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♻EPA Improving Performance of the Maryland Air Management Administration Ozone Model (OZIPM)

FINAL REPORT

EPA Contract No. 68-02-3511
Work Assignment No. 18
PES Project No. 566

IMPROVING PERFORMANCE OF THE MARYLAND
AIR MANAGEMENT ADMINISTRATION OZONE MODEL
(OZIPM)

Prepared by: Lowell G. Wayne
Joseph A. Cassmassi

Prepared for:

U.S. ENVIRONMENTAL PROTECTION AGENCY
Region III
6th and Walnut Streets
Philadelphia, Pennsylvania 19106
Edward A. Vollberg, Project Officer

February 1982

PACIFIC ENVIRONMENTAL SERVICES, INC.
1930 14th Street
Santa Monica, CA 90404
(213) 450-1800

ACKNOWLEDGMENT

EXECUTIVE SUMMARY

In response to a work assignment, PES studied the functioning of a photochemical air quality simulation model, OZIPM, which had been found by the Air Management Administration of the State of Maryland to yield unsatisfactory ozone isopleth curves in a test application in which a complex chemical kinetic mechanism was utilized. PES was assigned to determine the cause of the problem and recommend means to overcome it.

A major cause of the problem was found to consist in a discrepancy between the Users Manual directions and the actual structure of the OZIPM program. This discrepancy hinged on the distinction between molar and carbon-based units for the expression of concentrations of hydrocarbons; that is, between parts per million by volume (ppmV) and parts per million as carbon (ppmC). A method of correcting the discrepancy is recommended in this report, and alternative measures which involve slight revisions to the instructions in the Manual, but with no alteration to the existing program, are also described and discussed.

In a separate line of inquiry, the possibility that the chemical mechanism used in Maryland's application might be at fault was investigated. Results from a chamber simulation study done at the University of North Carolina were made available, prior to publication, by the Air Management Technology Branch, Office of Air Quality Programs and Standards, U.S. EPA. These results showed that isopleth curves based on the mechanism (CIT, devised by investigators at the California Institute of Technology) which was used by Maryland were similar in character to those based on other complex chemical mechanisms which have been provided for the same purpose. Although some of the reaction rate factors taken by the UNC investigators differed from those used by Maryland, it was

concluded that the CIT mechanism was not at fault in yielding isopleths of the type found in the Maryland application.

Study of the OZIPM output furnished by Maryland indicated that the isopleths were consistent with the proper functioning of the CIT mechanism and that the program itself functioned properly, except for the discrepancy already noted. Isopleth diagrams which represent simulations with no assumed hydrocarbons in air aloft, when interpreted three-dimensionally, may be expected to exhibit a ridge of ozone maxima, diagonally directed toward the plot origin. The lack of such a ridge in the Maryland isopleth diagram is a consequence of the conditions assumed in the program input, together with the program discrepancy noted.

In the Maryland application, a substantial level of hydrocarbons was assumed to be transported from aloft. At the same time, NOx was assumed to be absent from the transported air mass. Further, the effect of these transported hydrocarbons was magnified by an assumed large increase in mixing height during the day, which results in the final mixture consisting of nearly 90 percent air from aloft. Acting in the same direction, the program discrepancy erroneously multiplied the hydrocarbon concentrations in the air aloft by a factor of about 5. The net result of these circumstances was to displace the expected ozone ridge completely beyond the boundaries of the diagram produced by the computer.

In analogous circumstances in the atmosphere, the extent of reaction in the photochemical system would be severely limited by the availability of NOx and the quenching effect of excess hydrocarbons. Maryland's isopleth diagram correctly reflects these conditions, showing a large sensitivity of the ozone peak to initial NOx, but a low sensitivity to initial hydrocarbons.

A search was also made for possible errors in Maryland's version of OZIPM, which might have been introduced in the course of modifying OZIPM to accept the CIT mechanism. The program code as

applied by Maryland was compared in detail with that of an OZIPM program supplied by AMTB. A total of 43 revisions were identified, affecting 12 segments of the program. These revisions appeared to reflect two main purposes: to provide dimensions needed for the CIT mechanism, and to adjust internal parameters to minimize the occurrence of underflows. However, many of the changes were evidently directed toward reducing redundancy and improving the logic flow of the basic program.

None of these changes appeared inappropriate or likely to cause program malfunctions. It is concluded that, with manual and program corrections as suggested in this report, Maryland's OZIPM should operate as intended.

TABLE OF CONTENTS

1.0 INTRODUCTION

Pacific Environmental Services, Inc. (PES) was directed by Work Assignment No. 18 under EPA Contract No. 68-02-3511 to examine the ozone model, OZIPM, being used by the Maryland Air Management Administration as an aid in developing a control strategy for atmospheric ozone, in order to locate the cause of poor performance by the model in the isopleth generation mode, and to modify the model as necessary to bring its performance to an acceptable level.

This report describes findings by PES in response to Work Assignment No. 18. PES discussed the program, OZIPM, with personnel of the Maryland agency, most especially Mr. Mario Jorquera, and reviewed samples of OZIPM input and output as furnished by the Maryland agency, as well as the detailed coding of both Maryland's OZIPM computer program and a closely related program, also known as OZIPM, which has been under study by Mr. Gerald Gipson of the Air Management Technology Branch, Office of Air Quality Programs and Standards, U.S. Environmental Protection Agency.

Initial examination and discussion revealed an apparent flaw in the Users Manual for Maryland's OZIPM, in that it was ambiguous in regard to units to be used in specifying hydrocarbon concentrations in program input. At the suggestion of PES, Maryland undertook additional computer runs to test the effect of suggested changes in input. Based on verbal reports of the results of these exercises, PES arrived at a conclusion as to the cause and correction of the problem perceived by Maryland.

In a separate line of inquiry, PES reviewed the possibility that the apparent malfunction might be a consequence of the use, in Maryland's OZIPM, of a chemical kinetic mechanism known as CIT, devised by investigators at the California Institute of Technology for simulating the reactions which occur in photochemical air pollution. From AMTB, PES learned that investigators at the

University of North Carolina had recently compared the ability of several chemical kinetic mechanisms, including CIT, to simulate reactions in artificial smog systems, irradiated in an environmental chamber. PES requested and received from AMTB relevant excerpts of a draft report from UNC, dealing with these comparisons. From a review of these excerpts, PES concluded that the CIT mechanism, when applied using the parameters described in the draft report, produces isopleth curves which are comparable in shape and sensitivity to those obtained with other mechanisms.

In order to determine whether the reaction rate factors used by the UNC investigators in simulating photochemical ozone production by the CIT mechanism were consistent with those supplied to Maryland, PES compared them with those listed in the UNC draft report. Numerous differences were found, the largest representing a factor of about 5 in the rate factor applied for one of the 58 reactions in the mechanism. PES concluded, however, that the discrepancies encountered could not be mainly responsible for the problem of OZIPM performance as perceived by Maryland. (Appendix A presents a comparison of the factors used by Maryland and by UNC.)

Following sections of this report present more detailed discussion of PES findings and conclusions. The diagnosis of a relevant program flaw in OZIPM is described and discussed in Section 2.0, and a recommended program modification is shown in Appendix B.

In Section 3.0, we review the perceived defects in the isopleth diagram produced by Maryland's OZIPM, and show how the program flaw diagnosed in the previous section, together with conditions assumed by Maryland as input to the program, accounts for the general character and sensitivity of the ozone isopleth curves.

In Section 4.0, we review the differences in coding between OZIPM as used by Maryland and OZIPM as presently being studied by AMTB. A detailed comparison is presented in Appendix C.

Conclusions and recommendations are presented in Section 5.0.

2.0 CORRECTIONS TO OZIPM

By reviewing the computer printout provided by the Maryland Air Management Administration in conjunction with the Users Manuals for both Maryland and EPA versions of OZIPM, PES has located an inconsistency between the actual functioning of OZIPM and the instructions provided in the manuals. PES believes that this inconsistency has been largely responsible for the difficulties encountered by Maryland.

The inconsistency is as follows. In describing input values for the TRAN card and its successors (which are used to specify the concentrations and composition of contaminants in ambient air at the start of simulations and of air aloft which will enter the system as the inversion rises), the Maryland manual fails to specify the units to be used. The manual for EPA's OZIPM specifies that concentrations are to be entered as ppmC. Further, both manuals instruct the user to enter a "fraction vector" on the same card; one such card is to be used for the initial background hydrocarbons and another for the hydrocarbons in the air aloft. However, in the case of air aloft, the program is designed to perform calculations using concentrations in ppmV (not ppmC) and a "fraction vector" based on such concentrations; consequently, when the instructions are followed, the results will be wrong.

To correct this condition, various options are available. Without changing the program, correct results can be obtained by revising the instructions in either of two ways:

1. instruct the user to enter hydrocarbon concentrations (in air aloft) in terms of ppmV, and "fraction vectors" in terms of volume fractions, or

2. instruct the user to enter hydrocarbon concentrations in terms of ppmC; then, instead of a "fraction vector," to apply (for air aloft only) a composite vector, where each term is the product of the carbon-based fraction (for a given hydrocarbon) times the reciprocal of the carbon number.

Alternatively, the program can be modified to accept and act correctly on concentrations and fraction vectors specified in terms of ppmC, so that the instructions as given in the EPA manual would be correct. This can be done by inserting a statement in the main program which would retrieve the necessary carbon-number values from the previously read input and apply them to the corresponding specific hydrocarbons in the necessary manner. A recommended modification is shown in Appendix B.

It appears to us that this defect exists not only in Maryland's version of OZIPM, but also in EPA's version. Therefore, we believe, both versions should be modified by one or another of the methods described above.

The fact that OZIPM yields satisfactory results when run in a "default" mode might suggest that our recommended change is unnecessary, or even undesirable. To determine why the default mode might give reasonable results despite the existence of the inconsistencies described above, we studied the default data, which are embedded in the program. We found that, when the default mode is selected, the values which the program supplies to the array which accepts the user's "fraction vector" do not in fact constitute a fraction vector, but rather form a composite vector of exactly the type described in option 2, above. Thus it appears that the OZIPM program, in either the Maryland version or the EPA version, has been adjusted in such a manner that it works correctly in the default mode (using the Dodge mechanism), but not when an alternate mechanism is inserted.

3.0 REASONS FOR SHAPE OF ISOPLETH CURVES

Study of the OZIPM output forwarded to PES by M. Jorquera of the Maryland Air Management Administration indicates to us that the isopleths produced by the computer in this instance are consistent with the proper functioning of both OZIPM and the Caltech mechanism, except for the mistake in OZIPM which we have discussed above.

Isopleth diagrams produced by the OZIPM default mechanism, and by other mechanisms used with similar assumptions, often yield sets of curves which, when interpreted three-dimensionally, exhibit a ridge of ozone maxima, diagonally directed toward the origin. The isopleth diagram derived from Maryland's trial of OZIPM exhibits no such ridge. We conclude, however, that the absence of the ridge reflects no defect in the Caltech mechanism, but rather is a consequence of the conditions assumed in the program input, together with the program inconsistency discussed above.

In the application of OZIPM in the default mode, the Dodge mechanism is used and the assumption is made that no pollutants are transported into the atmospheric mixing layer from aloft. When this is done, the resulting isopleth chart displays a ridge of peak ozone values corresponding roughly to an initial ratio (of hydrocarbons, ppmC, to NOx, ppm) of 7 to 10. This is, in effect, a ratio of these contaminants in the irradiated air which, according to the Dodge mechanism, should give higher ozone maxima than any other ratio, so long as the concentration of hydrocarbons and NOx are assumed not to increase simultaneously.

When CIT or some other mechanism is taken, rather than the Dodge mechanism, it is to be expected that a similar ridge will exist, although it may occur at some other ratio than that found with the Dodge mechanism. However, even with the Dodge mechanism, the ratio of HC to NOx for highest ozone peaks is altered if contaminant transport is taken into account. If the transported

contaminants contain hydrocarbons without NOx, the ratio in the simulated air is increased, but the axes of the isopleth diagram do not reflect this increase. As a result, the ozone ridge is displaced toward higher initial NOx values, and corresponds (in the diagram) to lower ratios of initial HC to NOx.

In the Maryland application, unlike the OZIPM default case, a substantial level of hydrocarbons transported from aloft was assumed; at the same time, NOx was assumed not to be present in the transported air. Thus, for any set of initial concentrations, the ratio (HC/NOx) in the simulated air during the hours following initiation would increase as hydrocarbons from aloft were added to the mixing layer. This would result in the displacement of the ozone ridge on the isopleth chart toward higher initial NOx values; we believe that, in the Maryland application, this displacement was great enough to shove the expected ridge completely off the diagram.

This rather large displacement of the ozone ridge in the Maryland application is caused by a combination of three circumstances, which all reinforce the effect. First, Maryland assumed rather high concentrations of hydrocarbons transported aloft; the total hydrocarbon aloft was taken as 0.7 ppmC, which was 52 percent of the total (1.36 ppmC) of initial emitted hydrocarbons and initial background hydrocarbons present in the air at the start of simulation.

Second, the effect of the transported hydrocarbons was magnified by the large quantity of air aloft which was assumed to be incorporated in the mixing layer during the day. From an initial mixing height of 225 meters, the rising inversion was assumed to lift to 1,925 meters, at which point almost 90 percent of the air in the mixing layer would have originated in the contaminated, transported air aloft.

Third, the concentration of hydrocarbons specified in the air aloft was erroneously treated by the program as if it had been given

in ppmV rather than in ppmC. The result of this was that the program interpreted the entry 0.7 to represent ppmV and took it to be equivalent to almost five times as many ppmC as Maryland intended.

The effect of these circumstances on the ratio of HC to NOx was to cause a drastic increase within a short time after the start of simulation. Examination of the Maryland OZIPM output shows that HC/NOx was about 9 at the start of simulation, but increased to 75 after one hour, 750 after 2 hours, and much higher values still as the NOx provided in the initial ground-based layer of air was depleted by reaction as well as dilution.

Under these circumstances, the extent of reaction in the photochemical system would be severely limited by the availability of NOx and the quenching effect of excess hydrocarbons. The isopleth diagram obtained by Maryland correctly reflects these conditions, showing a large sensitivity of the ozone peak to the initial NOx, but a low sensitivity to initial hydrocarbons, which represent only a minor fraction of the hydrocarbons available in the system.

PES believes that isopleth diagrams representing the same assumptions but with the use of other mechanisms (such as Dodge) would show the same general character as the one obtained by Maryland using the CIT mechanism. Isopleth diagrams have been generated by investigators at the University of North Carolina to simulate reactions in a photochemical irradiation chamber, in which atmospheric transport is not a factor, and these show the expected ozone ridges for the Caltech mechanism as well as for the Dodge mechanism and two other mechanisms which involve several classes of hydrocarbons. We therefore conclude that the Caltech mechanism is not at fault in the Maryland application of OZIPM.

4.0 REVIEW OF OZIPM CODING

A comparison of the computer coding of OZIPM as applied by Maryland with that under study by EPA has been completed. A total of 43 differences have been identified. We assume that the Maryland version was generated by modifying a program originally identical to the EPA version of OZIPM.

The modifications affect 12 segments of the program. In our judgment, they reflect two main purposes: to allow for larger dimensions needed to accommodate the CIT mechanism, and to adjust certain internal parameters in the hope of minimizing underflows and similar operational impediments during execution. However, many of the observed changes were apparently undertaken mainly to reduce redundancy and improve the logic of the underlying program.

PES found no changes that appeared inappropriate or likely to cause malfunctioning of the program. It is our opinion that the Maryland version of OZIPM, including slight alterations inserted by the Maryland agency staff as well as those made before delivery to Maryland, should be expected to execute properly and to yield isopleth curves which correctly reflect consequences of the Caltech mechanism.

A review of the specific modifications detected by our study is given in Appendix C.

5.0 CONCLUSIONS AND RECOMMENDATIONS

PES concludes that the ozone isopleths obtained by the Maryland Air Management Agency are erroneous because of a discrepancy between the actual functioning of the OZIPM program and the input instructions given in the Users Manual, which Maryland followed. This discrepancy can be easily corrected; measures for correcting it are discussed in Section 2.0.

PES further concludes that the CIT mechanism is not inappropriate for the type of simulation embodied in OZIPM, although the reaction rate factors which have been used in the CIT mechanism as applied by Maryland may not constitute an optimum set.

Finally, PES concludes that the changes made in the OZIPM computer program to accommodate the CIT mechanism and to facilitate operation on Maryland's computer system are not such as to impair the operation of the program or to cause disorder in the generation of ozone isopleth diagrams when the program is used in the ISOPLETH mode.

Recommendations resulting from this study are the following:

1. The OZIPM program and Users Manual should be revised as specified as In Appendix C. Alternatively, without modifying the program, either of two options specified in Section 2.0 may be used. These are considered less desirable than the procedure given in Appendix C because, unless carefully understood and applied, they could confuse the user and lead to other errors.

2. The selection of reaction rate factors embodied in the CIT mechanism, as given in the Users Manual, should be reviewed and, where necessary, updated.

APPENDIX A

DISCREPANCIES IN REACTION RATE FACTORS FOR CIT MECHANISM

Reaction	Maryland[a] Number	Maryland[a] Factor	UNC[b] Number	UNC[b] Factor
$HNO_4 = HO_2 + NO_2$	14	21.8	17	4.37
$OLE + OH = RO_2$	28	89,100	35	59,500
$OLE + O = RO_2 + RCO_3$	29	22,100	36	39,300
$RO = HO_2 + HCHO(RCHO)^c$	39	360,000	42	200,000
$N_2O_5 = NO_2 + NO_3$	50	8.85	10	6.85
$O_3 + HO_2 = OH$	53	3.48	25	1.50
$OLE + O_3 = products^d$	30 to 35	0.136	37, 38	0.103

[a]Source: OZIPM output provided by Maryland Air Management Administration.

[b]Source: Excerpts from draft report of University of North Carolina project, provided by Air Management Technology Branch, Office of Air Quality Programs and Standards, U.S. EPA.

[c]UNC assumes the product is RCHO.

[d]The factors cited are totals of the rate factors for all reactions attributed to the reactants, OLE and O_3.

APPENDIX B

SUGGESTED MODIFICATION TO OZIPM

The purpose of this modification is to correct an error in program MAIN, which causes concentrations of hydrocarbons in air aloft to be treated as if given in ppmV, whereas other concentrations are read as ppmC. This change will allow the program to deal correctly with all input data regarding hydrocarbon concentrations when all such data are consistently entered as ppmC.

In program MAIN, follwoing Card No. 00002940, insert the following two cards:

```
    DO 171 I = 1, JAL                              00002941
171 FALHC(I) = FALHC(I)/CARB(I)                    00002942
```

In the Users Manual for OZIPM, two notes should be added, both in connection with the TRANSPORT option in Table 1. These are as follows:

1. The TRANSPORT option must not precede the MECHANISM option, which must include the vector of carbon numbers for hydrocarbon species (as already indicated in the Manual).

2. Total hydrocarbons entrained from aloft and total initial background hydrocarbons, in the TRANSPORT option, must be entered in terms of ppmC, not ppmV.

APPENDIX C

SUMMARY OF CHANGES MADE TO OZIPM BY
JAMES TILDEN (CALIFORNIA INSTITUTE OF TECHNOLOGY)
AND BY MARYLAND AIR MANAGEMENT ADMINISTRATION

Sections modified:

MAIN	1, 2, 4, 5
PHOT	1, 2, 4, 6
RLINE	3, 4, 5
SIM	4, 5
DRIVES	6
DIFFUN	3
LINER	2, 3, 4, 5
CURVE	2, 4
ISOPLT	2, 5
BLOCK DATA	6, 1
EMIS	2
EDGMX	3

Type of change:

1. Restructure data statements

2. Initialization and dimension

3. Routing of program flow

4. Omission of statements

5. Redefinition of programs or program simplification

6. Addition of data/change of data value

HIGHLIGHTS

MAIN: 1. Data statements have been moved from main program to block data statements.

2. Redefinition of PHOT - Large Core Memory (LCM)
   variable: IPH(9)   IPH(10);
               RFCT(8)   RFCT(10)
   to include extra photolytic species

3. Addition of SNLT1 (LCM) defining XJ1 array

4. Use of MT2DNV subroutine to create/initialize XJ array as transpose of XJ1

5. Option IDIL AMIX (1) = -3 is taken care of through Blk. data default

6. Option IRDY changes made to the definition of variable RTO(I) and XNLL(JK)

PHOT: 1. Data statements placed in Blk. data

2. Redefinition of CF(45,10) and P(15,10) arrays.

3. Inclusion of CONTINUE statement at end of loop.

RLINE 1. Change to equivalence statement made by Maryland
       Equivalence (NR, NRTO), (RTO, R)
                   (NR, NRTO), (RTO, R(1))

2. Deletion of statement IFG = 0

3. Inclusion of 45-CONTINUE statement

4. Reformatting of calculation of HCG ((statement 60 to 65)) apparent assumption and simplification

5. Similar treatment of variable RHO (1, I) as in No. 4.

6. ((Statements 270 to 280)) Deletion of redefinition of HCS = TOL * HCT(3)

7. Inclusion of CONTINUE statement at 280

8. Eliimination of dummy variable OZS ((Statement 285))

SIM: 1. Changes to data definitions

2. Deletion of TDIL = 0 from text

3. Statements 55 and 70,71 omitted (IF statements used to redefine if data not in order)

4. Deletion of redefinition of variable TOT if INX·NE·-3. ((Between Statements 90 and 95)).

DRIVES: 1. Value of UROUND is changed from 7.5 E-9 to 8.0 E-7

DIFFUN: 1. Definition of I slightly modified.

2. Slight recalculating of DILU/DILUT

3. Definition of RT-R(IR) if I.EQ.0 not addressed (i.e., changes to the DO 110 loop) not significant

LINER: 1. Changes made to the placement of variables in LCMs
/NEED/ XNLL:missing
/GEARC/ HCBP:missing

2. Value of array DUM1 expanded fro DUM1(274) to DUM1(294)

3. Deletion of initialization statement RPL (I, J) = -9 and loop

4. Deletion of several cards to print a new line if condition OZP(LS).LT.OC(4)

5. Restructure statements 85 NR1 = NR and definition clause NR1 = NR-1 that follows

6. Restructuring between statements 90 and 100 variables changed include: UNDIFF

7. Omission of definition of U(K) = HCBP(I) and V(K) = 0. ((Statements between 150 and 151))

8. Deletion of several lines of code calling curve production if U(IJ) and V(IJ)<0.0 code is used to redefine parameters for plotting the curve.

CURVE: 1. Exclusion of common statements with LCM /NEED/ and associated variables

           2. Deletion of statements preventing the calling of subroutines VVLBLF and VVLBLC under variable USX or USY out-of-bound conditions

ISOPLT: 1. Changes made to the dimensional sizes of variables DUM2 and DUM3

           2. Deletion of statement included to prevent definition of DUM(3), NR1 if (NPTO.NE.0)

BLOCK   1. Inclusion of value RONO (photolytic species name) in the
DATA   SPEC array

           2. Changes made to UROUND

           3. Inclusion of equivalence statements defining XJ1A to XJ1E

           4. Restructuring the data specification in those arrays. Also restructuring the SIGMA, PHI, and IW1 arrays.

EMIS: 1. Change size of variables dimensions
               EM(15) to EM(11)
               EC(58) to EC(38)
               IFLAG(15) to IFLAG(11)

EDGMX: 1. Exclusion of escape clause in DO 5 loop if conditions are not met

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16 ABSTRACT

The assignment was to study the functioning of a photochemical air quality simulation model which, in a test application, appeared to yield unsatisfactory ozone isopleth curves; to determine the cause of the problem and overcome it.

A major cause of the problem was found to consist in a discrepancy between the instructions given in the Users Manual and the actual functioning of the OZIPM program. A method of correcting the discrepancy is recommended, and alternative measures are discussed.

In a separate line of inquiry the possibility that the chemical mechanism used ("Caltech" mechanism) might be at fault was investigated. Results showed that isopleth curves based on the mechanism were similar in character to those based on other complex chemical mechanisms.

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