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GUIDE FOR USING THE EMPIRICAL KINETICS MODELING APPROACH INTERFACE (EKMAI)

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U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Technical Support Division
Source Receptor Analysis Branch
Research Triangle Park, NC 27711

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Notice

This report has been reviewed and approved for publication by the Office Of Air Quality Planning and Standards, U.S. Environmental Protection Agency. Mention herein of trade names or commercial products does not constitute endorsement or recommendation for use.

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The Empirical Kinetics Modeling Approach Interface (EKMAI) software was developed under contract by Computer Sciences Corporation.

CONTENTS

1. INTRODUCTION

The Empirical Kinetics Modeling Approach (EKMA)[1-4] has been used since the early 1980s to estimate emission reductions that are needed to achieve the ozone National Ambient Air Quality Standard (NAAQS). The 1990 Clean Air Act Amendments generally require that moderate and more severely polluted ozone nonattainment areas demonstrate that their proposed control strategies will be sufficient to attain the NAAQS for ozone by 1996. For moderate nonattainment areas contained solely in one state, the Environmental Protection Agency (EPA) has designated EKMA as one acceptable modeling technique which may be used to make this demonstration.[5] As a result, several moderate intrastate areas across the country plan to include EKMA modeling as part of their State Implementation Plan (SIP).

One of the problems with using EKMA in the past has been difficulty in specifying current boundary conditions and projecting these to future years. Boundary conditions in EKMA are defined as concentrations of ozone precursors aloft. Recently, the Regional Oxidant Model (ROM) has become operational. ROM is a photochemical grid model which is used to simulate regional scale control strategies applied to current or future years. Results of ROM simulations are being made available to State agencies,[6] where they may be used to specify present and projected boundary conditions for EKMA. The purpose of the EKMA Interface (EKMAI) software described in this guide is to provide a means by which stored ROM results may be accessed and made suitable for use with EKMA. In particular, the EKMAI program provides aloft concentrations of ozone (O_3), carbon monoxide (CO), nitrogen oxides (NOx), and nonmethane organic compounds (NMOC) for input to the EKMA model.

This guide provides the user with the information necessary

to run the EKMAI program. Section 2 gives an overview of the workings of EKMAI, and Section 3 walks the user through an example. In order for the user to understand how to access and process the ROM data for use with EKMAI, it is essential to refer to Chapter 4 of the Gridded Model Information Support System (GMISS) User's Guide Volume III[7] concurrently with this guide.

2. OVERVIEW

EKMAI uses gridded hourly species concentration data from previously run ROM simulations. The ROM data are currently stored in a database management system called the Gridded Model Information Support System (GMISS), and may be retrieved using the GMISS Model Concentration Data Retrieval Subsystem.

Accessing the Model Concentration Data Retrieval Subsystem to extract the desired data is the first step in using EKMAI. Directions for using the Retrieval Subsystem are provided in the GMISS User's Guide Volume III: Model Concentration Data Retrieval Subsystem (EPS-450/4-91-032)[7]. The Retrieval Subsystem should be used in conjunction with this EKMAI guide. It may be followed as written except for a few changes necessary for the specific case of retrieving data for EKMAI, which are explained in this guide.

The retrieval process begins with the extraction of data for a subdomain of the chosen ROM domain. The subdomain recommended for running EKMAI is an square array of 9 ROM grid cells (3 columns by 3 rows) or 25 ROM grid cells (5 columns by 5 rows) which covers the urban area to be modeled. The array is defined so that the center of the urban area is located somewhere in the center grid cell of the array. A ROM grid cell is 1/4° longitude by 1/6° latitude, or approximately 18.5 km by 18.5 km. A ROM domain and a 9 cell EKMAI subdomain covering parts of New York City are illustrated in Figure 1.

Using the GMISS Model Concentration Data Retrieval Subsystem, the user may choose to extract concentration data from any combination of Domains, Studies, Scenarios, and Dates from previously run ROM simulations as long as those data are in the subsystem and publicly available.

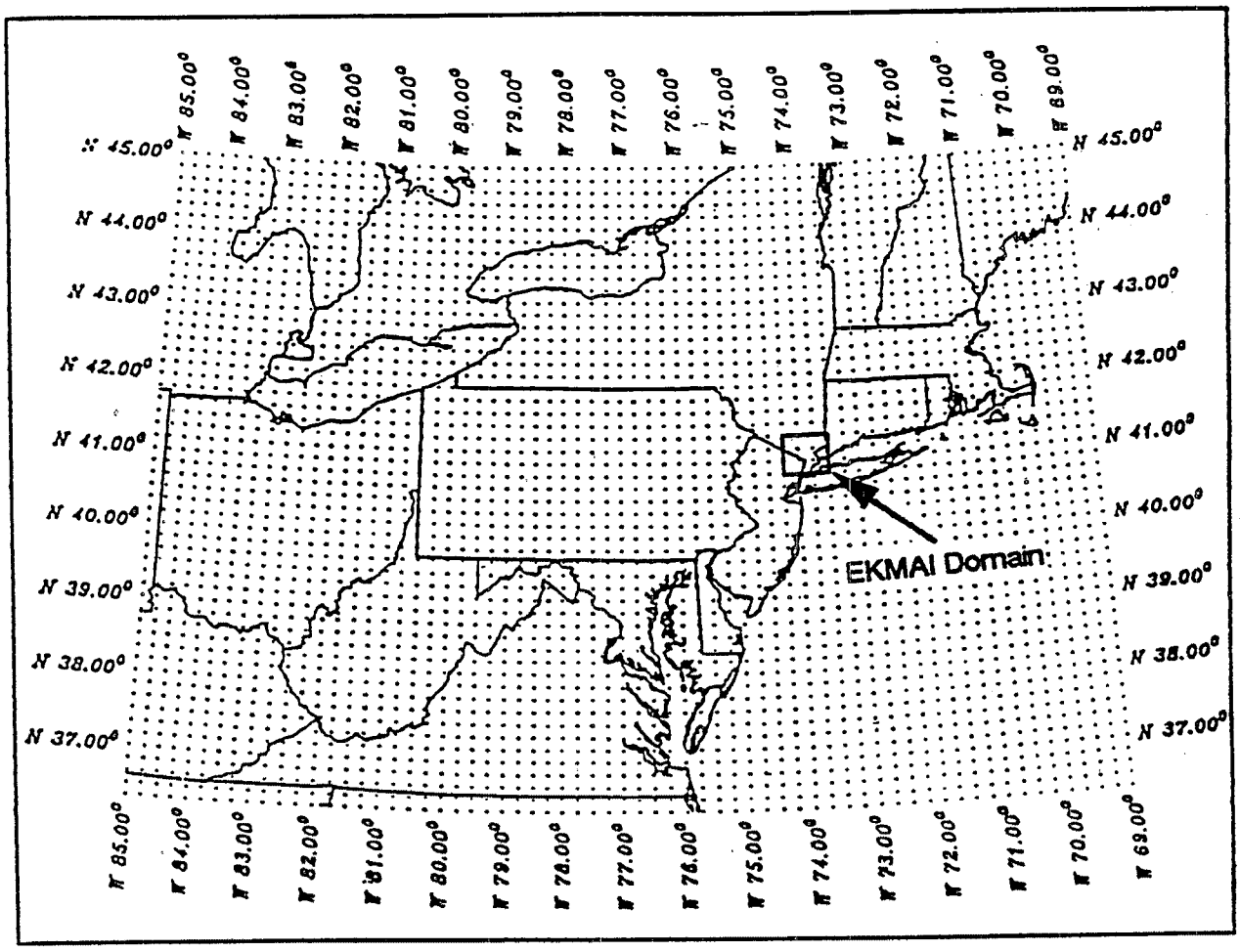

Figure 1. ROM Domain with a 9 Cell EKMAI Subdomain

When prompted for a ROM layer to extract from and which species to choose, however, the user is required by EKMAI to select layer 2 (aloft values) and the following 13 species: ALD2, CO, ETH, FORM, ISOP, NO, NONR, NO2, OLE, O3, PAR, TOL, and XYL.

When data retrieval is complete, the Model Concentration Data Retrieval Subsystem outputs an IBM ASCII formatted file with members INFO and DATA. INFO is a summary of the criteria used in creating the retrieval file, and DATA contains the hourly

concentrations for each species. The retrieval file serves as the input to the EKMAI program.

EKMAI resides on the IBM NCC Mainframe computer. It is accessed at the Time Sharing Option (TSO) "READY" prompt with the following command: **ekmai**. The screen which appears prompts for the name of the file produced by the GMISS Model Concentration Data Retrieval Subsystem, a bin number, and a print destination.

EKMAI takes the concentrations of each species in each grid cell and averages them over the three morning hours beginning at 8 am. This creates one value (a three hour average) for each species in each grid cell. An average value for each species is then calculated for the array as a whole by summing the value in each grid cell and dividing by 9 or 25 depending number of grid cells in the array. Finally, values for NMOC are calculated by multiplying the required organic species by their carbon numbers (i.e., the number of carbon atoms per molecule)[1] and summing.

The output of EKMAI is a system output report which contains a list of concentrations aloft for O3, CO, and NOx in ppm and NMOC in ppmC which may be used as input boundary conditions for the EKMA model.

3. USING THE EKMAI SYSTEM

This section provides an example for using EKMAI. The first part describes the method for using the GMISS Model Concentration Data Retrieval Subsystem to retrieve the data that EKMAI requires. The second part shows how to run EKMAI itself.

3.1 DATA RETRIEVAL

The example presented here follows the TUTORIAL provided in Chapter 4 of the Model Concentration Data Retrieval Subsystem in several ways, such as selecting the same Domain, Study, two Scenarios, and one Date for each scenario. It departs from the TUTORIAL, however, when it is necessary to specify the particular parameters required for running EKMAI. These are: a subdomain which is an array of 9 or 25 ROM grid cells with the center of the urban area located somewhere in the center grid cell, 13 specific chemical species, model layer 2, and the specific retrieval options "interactive" and "sequential". All of these are explained in detail in the example below.

Defining a Subdomain Array

To begin, follow the example in the Model Concentration Data Retrieval Subsystem TUTORIAL until you arrive at screen 3.1. (The screen number is located in the upper left corner of each menu). Your screen should look like Figure 2. Note that the screen shows ROMNET1 as the chosen ROM domain and that the column/row and longitude/latitude dimensions of this domain are displayed.

Screen 3.1 can be used in a special way to define the subdomain of ROMNET1 that EKMAI needs, which is an array of 9 or 25 ROM grid cells which overlay the EKMA urban area. The center grid cell of the array will contain the point that is the center

of the urban area. Figure 3 is a schematic of the grid cell arrays.

```
+3.1-------------------------------------------------------------------------+
|                  GMISS: Retrieve Model Concentration Data                  |
|                       Select Domain and Subdomain                          |
|                                                                            |
|      Specify the modeling domain for which you want to retrieve data,      |
|          then press ENTER.  To see a list of domains, enter "?".           |
|                                                                            |
|                              Domain: ROMNET1                               |
|                                                                            |
|                             -- Subdomain --                                |
|                                                                            |
|  Enter column-row or longitude-latitude ranges to define a rectangular     |
|  subdomain.  Erase (leave blank) all fields to select the entire domain.   |
|                                                                            |
|  West-to-East                    1    64      |          85 00    69 00   |
|  Dimension          Columns:  ___ - ___        |  Longitude: ___ __ - ___ __|
|                                                |                            |
|  South-to-North                  1    52      |          36 20    45 00   |
|  Dimension             Rows:  ___ - ___        |   Latitude: __ __ - __ __  |
|                                                |             dd:mm  dd:mm   |
|                                                                            |
|                    PF3/PF15 = Return to main menu                          |
+----------------------------------------------------------------------------+
```

Figure 2. Screen for Defining a Subdomain Array

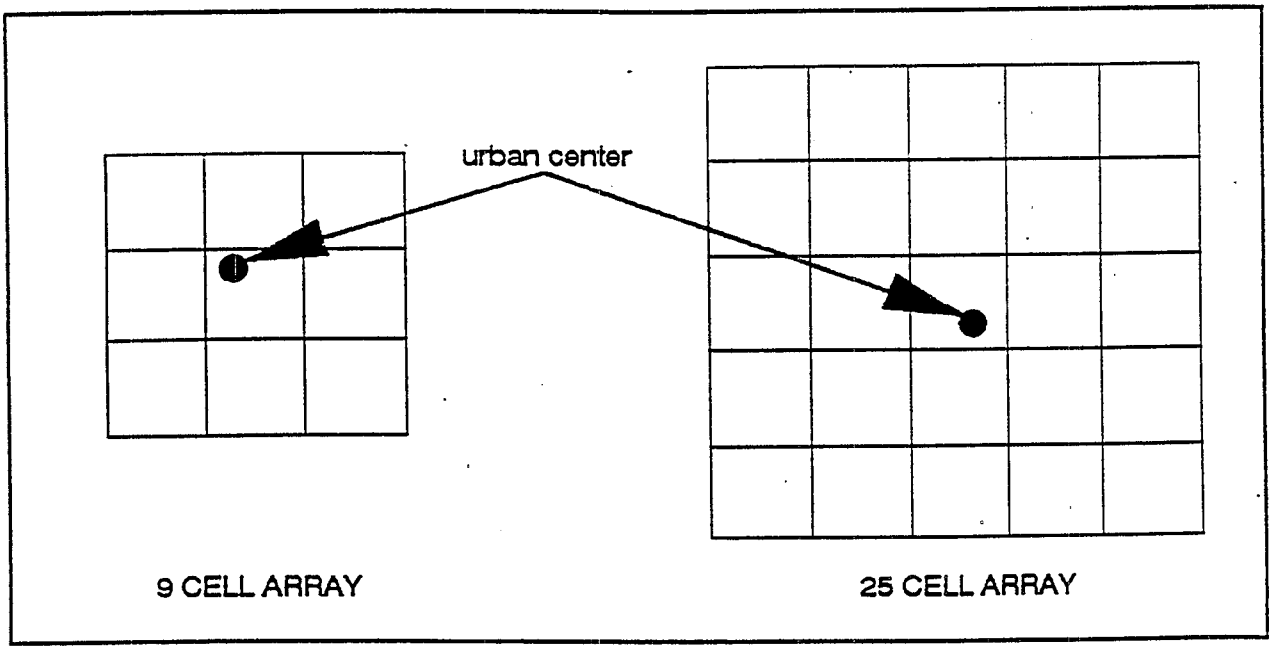

Figure 3. ROM Subdomain Arrays of 9 and 25 Cells

Suppose you will use EKMA to model New York City with the center of the urban area located at 74°00′ longitude and 41°00′ latitude. Enter the coordinates in screen 3.1. The screen should look like Figure 4. Press the ENTER key.

```
+3.1-------------------------------------------------------------------------+
|                GMISS: Retrieve Model Concentration Data                     |
|                       Select Domain and Subdomain                           |
|                                                                             |
|    Specify the modeling domain for which you want to retrieve data,        |
|       then press ENTER.  To see a list of domains, enter "?".               |
|                                                                             |
|                           Domain: ROMNET1                                   |
|                                                                             |
|                           -- Subdomain --                                   |
|                                                                             |
| Enter column-row or longitude-latitude ranges to define a rectangular      |
| subdomain.  Erase (leave blank) all fields to select the entire domain.    |
|                                                                             |
| West-to-East                    1    64  |              85 00     69 00    |
| Dimension           Columns: ___ - ___   |  Longitude: _74_ _00_ - ___ ___ |
|                                          |                                  |
| South-to-North                  1    52  |              36 20     45 00    |
| Dimension              Rows: ___ - ___   |   Latitude: _41_ _00_ - ___ ___ |
|                                                        dd:mm     dd:mm     |
|                                                                             |
|                    PF3/PF15 = Return to main menu                           |
+-----------------------------------------------------------------------------+
```

Figure 4. Entering Coordinates of Urban Center

Given a longitude and latitude, GMISS will fill in the corresponding column and row of the grid cell which contains that point. Your screen should now resemble Figure 5. Notice that the coordinates for the domain dimensions were carried through. Disregard these and concentrate only on the calculated column and row of the center cell, in this case column 45 and row 29.

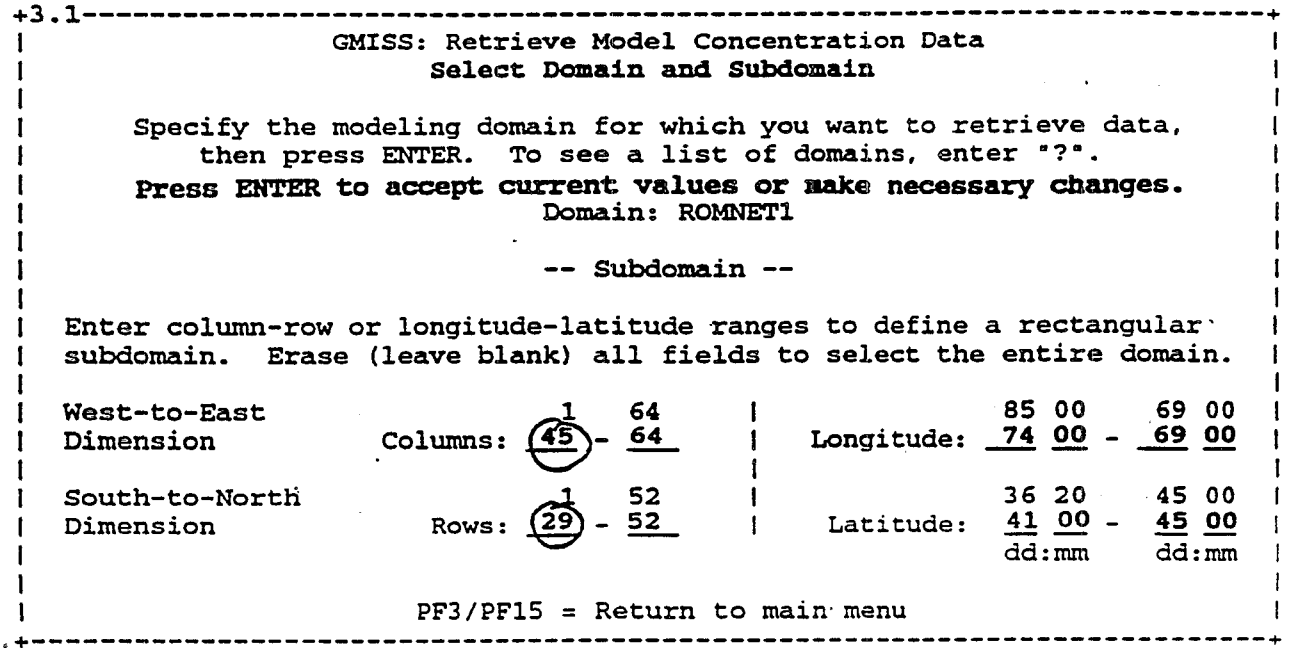

Figure 5. Column and Row of Array Center Cell

Now that you know the center grid cell of the array, you can use its coordinates to determine the dimensions of the whole subdomain array. Say for your New York example that you decide to extract data over the 9 grid cell array. As illustrated in Figure 6, you need to subtract and add 1 to the column number 45 to get the West-to-East Dimension of the array (44-46). Then subtract and add 1 to the row number 29 to get the South-to-North Dimension (28-30). (If you had chosen the array of 25 grid cells, you simply would have added and subtracted 2 from the center column and row to get the array dimensions.)

Now type the column and row dimensions of the 9 cell array into screen 3.1 as shown in Figure 7. Note that longitude and latitude will be overridden by the column and row coordinates, and longitude and latitude will be recalculated. Press the ENTER key.

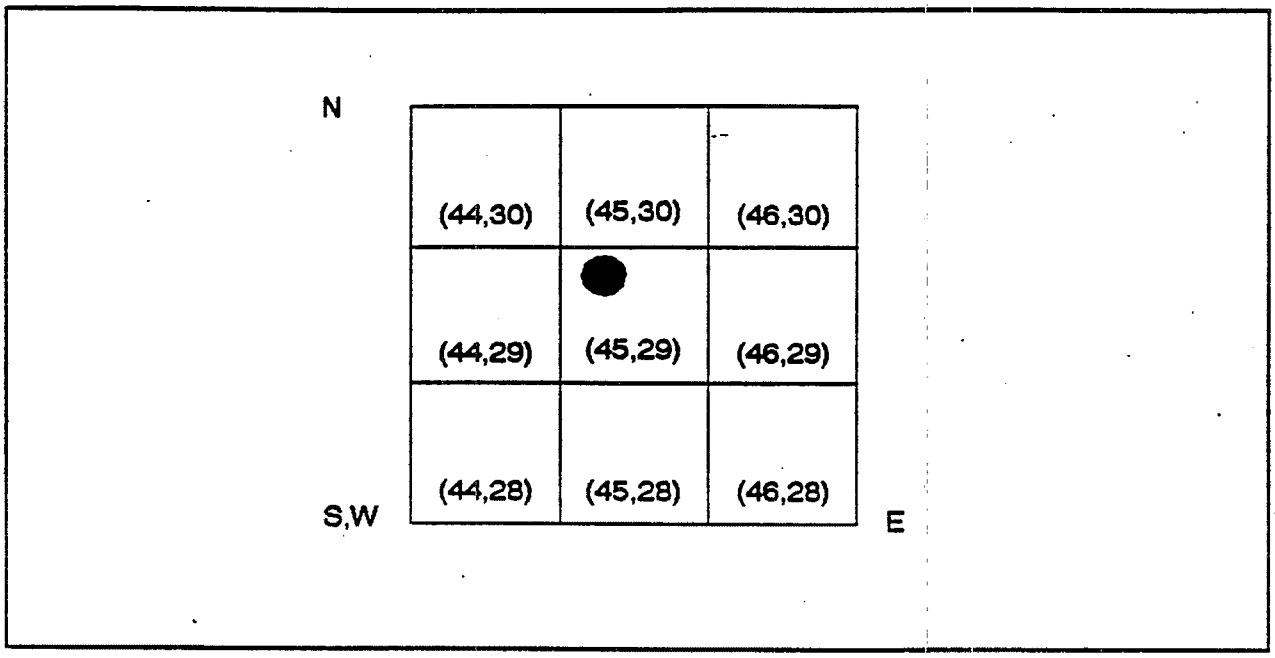

Figure 6. Calculating the Array Dimensions

```
+3.1-------------------------------------------------------------------------+
|                  GMISS: Retrieve Model Concentration Data                  |
|                        Select Domain and Subdomain                         |
|                                                                            |
|      Specify the modeling domain for which you want to retrieve data,      |
|          then press ENTER.  To see a list of domains, enter "?".           |
|      Press ENTER to accept current values or make necessary changes.       |
|                              Domain: ROMNET1                               |
|                                                                            |
|                             -- Subdomain --                                |
|                                                                            |
|  Enter column-row or longitude-latitude ranges to define a rectangular     |
|  subdomain.  Erase (leave blank) all fields to select the entire domain.   |
|                                                                            |
|  West-to-East                  1   64                  85 00    69 00      |
|  Dimension          Columns:  44 - 46      Longitude:   74 00 - 69 00      |
|                                                                            |
|  South-to-North                1   52                  36 20    45 00      |
|  Dimension             Rows:  28 - 30      Latitude:    41 00 - 45 00      |
|                                                         dd:mm    dd:mm     |
|                                                                            |
|                    PF3/PF15 = Return to main menu                          |
+----------------------------------------------------------------------------+
```

Figure 7. Entering the Array Column and Row Dimensions

Figure 8 shows the final coordinates of the 9 grid cell array over which the concentration data will be extracted.

```
+3.1-----------------------------------------------------------------------+
|                GMISS: Retrieve Model Concentration Data                  |
|                     Select Domain and Subdomain                          |
|                                                                          |
|     Specify the modeling domain for which you want to retrieve data,     |
|        then press ENTER.  To see a list of domains, enter "?".           |
|     Press ENTER to accept current values or make necessary changes.      |
|                          Domain: ROMNET1                                 |
|                                                                          |
|                          -- Subdomain --                                 |
|                                                                          |
|  Enter column-row or longitude-latitude ranges to define a rectangular   |
|  subdomain.  Erase (leave blank) all fields to select the entire domain. |
|                                                                          |
|  West-to-East                  1    64   |                85 00   69 00  |
|  Dimension          Columns:  44 -  46   |   Longitude:   74 15 - 73 30  |
|                                          |                               |
|  South-to-North                1    52   |                36 20   45 00  |
|  Dimension             Rows:  28 -  30   |   Latitude:    40 50 - 41 20  |
|                                                          dd:mm   dd:mm  |
|                                                                          |
|                   PF3/PF15 = Return to main menu                         |
+--------------------------------------------------------------------------+
```

Figure 8. Final Coordinates of the 9 Cell Array

Press the ENTER key. Then continue to follow the TUTORIAL example for screens 3.2 and 3.3 until you have duplicated its entries for Domain (ROMNET1), Model (ROM21), Study(ROMNET), Scenarios (BASE05 and CS01), and Dates (06/20/83 for BASE05 and 07/04/88 for CS01).

Note that the TUTORIAL example chooses two emission scenarios (BASE05 and CS01). Given this information, EKMAI will calculate and output the concentrations aloft for each scenario, one after the other. Up to 5 scenarios (or domains or studies) may be extracted from the GMISS database and used in one run of EKMAI. If more than one day is chosen for one scenario, EKMAI will calculate and output a set of concentrations for each day.

Up to 15 days can be extracted and processed for one scenario.

Selecting Species and Layer

At screen 3.4 it is necessary to depart from the TUTORIAL again because EKMAI requires specific selections. Type an "S" beside layer 2 and each of the following species: **ALD2, CO, ETH, FORM, ISOP, NO, NONR, NO2, OLE, O3, PAR, TOL, XYL.** Your screen should look like Figure 9. Press the ENTER key.

```
+3.4-------------------------------------------------------------------------+
|                  GMISS: Retrieve Model Concentration Data                  |
|                         Select Layers and Species                          |
|                                                                            |
|          Type "S" beside the model layers and chemical species             |
|                    you want to select, and press ENTER.                    |
|                                                                            |
|  Layers:                                                                   |
|  _ 1            S 2            _ 3                                         |
|                                                                            |
|  Species:                                                                  |
|  S ALD2         S CO           _ C2O3         S ETH          S FORM       |
|  _ HNO2         _ HNO3         _ HO2          _ H2O2         S ISOP       |
|  _ MTHL         S NO           S NONR         S NO2          _ NO3        |
|  _ N2O5         _ OH           S OLE          S O3           _ PAN        |
|  S PAR          S TOL          _ TRAC         _ XO2          S XYL        |
|  _ ........     _ ........     _ ........     _ ........     _ ........   |
|  _ ........     _ ........     _ ........     _ ........     _ ........   |
|  _ ........     _ ........     _ ........     _ ........     _ ........   |
|                                                                            |
|                    PF3/PF15 = Return to previous menu                      |
+----------------------------------------------------------------------------+
```

Figure 9. Selecting Layer 2 and Species

Specify Retrieval Options

At the next screen, 3.5, select "I" for Interactive Data Retrieval Mode and "Q" for seQuential Retrieval File Type for the purposes of EKMAI. You may specify your own name for the output file or use the default provided. Either way, write down this filename because you will need to enter it as input to EKMAI. Figure 10 shows what this screen should look like. Press the ENTER key. The retrieval will take place.

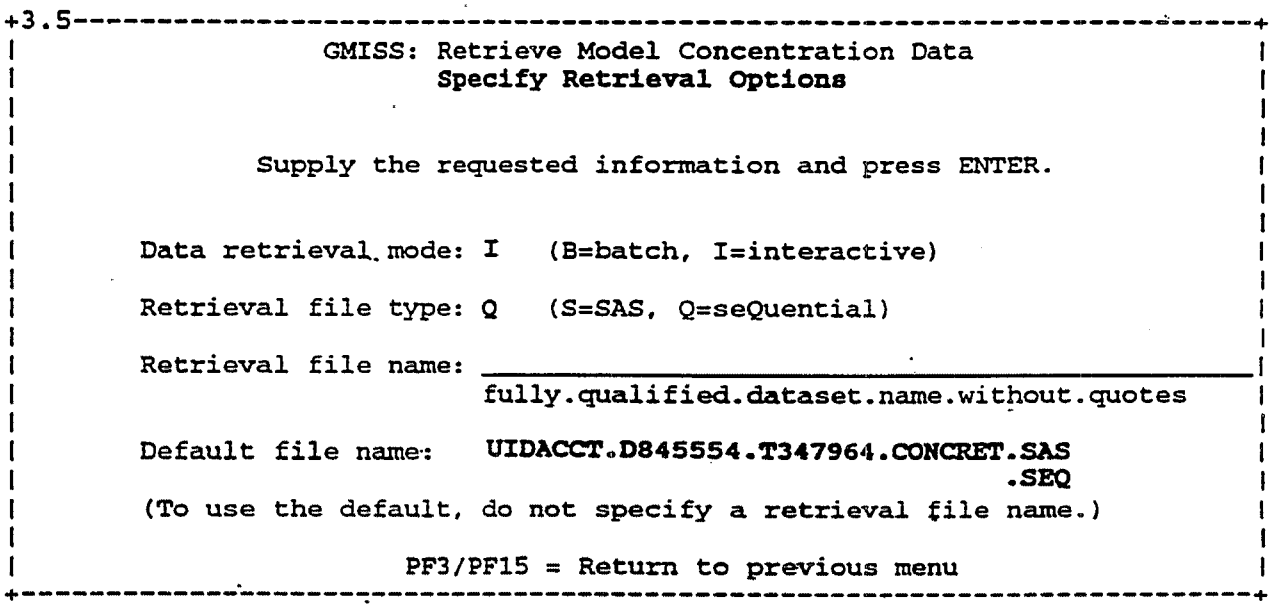

Figure 10. Specifying Retrieval Options

Follow the instructions in the TUTORIAL to exit from GMISS.

3.2 RUNNING EKMAI

Having obtained the hourly concentration data for the required species over a defined subdomain array, you are ready to run EKMAI. Type the following (in either upper or lower case letters) at the TSO "READY" prompt: **ekmai**. Press the ENTER key, and an introductory screen will appear. Press the ENTER key again to continue. The EKMAI screen will appear as in Figure 11.

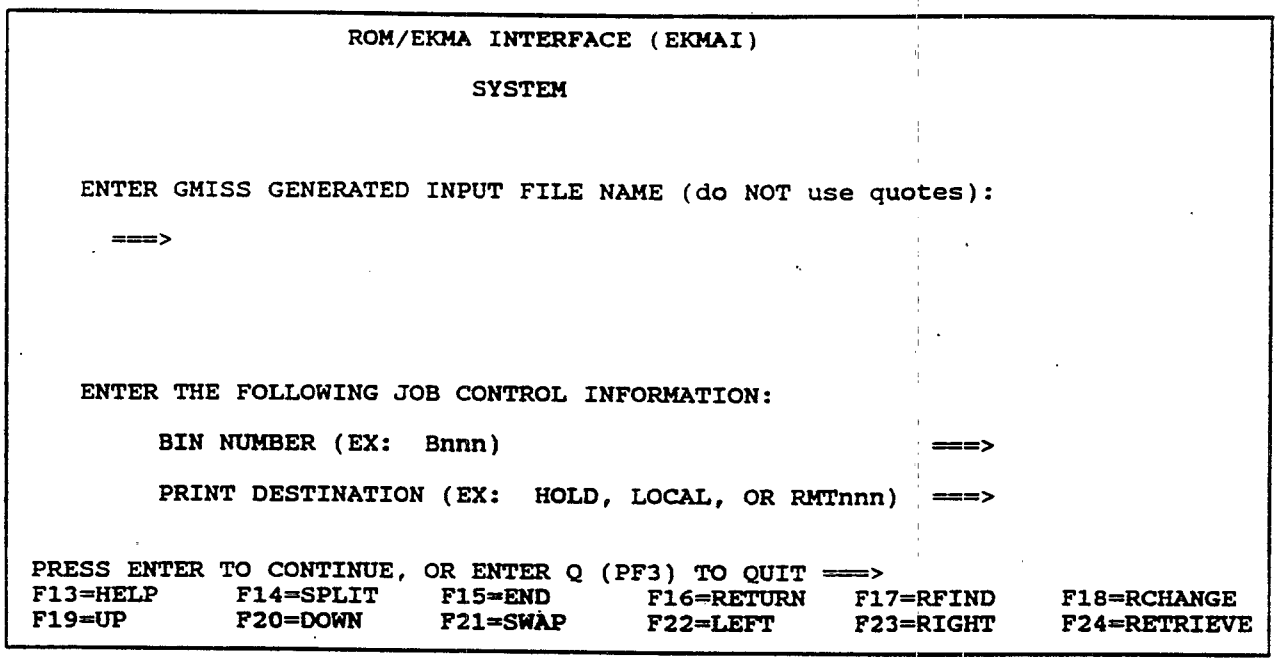

Figure 11. The EKMAI Screen

Type in the name of the file you created with the GMISS Model Concentration Data Retrieval Subsystem. Also type in a bin number and print destination as prompted. Figure 12 shows a completed screen.

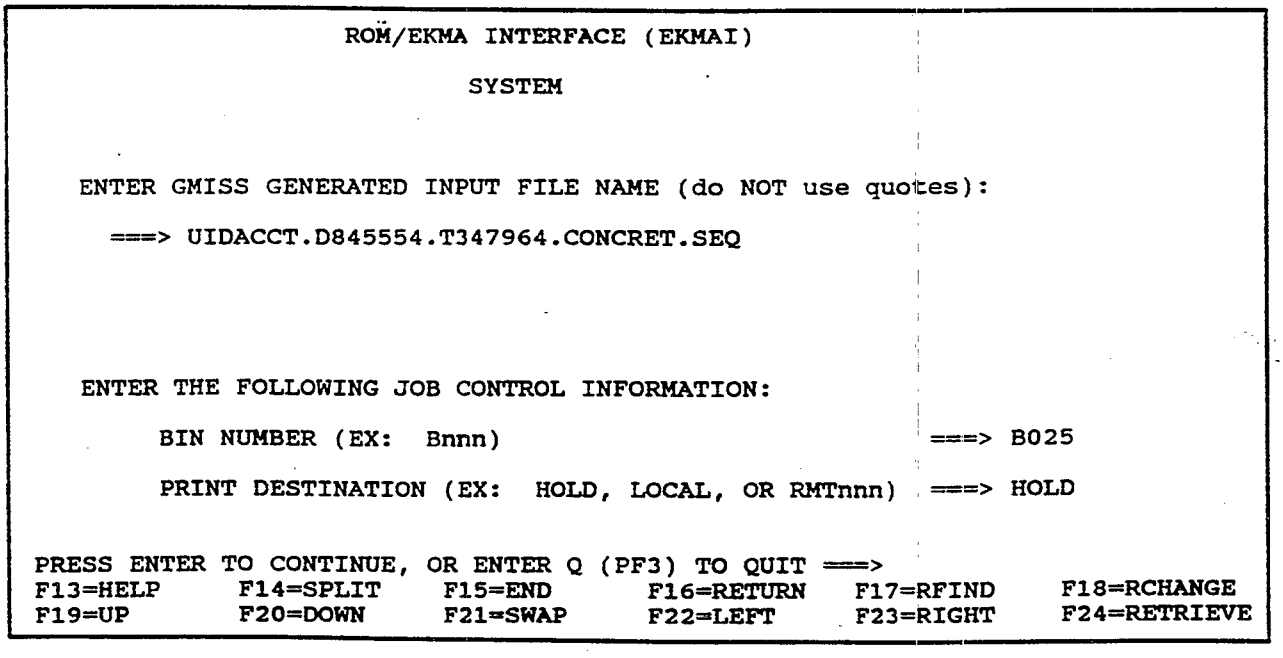

Figure 12. Completed EKMAI Screen

Press the ENTER key and your job will be submitted by EKMAI. (At this point you may encounter a TSO Interactive System Productivity Facility (ISPF) screen for specifying the disposition of the IBM Mainframe log data set. As the screen directs, you may press the ENTER key to continue or enter the END command to return to EKMAI. Options are available in ISPF to prevent the appearance of this screen. If you need assistance with this or have other ISPF or IBM Mainframe questions, contact the EPA National Computer Center (NCC) user support at (919) 541-7862 or (800) 334-2405.)

You will need to use ISPF to view the system output report. Again, if you need assistance using ISPF contact user support at the numbers mentioned above. After paging down to the bottom of the system output report, your output for this example should look similar to Figure 13. If EKMAI ran without any problems, the message NORMAL SUCCESSFUL COMPLETION OF PROGRAM will appear, followed by a set of aloft concentration values for each set of requests retrieved from GMISS. Note, for example, that because you chose two scenarios your output produced a set of values both scenarios. If you had chosen more than one date in a scenario, a set of concentrations would have been output for each day. In any case, you will need to **write down the values for O_3, CO, NOx, and NMOC** and use them as input boundary values for EKMA.

```
NORMAL SUCCESSFUL COMPLETION OF PROGRAM

FOR THE DOMAIN : ROMNET1
AND THE MODEL VERSION : ROM21
AND THE STUDY  : ROMNET
AND THE SCENARIO : BASE05
AND THE DATE  : 06/20/83

THESE ARE THE AVERAGED ROM VALUES TO BE USED
AS ALOFT CONCENTRATION INPUTS TO EKMA

   O3     :  0.64478E-01 ppm.
   CO     :  0.20309E+00 ppm.
   NOX    :  0.20764E-02 ppm.
   NMOC   :  0.61463E-01 ppmC.



NORMAL SUCCESSFUL COMPLETION OF PROGRAM

FOR THE DOMAIN : ROMNET1
AND THE MODEL VERSION : ROM21
AND THE STUDY  : ROMNET
AND THE SCENARIO : CS01
AND THE DATE  : 07/04/88

THESE ARE THE AVERAGED ROM VALUES TO BE USED
AS ALOFT CONCENTRATION INPUTS TO EKMA

   O3     :  0.46698E-01 ppm.
   CO     :  0.15224E+00 ppm.
   NOX    :  0.10245E-01 ppm.
   NMOC   :  0.43873E-01 ppmC.
```

Figure 13. Output from EKMAI

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16. ABSTRACT

The Empirical Kinetics Modeling Approach Interface (EKMAI) is a computer program which uses species concentration data from previous runs of the Regional Oxidant Model (ROM) to create input boundary conditions for the EKMA model. This manual describes how a user may extract the ROM data using the Gridded Model Information Support System (GMISS) Model Concentration Data Retrieval Subsystem and use EKMAI to produce boundary concentrations aloft of ozone, carbon monoxide, nitrogen oxides, and nonmethane organic compounds for input to EKMA.

17. KEY WORDS AND DOCUMENT ANALYSIS

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