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Project Summary

User's Guide for Executing OZIPR

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A new, trajectory-type, air quality simulation model called OZIPR has been developed. OZIPR is based on previous versions of EPA's Ozone Isopleth Plotting Program (OZIPP) Model but contains improved and expanded capabilities that make the model useful for research purposes. OZIPR serves the dual purpose of providing: (1) a simple trajectory model capable of using complex chemical mechanisms, emissions, and various meteorological parameters, and (2) procedures through which the Empirical Kinetics Modeling Approach (EKMA) can be implemented to calculate emission reductions for compliance with the National Ambient Air Quality Standard for ozone. While these capabilities were included in earlier versions of OZIPP, the new OZIPR contains major improvements that expand the program's capability to input, utilize, and output a much larger range of information.

The Project Report serves as a user's manual for OZIPR. It contains a description of the model, along with input and output requirements and options. The input and output files for nine examples are also included. A floppy disk of the executable program, the code, and input and output files are provided.

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

Introduction

This project consisted of the development of a new, research-oriented version of EPA's OZIPP (Ozone Isopleth Plotting Program) computer program. The OZIPP series of programs employs a trajectory-based air quality simulation model, in conjunction with the Empirical Kinetics Modeling Approach (EKMA), to relate ozone concentrations to emissions of volatile organic compounds (VOC) and oxides of nitrogen (NO_x). While the aim of earlier versions was to provide a rigid structure within which State Implementation Plans could be formulated, the goal of OZIPR is to furnish a more comprehensive research tool that is of use to Agency planners and model developers. This version, called OZIPR (R for research), is specifically enhanced to provide more complex input, output, and calculation capabilities than exist in the earlier versions.

Description of OZIPR

OZIPR simulates the complex chemical and physical processes of the lower atmosphere through use of a trajectory model. The physical representation is a well-mixed column of air extending from the ground to the top of the mixed layer. This idealized air column moves with the wind (along the wind trajectory) but cannot expand horizontally. Emissions from the surface are included as the air column passes over different sources, and air from above the column is mixed in as the inversion rises during the day. Very complex chemical mechanisms may be used with OZIPR to describe the chemical processes that occur within the modeled air mass.

Besides individual wind trajectory simulations, the program can use the EKMA procedure to automatically estimate the amount and type of precursor emission reductions expected to achieve a specified ozone level. In this procedure, OZIPR performs multiple simulations with different levels of organic and NO_x precursor emissions to estimate the effect of reduced emissions on maximum ozone concentrations. The program can also perform a specified set of simulations used to calculate ozone levels at fixed intervals. This allows for the plotting of fixed ozone concentration lines (isolines) as a function of initial precursor and emission levels.

Although the structure of the program is similar to earlier versions of OZIPP, OZIPR was enhanced in this study to provide expanded yet simpler input capability, more calculation options, greater calculation speed, and enhanced output options. These improvements are described in the following sections:

Using OZIPR

The structure of OZIPR has been altered to execute in batch mode on a personal or mainframe computer. Fixed-column oriented input has been eliminated in favor of free-format style. In addition, many redundant options were eliminated, and a new command structure was devised. The input file is a text file consisting of a series of OPTIONS and COMMANDS. In addition, the input file can contain the names of commonly used "include" files that are inserted into the text of the input file. This is done by inserting the character "@," followed by the complete filename of an include file at the location in the input file where the text of the include file is desired. Comments are also now allowed on input between { } and ( ), or on lines with the first character "!."

In previous versions of OZIPP, a fixed amount of input was allowed for each option, such as 20 photolysis reactions, or 24 hours of temperature, etc. These numbers were deeply buried in the computer code and could not be changed. One result of this study was to uncover these numbers and bring them to the top of the program so that they may now be easily changed if the user wishes to expand the program's capabilities. The parameters that can now be easily varied and their current limits are:

Hours of input =	24
Total Reactions =	160
Photolysis Reactions =	23
Reaction Products =	12
Total Species =	65
VOC Species =	20
Emitted Species =	10
Isopleth Species =	12
Deposition Species =	10
Printed Species Names =	20
Average Species Names =	10
Dump Names =	12
Dump Rates =	12
Filed Species Names =	20

Command Options

The command options were reorganized and enhanced in OZIPR. The following list summarizes the improved features added in this project:

ECHO of input commands into the output file.

Optional output printer WIDTH of 80 or 132 columns.

Optional listing of the chemical mechanism used, a list of rate constants at standard conditions, and a list of the kinetic expressions and rate parameters.

Expanded chemical MECHANISM input, including:

- Elimination of the default CBM-IV Mechanism;
- Free format input of reactions and kinetics for any mechanism;
- Use of N_2, O_2, and M as known concentrations;
- Three reactants and twelve products with stoichiometry;
- Negative product stoichiometry;
- Kinetics in either ppm-min or molec-cc-sec units;
- Standard kinetic expressions such as $k = A \times (T/300)^B \times e^{(-E/T)}$;
- Falloff type kinetic expressions;
- Special kinetic expressions designed to represent unique pressure and temperature dependency;
- Linear dependence of one rate on another;
- Calculation of reverse equilibrium rates using the equilibrium constant as input;
- Dependence of reaction rates on solar zenith angle and spectral distribution of actinic flux.

Tabular input of either absolute or relative solar ZENITH angle dependence for rate constants.

Expanded input for METEOROLOGICAL conditions, including:

- Free format input of all options;
- Dilution curve or hourly mixing height input;
- Temperature table input;
- User supplied atmospheric pressure;
- Water vapor concentration from either concentration or relative humidity tables;
- Simplified input of constant temperature, pressure, and water levels.

New grouping of input for BOUNDARY conditions input, including:

- Free format input of all options;
- VOC reactivity;
- Optional NO-to-NO_2 ratios for both initial and emitted NO_x;
- Input of surface and aloft transported levels of O_3, VOC, NO_x, and CO;
- Input of surface and aloft transported concentrations other than the specific controllable substances noted above;
- Expanded deposition rate profiles;
- Simplified input of constant deposition rates.

Reformulated EMISSIONS options, including:

- Elimination of the MOLE option;
- Simplification of MASS type input (kg/km^2/hr);
- Expansion of the MASS option to allow input of mass emissions for any species;
- Printed hourly output of both emission ratios and mass per unit area emissions for each emitted species;
- Improvement of the emission algorithm to account for changing MASS emission rates with changing temperature and pressure;
- Simplified input of CO emissions.

CO is now included as a main, controllable species (like NO_x and VOC) in the CALC, EKMA and ISOP commands.

Expanded user control of output characteristics for the single CALCULATION option, including:

- Print control options allowing individual control over specific aspects of output, such as printing of concentrations, net rates of change of species, hourly photolysis rates, and net rates of each reaction;
- Time control of first printing of output and time interval between printing output;
- Printing of concentrations for only a limited number of species;
- Calculation of the maximum concentration of a variable number of species over a user supplied time interval (e.g., an 8-hour average maximum);
- Optional table of hourly concentrations or reaction rates printed at the end of the simulation;
- Optional output of concentrations for user specified species in a file suitable for importing into spreadsheet programs.

Reorganization and expanded user options for the EKMA option, including:

- Inclusion of CO directly in the EKMA command;
- Ability to reduce future CO emissions;
- Merger of EKMA and EMISSIONS options for CO;
- Input of future surface and aloft transported O_3, VOC, NO_x, and CO;
- New formulation for generating incremental VOC, CO, or NO_x reduction tables;
- Optional input of the number of tries for program to attempt solution of design and control convergence.

Minimization of computer code size and increase in speed by removing isopleth diagram generation from OZIPR and creating a post-processor program named ISOPLOT.

Expansion of isopleth plotting options, user interaction, and provisions for high quality graphics output in the ISOPLOT program.

Examples

Input and output files are provided for nine examples, along with the program source and executable files. The examples use three different chemical kinetics mechanisms, all major inputs, functions, and output options.

Summary

An expanded, research-oriented version of EPA's OZIPP computer program has been developed. The new program, OZIPR, allows increased input of information, including free-format input of chemical kinetics mechanisms, and extensive expansion of kinetics input and optional output. The use of the computer code is fully described in the user's manual.

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The complete report, entitled "User's Guide for Executing OZIPR," (Order No. PB91-175877/AS; Cost: $23.00, subject to change) will be available only from:
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