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Project Summary

User's Guide for Executing OZIPM-4 with CBM-IV or Urban and Regional Modeling

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In a recent study, Systems Applications developed a new chemical mechanism called the Carbon-Bond Mechanism-IV (CBM-IV), which provides a complete and verified description of urban smog chemistry. In this study, the CBM-IV has been incorporated into a new computer program called Ozone Isopleth Plotting with Option Mechanisms -- Version 4 (OZIPM-4). This program is designed to be used with EKMA to calculate the emission reductions needed to achieve the air quality standard for ozone. The OZIPM-4 can accept as input chemical mechanism other than the CBM-IV. Recent updates and improvements to the OZIPM-4 are discussed along with the CBM-IV mechanism. OZIPM-4 expands on earlier codes by providing a wider compatibility between computers, an improved isopleth plotting package, expanded user interaction with control strategy calculations, and a new option for determining credits for carbon monoxide emissions reductions. Volume 1 serves as the User's Manual for OZIPM-4. It contains both a detailed description of OZIPM-4 and a discussion of the input and output requirements and options available for exercising either the default CBM-IV mechanism or an optional mechanism. Five examples of OZIPM-4 input and output files are also included. Volume 2 contains the listing of the FORTRAN computer code. A magnetic tape or floppy disk of this code is also available from Systems Applications.

This Project Summary was developed by EPA's Atmospheric Sciences Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in two separate volumes of the same title (see Project Report ordering information at back).

Introduction

This project consisted of the development of a new version of the OZIPM (Ozone Isopleth Plotting with Optional Mechanisms) computer program, which is recommended by the U.S Environmental Protection Agency (EPA) for formulating State Implementation Plans (SIPs) for attainment of the ozone National Ambient Air Quality Standard (NAAQS). OZIPM utilizes the Empirical Kinetics Modeling Approach (EKMA) to relate levels of ozone to levels of nonmethane organic compounds (NMOC) and oxides of nitrogen (NO_x). The current version is known as OZIPM-4 because the Carbon-Bond Mechanism-IV (CBM-IV) is the default photochemical kinetics mechanism (though alternate chemical mechanisms may be used). In addition to development of the OZIPM-4 computer code, this project involved creation of a user's manual containing (1) a technical description of the model and the various input and output options, (2) guidance on the selection of input options, (3) a quick reference section, and (4) example simulations that demonstrate certain model features.

Description of OZIPM-4

OZIPM-4 consists of two distinct components: the first is a trajectory-based photochemical kinetics simulation model that mathematically simulates physical and chemical processes in the atmosphere; these results are then used as part of the EKMA procedure to calculate emission control requirement for a specific test case or to construct an ozone isopleth diagram.

In the OZIPM-4 photochemical kinetics model a column of air containing ozone and precursors is transported along an assumed trajectory. As the column moves, it encounters fresh precursor emissions that are uniformly mixed within the column, which is assumed to extend from the earth's surface through the mixed layer. The assumed horizontal dimensions of this column are such that the concentration gradients are small enough to make the horizontal exchange of air between the column and its surroundings insignificant. The air within the column is assumed to be uniformly mixed at all times.

At the beginning of a simulation, the column is assumed to contain some specified initial concentrations of NMOC and NO_x. As it moves along the assumed trajectory, the height of the column can change due to temporal and spatial variations in mixing height; it is assumed to change with time during a user-selected period, and to be constant before and after that period. As the height of the column increases, its volume increases, and air from the inversion layer above is mixed in. Pollutants above the mixed layer are described as "transported above the surface layer" or "transported aloft." Any ozone or ozone precursors above the mixed layer that are mixed into the column as it expands are assumed to be rapidly mixed throughout the column. The photochemical kinetics model in OZIPM-4 considers emissions of VOC, NO_x, and CO into the column as it moves along its trajectory. The concentrations of these species within the column are physically decreased by dilution due to the inversion rise, and physically increased by both entrainment of pollutants transported aloft and fresh emissions. All species react chemically according to the kinetic mechanism selected. The photolysis rates within the mechanism are functions of the intensity and spectral distribution of sunlight and they vary diurnally according to time of year and location.

The EKMA Procedure

The EKMA procedure was developed to relate levels of photochemical oxidants (expressed as ozone) to levels of NMOC and oxides of nitrogen NO_x. It utilizes a set of isopleths that depict maximum afternoon concentrations of ozone as a function of the following parameters:

Morning concentrations of NMOC and NO_x (which may include precursors transported from upwind sources);

Emissions of volatile organic compounds (VOC), NO_x, and other species (such as carbon monoxide) occurring during the day;

Meteorological conditions; and

The reactivity of different VOC and NMOC mixtures.

The EKMA procedure utilizes multiple computer simulations with different levels of NMOC and NO_x concentrations to predict the resulting maximum hourly ozone concentrations. These ozone concentrations are then used to generate ozone concentration isolines that are plotted as a function of initial precursor concentrations. These isopleths are used to compute the percent reduction in emissions that is needed to lower peak ozone to the NAAQS of 0.12 ppm. It is not necessary to use isopleth diagrams to perform EKMA calculations because the EKMA option in OZIPM-4 will do this internally and report a control value. However, though use of the EKMA option will provide the target VOC control requirements, in some cases an isopleth diagram can provide additional diagnostic information.

The Chemical Kinetics Mechanism

As noted earlier, the CBM-IV is internally stored in the OZIPM-4 program. However, the program can accept a chemical mechanism other than the default CBM-IV. This optional kinetic mechanism cannot contain more than 135 reactions and/or 60 species. To input a different kinetic mechanism, the user must specify certain parameters:

The total number of photolysis reactions (maximum of 20) and the reaction numbers that identify the photolysis reactions in the mechanism.

The total number of organic species included in the initial NMOC mix (maximum of 20), the names that identify these species, and th number of carbon atoms in each.

The fraction of total carbon that eac organic species represents.

Mechanisms are included in th OZIPM-4 through the use of variou input options. These options and other are described next.

Input and Output Options

Input parameters (options) that ca be specified by the user whe performing an OZIPM-4 calculatio include:

A new chemical kinetic mechanism;

The zenith-angle-dependence c the photolytic rates for the chemic mechanism;

Latitude, longitude, time zone an date;

Morning and afternoon mixing height (also called mixing depths) or hourl mixing depths;

Hourly temperature variation;

The simulation start and stop times;

Concentrations of NMOC, NO_x, C ozone, and up to 10 other species the air above the mixed layer due transport aloft (note that these cann be varied in time);

Concentrations of NMOC, NO_x, C ozone, and any other chemic species transported in the surfac layer;

Background concentrations of NMO NO_x, and ozone. The backgrour represents the minimum levels in bo the surface layer and aloft that cou be achieved if all urban emissio were reduced to zero (i.e., continen background);

VOC, NO_x, and CO emissions at ea hour;

Organic reactivity. Four reactiviti can be specified: background, initi aloft, and emitted. However, each ty of reactivity is fixed in time for ea diagram point and at every point the diagram;

NO_x reactivity (initial fraction of N that is NO_2);

Surface deposition as a function time for up to 10 species.

In addition, the user may va individual reaction rates, alter the er tolerance of the calculations, and in simulation results from previous ru The major function of OZIPM-4 is

Estimate the VOC reductions needed to achieve the ozone air quality standard. The output depends on the option selected by the user. Three types of output can be requested:

(1) Perform a single calculation for a specified set of initial concentrations.

(2) Compute VOC emission reduction needed to achieve the 0_3 standard of 0.12 ppm without generating an 0_3 isopleth.

(3) Generate an 0_3 isopleth.

In addition, the user may generate isopleths for species other than ozone, and perform off-line (CALCOMP) plotting.

Limitations of the OZIPM-4/EKMA

OZIPM-4 has a limited applicability to ozone problems within, or immediately downwind of, large urban areas and thus should not be applied to the following situations unless special attention is given to current limitations and assumptions:

The rural ozone problem;

Situations in which transported ozone and/or precursors are clearly dominant (i.e., multiday transport situations);

Cases in which the maximum ozone concentration occurs at night or in the early morning; and

The development of control strategies for single or small groups of emission sources.

The validity of an ozone isopleth diagram generated by OZIPM-4 for a particular city may be limited by the following considerations:

The kinetic mechanism used to describe the transformations of NMOC and NO_x;

The physical assumptions used to formulate the trajectory model coded into OZIPM-4;

The meteorological data and assumptions used to specify required OZIPM-4 parameters;

The availability and reliability of current ozone data, precursor concentration data, and VOC, NO_x, and CO emission inventories;

The mathematical assumptions needed to integrate the differential equations formulated within OZIPM-4; and

The interpolations needed to generate isopleths from the results of a number of computer simulations.

Summary

A new version of the Ozone Isopleth Plotting Package with optional Mechanisms (OZIPM-4) computer code has been developed for use in the Empirical Kinetic Modeling Approach (EKMA). The OZIPM-4 contains the Carbon-Bond Kinetics Mechanism-IV (CBM-IV) and additional capabilities not present in earlier versions of OZIPM. The use of the computer code is fully described in the user's manual.

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***Marcia C. Dodge** is the EPA Project Officer (see below).*
The complete report consists of two volumes and a computer tape, entitled "User's Guide for Executing OZIPM-4 with CBM-IV or Optional Mechanisms," EPA/600/8-88-073a, b, and c.
"Volume1. Description of the Ozone Isopleth Plotting Package Version 4," (Order No. PB 88-221 957/AS; Cost $25.95)
"Volume 2. Computer Code," (Order No. PB 88-221 965/AS; Cost: $19.95)
"OZIPM-4 Source Code (Computer Tape)" (Order No. PB 88-221 940/AS; Cost: $800.00--cost of tape includes paper copy of reports)
The above reports and computer tape will be available only from: (cost subject to change)

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

The EPA Project Officer can be contacted at:

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