
 &SAME INUMB=4,IYEAR=78,IDAY=165,IHOUR=1,IGRIDS=1,&END
FIND
 &SAME INUMB=4,IYEAR=78,IDAY=165,IHOUR=2,IGRIDS=1,&END
FIND
```

```
 &SAME INUMB=4,IYEAR=78,IDAY=165,IHOUR=3,IGRIDS=1,&END
ADD1
 &SAME IRUN=1,DISK=1,&END
ADD1
 &SAME IRUN=2,DISK=1,&END
ADD1
 &SAME IRUN=3,DISK=1,&END
```

3. MESOPLOT DESCRIPTION

MESOPLOT is a contour plotting package designed to produce simultaneous Calcomp and line printer contour plots of any two-dimensional scalar field array, for example, ambient concentrations, PGT stability class, or mixing heights. Both line printer and Calcomp plots are made available because the contour lines in the Calcomp plots are not labeled; the line printer plots enable the user to easily identify the contour lines. (Modifications of the Calcomp contour plotting routine may be necessary to make MESOPLOT compatible with the user's plotting facilities.) Samples of the Calcomp and line printer plot are shown in Figure 3-1.

Any scalar field which is stored on the direct-access disk File 25 (MESOFILE output file) can be contour plotted by specifying IVAR = 1 and the first and last disk file record number containing the appropriate fields (see Table 3-1). The PGT stability and mixing height fields, output from the MESOPAC meteorological preprocessor, may be plotted by specifying IVAR = 2 or 3, respectively. It is assumed that the stability and mixing height fields are stored on a data set corresponding to Logical Unit 2. For convenience, different default contour values are defined for each value of IVAR (see Table 3-2). The hour, Julian day, and year of the first stability or mixing height field to be plotted, the number of fields to be plotted, as well as the time interval (DELTAT) over which subsequent fields are to be plotted must be specified via the DATE NAMELIST (see Table 3-3) if IVAR = 2 or 3.



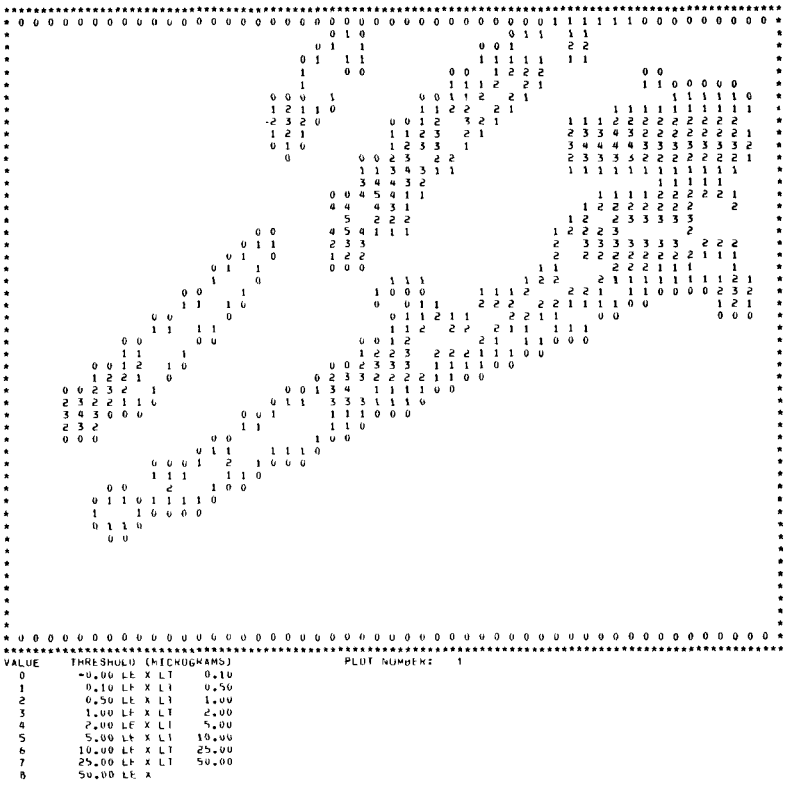
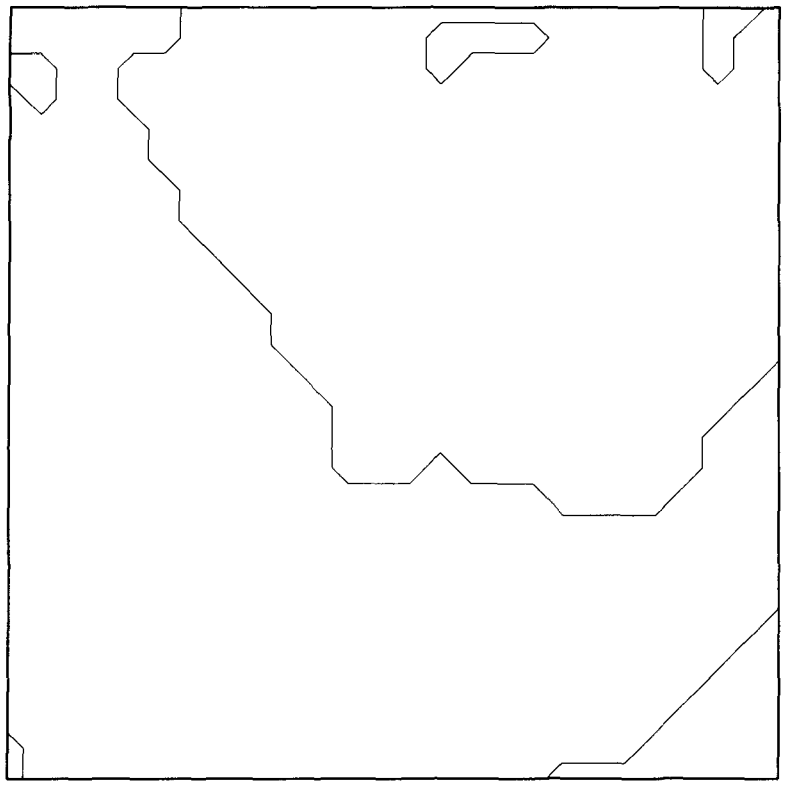


Figure 3-1(a) Sample MESOPLOT Contour Plots - Concentration Fields



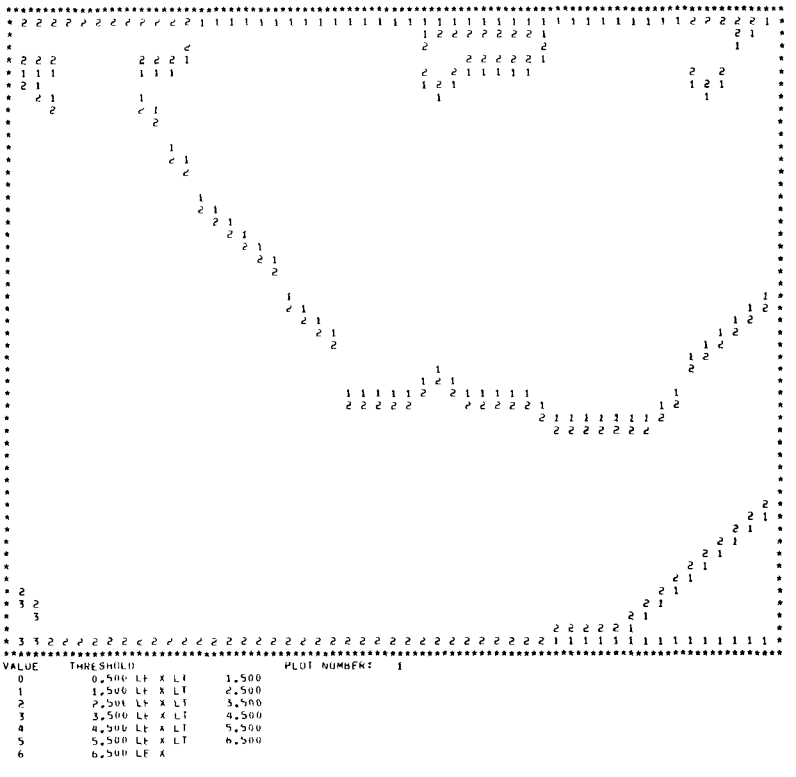
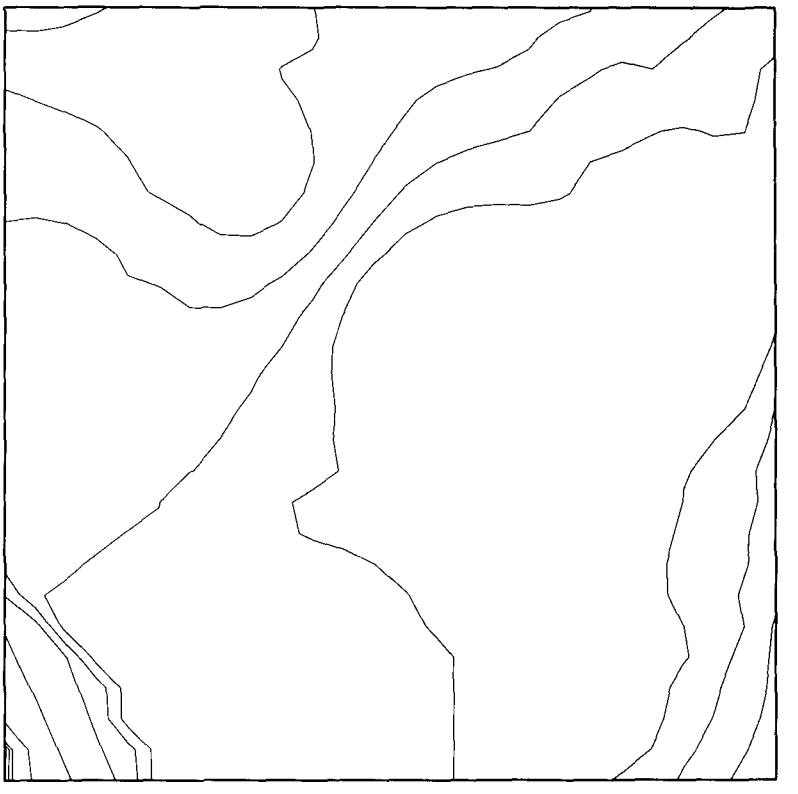


Figure 3-1(b) Sample MESOPLOT Contour Plots - Stability Class Fields



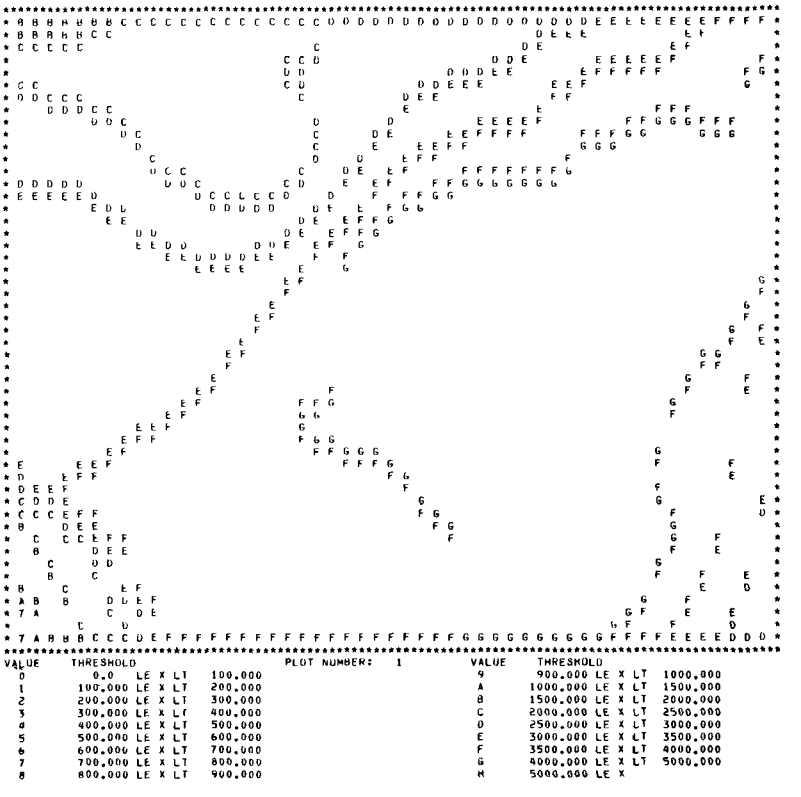


Figure 3-1(c) Sample MESOPLOT Contour Plots - Mixing Height Fields

TABLE 3-1

CARD INPUTS TO MESOPLOT--'SAME' NAMELIST

NAMELIST TITLE - SAME

Parameters	Type	Definition	Default
IVAR	INTEGER	Variable plotted (for concentration or other scalar fields from File 25, IVAR = 1; for P-T stability fields, IVAR = 2; for mixing height fields, IVAR = 3.)	1
IMAX	INTEGER	Number of elements in the X direction of the grid to be plotted (_ 40).	26
JMAX	INTEGER	Number of elements in the Y direction of the grid to be plotted (_ 40).	26
CALCOMP	LOGICAL	If .TRUE., Calcomp plots and line printer plots are produced; if .FALSE., only line printer plots are produced.	.FALSE.
NSTART	INTEGER	Disk record number on File 25 of the first field to be plotted (used if IVAR = 1).	-
NSTOP	INTEGER	Disk record number on File 25 of the last field to be plotted (used if IVAR =1).	-
NPLOTS	INTEGER	Number of data fields to be plotted (used if IVAR = 2,3).	
METCOD	INTEGER	4-digit identifying meteorological data code number.	1003
DELTAT	REAL	Field will plotted every DELTAT time steps (used if IVAR = 2,3).	1.
NEWV	INTEGER	Plotter contour values control variable. NEWV = 1--user input contour values (If NEWV = 1, the user must insert a DIFF NAMELIST card with the appropriate contour information--see Table 3-2); NEWV = 0--default contour values.	0

TABLE 3-2

CARD INPUTS TO MESOPLOT--'DIFF' NAMELIST

NAMELIST TITLE - DIFF

(included only if NEWV = 1)

Parameter	Type	Definition	Default
N	INTEGER	Number of contour levels (must be _ 20)	see below
THR (20)	REAL ARRAY	Contour values	see below

The default values of N and THR depend on the value of IVAR (see Table 3-1). The defaults for each value of IVAR are:

IVAR	Field	N	THR*
1	Concentrations or other scalar from File 25	9	$-1.\times10^{-10}$, 0.1×10^{-6}, 0.5×10^{-6}, $1. \times 10^{-5}$, $2. \times 10^{-6}$, $5. \times 10^{-6}$, $25. \times 10^{-6}$, $50. \times 10^{-6}$
2	P-G-T stability	7	0.5, 1.5, 2.5, 3.5, 4.5, 5.5, 6.5
3	Mixing height	18	0., 100., 200., 300., 400., 500., 600., 700., 800., 900., 1,000., 1,500., 2,000., 2,500., 3,000., 3,500., 4,000., 5,000.

*The first element of THR should be less than the minimum value of the field being plotted.

TABLE 3-3

CARD INPUTS TO MESOPLOT--'DATE' NAMELIST

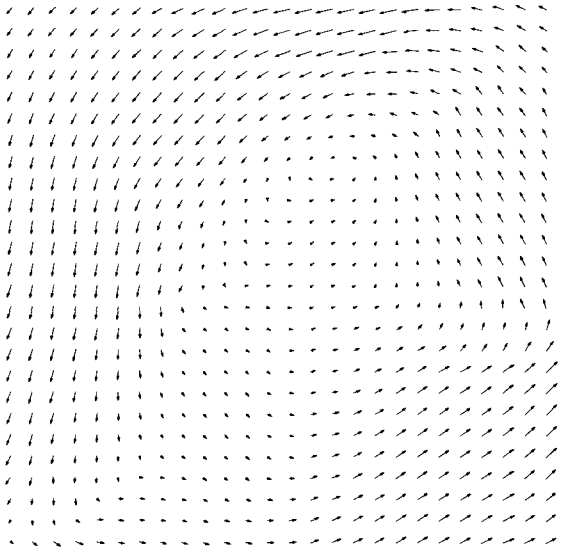
NAMELIST TITLE - DATE

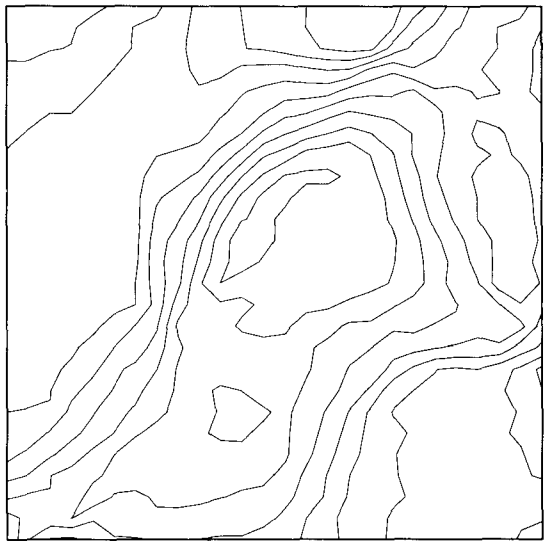
(included only if IVAR = 2 or 3)

Parameter	Type	Definition	Default
JHOUR	INTEGER	Hour of first field to be plotted.	-
JDAY	INTEGER	Julian day of first field to be plotted.	-
JYEAR	INTEGER	Year of first field to be plotted (last two digits only.	-

4. PLOTVEC DESCRIPTION

PLOTVEC is a vector and isotach contour plotting routine for use with the wind field data generated by the MESOPAC program. PLOTVEC may require modification to make the Calcomp vector and contour plotting routines compatible with the user's plotting facilities. PLOTVEC reads u and v gridded velocity components from a data set corresponding to Logical Unit 2. These velocity components are converted to fields of wind direction (measured positive counterclockwise from the x-axis) and wind speed in meters per second (m/s). Calcomp vector plots and isotach contour plots are then generated (see Figure 4-1). A line printer isotach plot is produced for each Calcomp plot, thus allowing the contour levels of the Calcomp plot to be easily identified. All the vectors are scaled such that a length of one grid spacing corresponds to a wind speed of 25 m/s. The direction of the wind is indicated by the vector direction. A description of PLOTVEC's input parameters is contained in Tables 4-1 and 4-2.





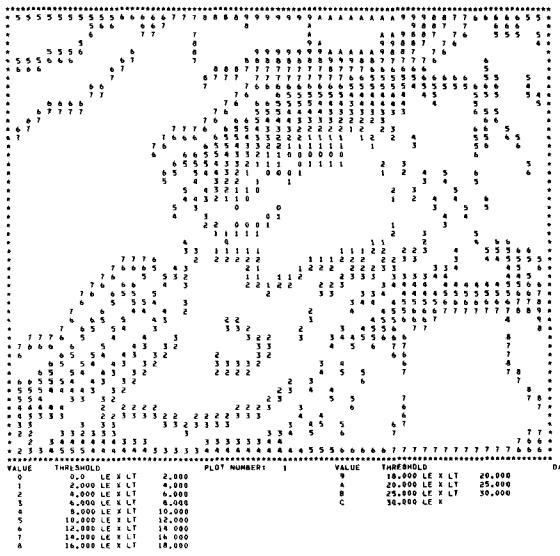


Figure 4-1 Sample PLOTVEC Vector and Contour Plots

TABLE 4-1

CARD INPUTS TO PLOTVEC--'SAME' NAMELIST

NAMELIST TITLE - SAME

Parameter	Title	Definition	Default
IMAX	INTEGER	Number of elements in the X direction of the grid to be plotted (40).	26
JMAX	INTEGER	Number of elements in the Y direction of the grid to be plotted (40).	26
METCOD	INTEGER	4-digit identifing meteorological data code number.	1003
JHOUR	INTEGER	Hour of the first field to be plotted.	-
JDAY	INTEGER	Julian day of the first field to be plotted.	-
JYEAR	INTEGER	Year of the first field to be plotted (last two digits only).	-
NPLOTS	INTEGER	Number of data fields to be plotted.	1
DELTAT	REAL	Fields will be plotted every DELTAT time steps.	12.
NEWV	INTEGER	Plotter contour value control variable. NEWV = 1--user input contour values (if NEWV = 1, the user must insert a DIFF NAMELIST card with the appropriate contour information--see Table 4-2); NEWV = 0--DEFAULT contour values.	0

TABLE 4-2

CARD INPUTS TO PLOTVEC--'DIFF' NAMELIST

NAMELIST TITLE - DIFF

(included only if NEWV = 1)

Parameter	Title	Definition	Default
N	INTEGER	Number of contour levels (must be 20).	13
THR(20)	REAL ARRAY	Contour values.	0., 2., 4., 6., 8., 10., 12., 14., 16., 18., 20., 25., 30.

5. BACKUP01 AND ZERO50 DESCRIPTION

Each mesoscale diffusion model run that outputs SO_2 and $SO_4^=$ concentration data to disk is automatically recorded in a run log (Library File 13) by the file management system. The disk file record numbers of the disk output data and all the related run log information is stored on disk, and can be accessed by the user by subroutine ECHO of the MESOFILE program (see Section 2.2.1). Figure 2-1 is a sample of this file management run log.

As indicated in Section 2.2.1, a normal run termination indicator ICHECK is one of the variables displayed with the run log information. The file management system determines the proper locations (disk file record numbers) of the output concentration fields before these arrays are actually written on the disk file. A check is made at the end of the run to verify that all the concentration fields have been written to disk; the normal termination indicator is then assigned a value of 1. If, however, the run terminated abnormally, ICHECK retains a value of 0. An abnormally terminated run* must be erased from the run log (library file) before more model runs are made. BACKUP01 accomplishes this by decrementing the appropriate run pointer in the direct-access disk storage system files. An attempt to run one of the models when a previous run terminated abnormally will result in the following message:

ERROR: INCORRECT VALUE IN FILE 13 OF PARAMETER = ICHECK
(Previous run normal completion flag)

BACKUP01 requires no user card inputs. It should be emphasized that BACKUP01 will remove from the run log the record of the last run made, making the concentration data produced by the run inaccessible.

When the record of a run has been removed from the run log by BACKUP01, the disk space occupied by the output of this run is again available for subsequent model runs. Another application of BACKUP01, therefore, is to remove model runs where output is no longer needed from the run log, thus releasing their disk space for future runs.

---

*Runs that terminate abnormally caused by errors in the user's card input data may not require the use of BACKUP01. The mesoscale diffusion models call the file management subroutine, FILMAN, after all the user's card inputs have been read. It is FILMAN that enters a record of the run in the run log; if FILMAN has not been called, it is not necessary to run BACKUP01. It is suggested, therefore, that the user verify an ICHECK = 0 with an ECHO of the run log before running BACKUP01.

Although multiple runs of BACKUP01 is allowed, it may be desirable to remove in one run the record of all the model runs made on a particular set of disk files. ZERO50 is a program that erases the entire run log, thereby yielding a 'clean slate' on which further model runs may be made.

The most useful application of ZERO50 is in a situation in which the disk files have been filled with data from model runs. It is possible to spool to tape the entire set of disk files; ZERO50 can then be run, clearing the run log and releasing the direct-access disk space for subsequent model runs. The data from the first set of model runs may be accessed by the file management system by transferring the set of files on tape back to direct-access disk, and then using MESOFILE for post-processing operations. As with BACKUP01, ZERO50 requires no user card inputs. Care should be taken to ensure that the data stored on the disk files are transferred to tape <u>before</u> running ZERO50, because once the run log is erased, the disk file data are inaccessible by the MESOFILE program.

REFERENCES

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16. ABSTRACT

The MESOscale FILE management and analysis package (MESOFILE) is a highly flexible post-processing system designed especially for interface with the MESOPLUME, MESOPUFF, and MESOGRID regional-scale air quality models, and the MESOPAC meteorology package. The MESOFILE package is composed of five distinct program modules consisting of file management, file merging, file manipulation, statistical analysis, and graphical display.

The file management system automatically catalogues input parameter values and output file locations of all regional-scale model simulations; any set of regional-scale model output can, therefore, be easily accessed for postanalysis. Postprocessing capabilities include multiple file averaging, multiple file addition, point-by-point and bulk statistical comparison of two files, contour plots of concentration and most meteorological fields, and vector plots of wind fields.

A complete set of users instructions and a full FORTRAN listing are provided.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
*Air Pollution		13B
*Algorithms		12A
*Atmospheric Models		04A

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