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Project Summary

Guidelines for Using OZIPM-3 With CBM-X or Optional Mechanisms

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The U.S. Environmental Protection Agency is continuing to recommend the use of the Empirical Kinetic Modeling Approach (EKMA) as a procedure for relating levels of photochemical ozone to levels of organic compounds and oxides of nitrogen. In an earlier study, Systems Applications developed a new chemical mechanism that is suitable for use in EKMA. The mechanism, called the extended Carbon Bond Mechanism (CBM-X), provides the most up-to-date and verified description of urban smog chemistry currently available. In the study reported here, a new computer program, called Ozone Isopleth Plotting with Optional Mechanisms—Version 3 (OZIPM-3), was developed to enable the use of the CBM-X mechanism for EKMA control strategy calculations. The OZIPM-3 program also has the capability to accept a chemical mechanism other than the default CBM-X that is internally stored in the program. Volume 1 serves as the User's Manual for OZIPM-3. It contains a detailed description of how OZIPM-3 operates. It also contains a thorough discussion of the different input and output options available to the user when exercising either the default CBM-X mechanism or an optional mechanism. Five examples of OZIPM-3 simulations are presented. Input and output files for each example are included. Volume 2 contains the FORTRAN listing of the computer code. A magnetic tape of this code is also available.

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 and a magnetic tape of the same title (see Project Report ordering information at back).

Introduction

For several years, the EPA has used the Empirical Kinetic Modeling Approach (EKMA) to estimate reductions in emissions of volatile organic compounds (VOC) needed to achieve the National Ambient Air Quality Standard (NAAQS) for ozone. The objective of the study reported here was to develop a computer program to enable the use of the latest photochemical kinetics mechanism in EKMA for control strategy calculations. This mechanism is called the extended Carbon-Bond Mechanism (CBM-X). It is described in the report "Modeling of Auto Exhaust Smog Chamber Data for EKMA Development" (EPA/600/3-85/025). The computer code developed is called Ozone Isopleth Plotting with Optional Mechanisms—Version 3 (OZIPM)-3). It expands on earlier codes by providing a wider compatibility between computers, a feature to calculate VOC reduction without drawing an isopleth diagram, and easier input of photolysis rates when operational chemical mechanisms are selected.

Features of the CBM-X

The expanded mechanism was comprehensively developed and tested to provide the most up-to-date and verified description of urban smog chemistry currently available. In addition to testing of the whole mechanism, independent testing of various parts of the CBM-X was

conducted. In particular, the inorganic reactions, common to all smog chemistry, were tested against a wide range of smog chamber experiments involving various combinations of NO, NO_2, CO, formaldehyde, temperature, humidity, and light conditions. The same inorganic reactions were then combined with each of the subsets (such as acetaldehyde, ethene, toluene, and xylene) to verify each chemistry subset using smog chamber data specific to each. Finally, the whole CBM-X was tested by simulating auto exhaust and synthetic urban mixtures in single- and multiple-day experiments. Since the reaction set includes, directly or indirectly, all the key reactions that have been recommended and independently evaluated for smog photochemistry, the CBM-X is currently the most evaluated and tested mechanism available. Other mechanisms are being developed, however, and the CBM-X is still being tested and refined. In particular, the CBM-X is being evaluated under dynamic conditions intended to simulate entrainment of pollutants into the mixed layer from either aloft or fresh emissions. The fresh emissions also vary widely in reactivity in the new tests.

Features of the New Computer Code

Some of the features in the new computer code OZIPM-3 expand the EKMA model itself. These features include the ability to specify the following: the zenith angle dependence of photolysis reactions; hourly temperature variations; optional start and stop times; different mixtures of precursors and ozone plus other species for initial, aloft, and background conditions and for emissions; and surface deposition (which can vary in time for up to 10 species). The model still has the features of optional kinetic mechanisms, automatic zenith angle generation, and diurnally variable emission rates. The outputs are similar to previous OZIPM versions in that single trajectory calculations can be performed, VOC reduction estimates can be computed independently of an O_3 isopleth diagram if needed, and isopleth diagrams can be prepared for any species, including O_3.

The computer code is limited by the timewise fixed reactivities or concentrations from the precursors in emissions or aloft. Limitations on model formulation include those on trajectory models in general, such as horizontal mixing, windshear effects, eddy diffusion, heterogeneous chemistry, and aerosol light scattering. Also, EKMA modeling is not designed to treat plumes, rural ozone problems, or situations dominated by transport of ozone or its precursors. OZIPM-3 has been prepared using FORTRAN-66 to make it adaptable to a wide range of computers. However, the 7000 lines of code may require computers of moderate size.

Summary

The new CBM-X mechanism and its use in the new computer code, OZIPM-3, are described in detail in the project report. The report provides guidance for using the new chemistry and code in the EKMA procedure developed by the EPA for estimating VOC reductions needed to meet the ozone standard. It should be noted, however, that the CBM-X is still undergoing additional testing and refinement, which will not be completed until late 1987. Until that time, it is recommended that OZIPM-3 with the CBM-X mechanism be used only as a research tool.

The new CBM-X was developed and tested to provide the most up-to-date and detailed chemistry suitable for use in EKMA. Although the new code contains the CBM-X embedded as a default mechanism, other mechanisms can be utilized.

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The complete report consists of two volumes and software for Volume 2, entitled
"Guidelines for Using OZIPM-3 with CBM-X or Optional Mechanisms:"
"Volume 1. Description of the Ozone Isopleth Plotting Package/Version 3," (Order No. PB 86-187 770; Cost: $22.95)
"Volume 2. Computer Code," (Order No. PB 86-194 248; Cost: $16.95)
"OZIPM-3 Source Code (software for Volume 2)," (Order No. PB 86-187 788; Cost: $685.00, includes paper copy)

The above items will be available only from: (cost subject to change)
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

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