# USER'S GUIDE TO THE OZONE TOOL:

# OZONE SOURCE APPORTIONMENT TECHNOLOGY FOR UAM-IV

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# 1. INTRODUCTION

## Background

Photochemical grid models, such as the Urban Airshed Model (UAM), are used to design control strategies for reducing emissions of volatile organic compounds (VOCs) and nitrogen oxides ($NO_X$) emission to achieve ozone air quality standards. Developing an effective ozone attainment strategy involves many cycles of changing the emission inventory and then re-running the photochemical grid model to determine which geographical source areas, source categories, and pollutant types (i.e., VOC and $NO_X$) should be controlled to effectively reduce ozone. This process may be thought of as laboriously mapping out the relationships between ozone and groups of emission sources by means of a long series of sensitivity tests. Because photochemical grid model simulations are computionally demanding, not all permutations of controls can be analyzed by this approach and the potential exists for controlling sources that contribute little to the high ozone concentrations or, conversely, not controlling sources that do contribute significantly. The ozone source apportionment technology (OSAT) for UAM (the Ozone Tool)[1] has been designed to address this issue by providing modelers with a means of estimating the contributions multiple of source areas/categories/types to ozone formation in a *single model run*. Since the cost-effectiveness of control strategies may be enhanced in some cases by temporally targeting the control measure, the Ozone Tool also includes a methodology for diagnosing the temporal relationships between ozone and emissions from groups of sources. The capabilities of the Ozone Tool are summarized below along with an assessment of the strengths and limitations of the approach. Some familiarity with the concepts of photochemical grid modeling (NRC, 1991) and the UAM (EPA, 1990) is assumed.

The main challenges in developing and implementing a methodology to track the spatial and temporal relationships between separate groups of emission sources and ozone formation are:

- Accounting not only for the presence of ozone precursors from a given source region at a given receptor location, but also accurately estimating the cumulative contribution to ozone production of those precursors while they were en-route to the receptor.

- Insuring compatibility with the underlying UAM formulation so that derived source-receptor relationships will be consistent with UAM response to emission changes.

- Providing sufficient spatial and temporal resolution while managing, within practical constraints, the computer resources required to run the software tool.

## Capabilities of the Ozone Tool

The Ozone Tool uses multiple tracer species to track the fate of ozone precursor emissions (VOC and $NO_X$) and the ozone formation caused by these emissions within a UAM simulation. The tracers operate as spectators to the normal UAM calculations so that the underlying UAM predicted relationships between emission groups (sources) and ozone concentrations at specific

[1]The Ozone Tool contains code copyrighted by SAI and ENVIRON, all rights reserved.

locations (receptors) are not perturbed. Tracers of this type are conventionally referred to as "passive tracers," however it is important to realize that the tracers in the Ozone Tool track the effects of chemical reaction, transport, diffusion, emissions and deposition within the UAM. In recognition of this, they are described here as "ozone reaction tracers." The ozone reaction tracers allow ozone formation from multiple "source groupings" to be tracked simultaneously within a single simulation. A source grouping can be defined in terms of geographical area and/or emission category. Figure 1-1 provides an example of the way that a UAM domain can be sub-divided into multiple source areas -- 17 in this example. Also, the emission inventory could be sub-divided into several source categories -- two emission categories over 17 source regions would produce 34 separate source groupings. So that all sources of ozone precursors are accounted, the UAM boundary conditions and initial conditions are always tracked as separate source groupings. The methodology is designed so that all ozone and precursor concentrations are attributed among the selected source groupings at all times. Thus, for all receptor locations and times, the ozone (or ozone precursor concentrations) predicted by the UAM are attributed among the source groupings selected for the Ozone Tool run. The methodology also estimates the fractions of ozone arriving at the receptor that were formed en-route under VOC- or $NO_X$-limited conditions. This information indicates whether ozone concentrations at the receptor will respond more to reductions in VOC or $NO_X$ precursor emissions.

In addition to using ozone reaction tracers to apportion ozone formation, the Ozone Tool uses separate families of timing tracers to allow source-receptor transport times to be estimated. Unique timing tracers are released from each geographical area selected for ozone source apportionment. Thus, if the ozone formation tracers show that emissions from a given source area contributed to ozone at any receptor of interest, the timing tracers can then be used to estimate the time at which the emissions were released. This provides a way of investigating temporal features of the source-receptor relationships and even developing temporally targeted control strategies.

An example display of ozone source apportionment information provided by the Ozone Tool is shown in Figure 1-2. The figure shows information for the location of the region wide maximum hourly average ozone concentration (the hourly peak) for an example Ozone Tool run (this run had 17 geographical source areas as shown in Figure 1-1 and a single emission group). Summary information for scenario and receptor is shown in the center. At top left, a bar chart shows how the total amount of ozone was attributed between initial conditions, boundary conditions and emissions, with the emissions contribution being divided between ozone formed under VOC and $NO_X$ limited conditions. At top right, a pie chart shows the relative ozone contributions from initial conditions, boundary conditions and emissions, with the emissions contributions broken out by numbered geographical source areas. Only the source areas with the largest ozone contribution are shown, the remaining source areas are lumped together under "All Others." At bottom, there is a tabular summary of ozone contributions underlying the charts at the top. The tabular summary also shows the estimated release times for the emissions from different source areas impacting the receptor (under the "Time Emitted" column). The release times are estimated using the timing tracers. The timing tracers are also used to estimate whether there is more than one significant source-receptor pathway between each source area and the receptor, i.e. if timing tracers of different ages from the same source area are present at the receptor it is likely that recirculation of emissions is occurring. The display shown in Figure 1-2 is only one of many ways in which the Ozone Tool results can be displayed to gain insight into ozone source-receptor

relationships predicted by the UAM. Figure 1-2 is shown here to illustrate the types of information available. Displays like Figure 1-2 are generated using the post-processing software described in section 4.

The intended purpose of the Ozone Tool is to aid in the design of optimally effective ozone control strategies. Displaying the ozone source apportionments estimated by the Ozone Tool shows clearly the major source groupings contributing to high ozone levels so that control strategies can focus on these sources.

**Strengths and Limitations**

An important feature of the ozone reaction tracer approach used in the Ozone Tool is that the normal UAM calculations are not perturbed. Thus, the Ozone Tool estimates the same ozone and precursor concentrations as the standard UAM. Further, since the same inputs are used for meteorology, emissions etc., and the same numerical methods are employed throughout the model, the source-receptor relationships developed by the Ozone Tool inherently have a high degree of consistency with those present in the standard UAM. (Source-receptor relationships are present within standard UAM simulations, they just are not readily apparent and can only be discerned by observing the response of the UAM to a perturbation in inputs). The level of consistency between the source-receptor relationships developed by the Ozone Tool and the standard UAM is limited by three factors:

- The completeness of the conceptual methodology underlying the source apportionments
- The limitations of the numerical methods employed by UAM
- The non-linear nature of the ozone formation process

The completeness of the source apportionment methodology was evaluated by performing a series of evaluations of Ozone Tool results against UAM sensitivity tests (Yarwood et al. 1996). These tests showed that the Ozone Tool performed well in predicting both the spatial area of impacts of emissions from given source regions and the relative contributions of separate emission regions/groups to ozone.

The Ozone Tool cannot overcome numerical limitations inherent to the UAM (as well as other gird models) since it is based on the UAM. The evaluation tests referred to above suggested that a potential serious numerical limitation in UAM is the Smolarkeiwicz horizontal advection solver (Smolarkeiwicz, 1982). As discussed below, the numerical limitations of the Smolarkeiwicz algorithm are addressed in the Ozone Tool design, and we believe that they probably pose greater problems for the use of UAM in conventional control strategy evaluations than for the Ozone Tool (Yarwood et al., 1996). The preferred option would be to move on to a more robust advection solver in UAM, as discussed by Odman et al. (1996) for example.

The biggest limitation of this, or any other, ozone source apportionment approach likely results from the third factor mentioned above: namely, the non-linear nature of the chemical interactions between emissions from different source groupings means that as soon as the emission inventory is perturbed, the source receptor relationships begin to change. Thus, the Ozone Tool can only

estimate the contribution to ozone from a specific source grouping under the current emissions scenario. The Ozone Tool cannot directly quantify the ozone reductions that will result (in UAM) from an emission control strategy because the UAM response may well be non-linear with the magnitude of the control applied (e.g. 20 percent or 60 percent control) and the presence/absence of other simultaneous controls on other source groupings. However, this fundamental truth of photochemical modeling does not limit the usefulness of the Ozone Tool: arguably it increases the usefulness. At any rate, it suggests the following approach to control strategy development with the Ozone Tool. For the base UAM scenario, the Ozone Tool could be used to identify specific source groupings for which ozone reductions from emissions controls would be maximized. Just as important, the Ozone Tool will identify source groupings for which emissions controls are not effective at reducing ozone concentrations. The most effective and feasible control measures identified in this way can be applied to the emission inventory, leading to a revised UAM scenario with different (lower) emissions. If additional controls are needed, the Ozone Tool could be applied again to identify the most effective control measures under the new conditions. Development of the control plan will still proceed by an iterative process, but the Ozone Tool can be used to guide the process to develop (and justify) more refined, better targeted and more cost-effective ozone control strategies.

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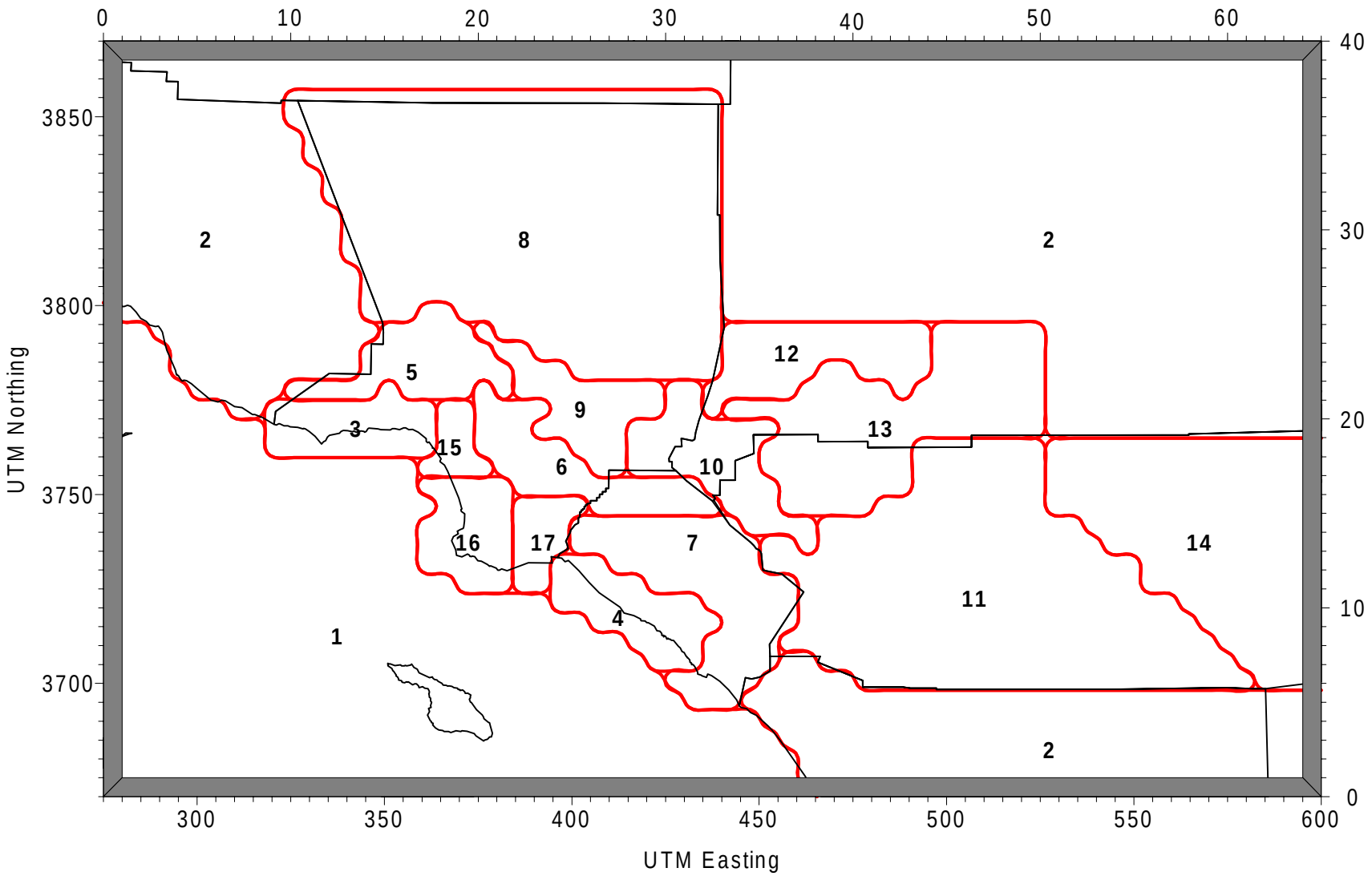
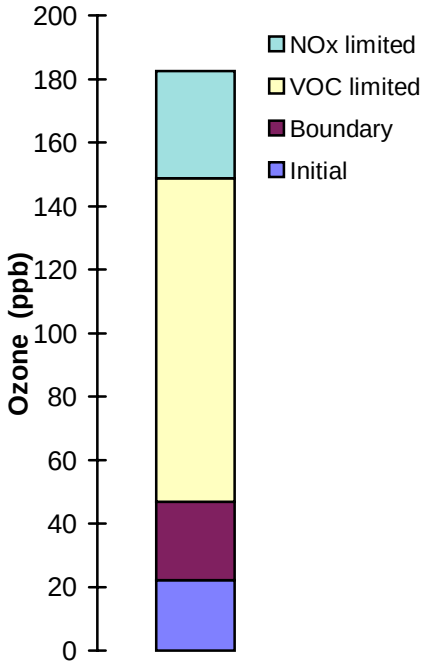
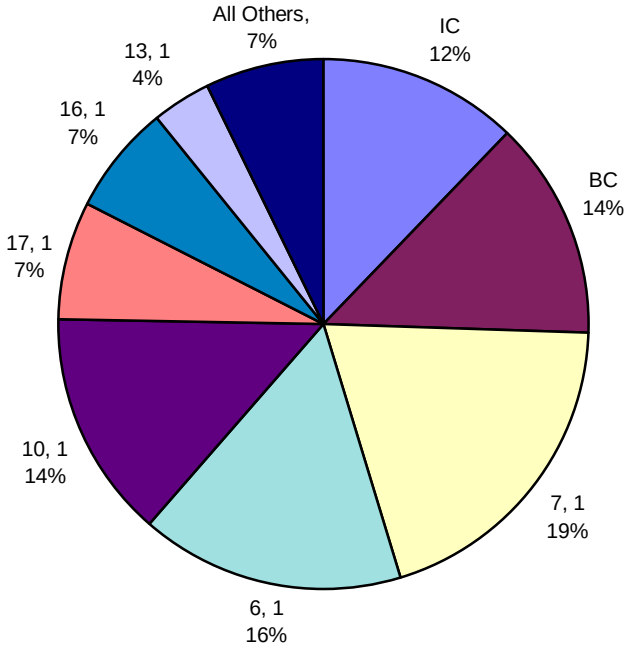



**Figure 1-1.** Example of the sub-division of a UAM domain into separate areas for geographic source apportionment.

Contributions By Type




Contributions By Source Area




| | | |
|---|---|---|
| **Receptor** | **=** | **HourlyPeak** |
| **Time** | **=** | **16 To 17** |
| **Date** | **=** | **8/28/87** |
| **Scenario** | **=** | **Evaluation Test** |
| **Total Ozone** | **=** | **183 ppb** |

Detailed Ozone Apportionment

| *Source Area* | *Emission Group* | *Percent Ozone from NOx* | *VOC* | *Total* | *Time Emitted* | *Recirculation Likely* |
|---|---|---|---|---|---|---|
| IC | | | | 12% | | |
| BC | | | | 14% | | |
| 7 | 1 | 3% | 17% | 20% | 8/28 5 am | No |
| 6 | 1 | 4% | 13% | 16% | 8/28 6 am | No |
| 10 | 1 | 7% | 7% | 14% | 8/28 7 am | No |
| 17 | 1 | 1% | 6% | 7% | 8/27 1 pm | No |
| 16 | 1 | 1% | 6% | 7% | 8/27 6 am | No |
| 13 | 1 | 2% | 1% | 4% | 8/28 2 pm | No |
| All Others | | | | 7% | | |

**Figure 1-2.** Example display of ozone source apportionment information provided by the Ozone Tool for a run with 17 source areas (as shown in Figure 2-1) and 1 emission group.

# 2. MODEL FORMULATION

The UAM has been extended to accommodate extra tracer species needed to perform ozone source apportionment. For each user specified source grouping (geographical area/emissions category) there are two distinct types of tracer species, "timing tracers" and "ozone reaction tracers." The timing tracers are used to track the temporal relationships between precursor emissions and ozone formation. The ozone reaction tracers track the fate of ozone precursors ($NO_X$ and VOC) emissions from each source grouping plus the ozone formation attributed to those emissions. The methodology requires that all ozone precursors be tracked so that all contributions to ozone can be accounted for, thus ozone and precursors originating from the model boundary and initial concentrations are also tracked as separate source groupings (however, no timing tracers are allocated to the initial or boundary conditions).[1] The following sections describe the methodologies employed for the timing and ozone reaction tracers.

## TIMING TRACERS

There are two types of "timing" tracers called inert and decay-companion tracers. Inert and decay-companion tracers are used in tandem to identify the age of emissions from any source area. Timing tracers are emitted into every surface grid cell at a constant rate. Timing tracers have unique names that identify the source area in which they were released. After release, the decay-companion tracers decay exponentially with a constant lifetime. Since the inert and decay-companion tracers are affected identically by transport and diffusion, differences in predicted concentrations between the two are due only to the first-order decay of the decay-companion tracer. The presence of inert tracer from a given source area (A) at a receptor (B) indicates that a transport pathway exists from A to B. The amount of tracer decay that has occurred since release (i.e. the ratio of the decay companion tracer to its matched inert tracer) can be used to calculate the transport time from A to B and therefore the time period during which emissions at source area A can potentially impact receptor B.

To resolve ambiguities in timing calculations that could result from wind flow reversals (e.g., land/sea breezes) or other recirculation patterns, new sets of inert and decay-companion tracers can be released at user specified time periods. When a new set of timing tracers (i.e. one pair for each source area) is released, emissions of the previous set cease. Old timing tracers are still carried in the model to track emissions from those source areas and time period as they age. Thus, as a simulation progresses the number of timing tracers being carried increases as new sets are released. The names of timing tracer species identify the species type and source area/time period in which the tracer was released:

$I_{i,t}$ = Inert timing tracer for region *I* and time period *t*. Emitted at a constant rate during that time period.

[1]The implementation of timing tracers and ozone reaction tracers is independent, and the model supports the option of running with only ozone reaction tracers if temporal resolution is not required.

$D_{i,t}$ =Decay companion timing tracer for region *I* and time period *t*. Emitted at a constant rate during that time period. Decays exponentially with a constant lifetime of 12 hours after release.

This method is more computationally efficient than the simpler alternative of releasing non-decaying tracers many short time periods, since the latter approach would rapidly lead to an impossibly large number of tracers.

## OZONE REACTION TRACERS

The second category of tracers are called "ozone-reaction" tracers. There are four ozone-reaction tracers per source area to account for the contributions of emissions of separate source areas to the complex process of the ozone formation activity. It is important to recall that the mass of $NO_X$ or VOC from a given source area that may be present at a given receptor at a selected hour is often not particularly relevant to the amount of ozone present there at that time. Rather, it is the contribution to ozone formation activity of source areas' $NO_X$ and VOC emissions en-route to a receptor that must be determined. The ozone-reaction tracers are designed to integrate these en-route contributions to ozone production/destruction activity.

Ozone formation involves both $NO_X$ and VOCs, and the $NO_X$ and VOCs participating in ozone formation in any particular grid cell/time step may have originated from different source groupings. The ozone formation process can be controlled more by the availability of VOCs or $NO_X$ depending upon the relative abundance of both precursors and ozone formation is described either as VOC limited or $NO_X$ limited, respectively. When ozone production at a given location and time is $NO_X$ limited it makes sense to attribute ozone production to source groupings based on their contributions to the local $NO_X$ and similarly to allocate based on VOC contributions when ozone formation is VOC limited. Consequently, separate tracers are used to track ozone formation occurring under $NO_X$ and VOC limited conditions. The criterion used to determine whether ozone formation is occurring under locally $NO_X$ or VOC limited conditions is described in detail in a separate section below.

The four types of ozone-reaction tracers that are tracked for each source grouping (i.e., geographic area/source category, boundary conditions or initial conditions) are explained below. The name of each tracer uniquely identifies the source grouping it represents:

$N_i$ = $NO_X$ tracer for source grouping *I*. Emitted with the same spatial and temporal distribution as $NO_X$ emissions for source grouping *I*. Decays with local $dNO_X/dt$ for each grid cell/time step.

$V_i$ = VOC tracer for source grouping *I*. Emitted with the same spatial and temporal distribution as VOC emissions for source grouping *I*. Decays with local dVOC/dt for each grid cell/time step. Note that VOC tracers are defined as single carbon species, so their concentrations are numerically equal in ppb and ppbC units.

$O3V_i$ = Tracer of ozone formation under VOC limited conditions attributed to source grouping *I*. If ozone formation is determined to be VOC-limited for a given grid cell/time step, $O3V_i$ is formed in proportion to local $dO_3/dt$ in proportion weighted by the distribution of VOC precursors ($V_i$).

$O3N_i$ = Tracer of ozone formation under $NO_X$ limited conditions attributed to source grouping *I*. If ozone formation is determined to be $NO_X$-limited for a given grid cell/time step, $O3N_i$ is formed in proportion to local $dO_3/dt$ in proportion weighted by the distribution of $NO_X$ precursors ($N_i$).

The methods by which ozone reaction tracers are treated in the separate components of the UAM are described in detail below.

**Mass Consistency with UAM**

The ozone reaction tracer methodology was designed to be inherently mass consistent with UAM. In other words, the sums of the $NO_X$, VOC and ozone tracers should remain consistent with their standard UAM counterparts as follows:

$$\Sigma\ N_i = NO + NO2$$

$$\Sigma\ V_i = \Sigma\ CBM\text{-}IV\ VOCs$$

$$\Sigma\ O3V_i + \Sigma\ O3N_i = O3$$

The validity of these relationships was tested and evaluated and it was found that the chemistry, emissions, deposition and vertical transport/diffusion algorithms maintained mass consistency on an overall and cell by cell basis. However, it was found that the horizontal advection/diffusion algorithm (Smolarkiewicz, 1983) inherently maintained mass consistency on an overall basis, but not a cell by cell basis. Accordingly, the horizontal advection/diffusion algorithm for the ozone reaction tracers was modified as described below to maintain mass consistency.

**Emissions**

The tracer families, $N_i$ and$V_i$, track $NO_X$ and VOC emissions from each source grouping to allow attribution of ozone formation as it occurs throughout UAM. The rates of emission of the $N_i$ and $V_i$ tracers are set equal to the total $NO_X$ and VOC emissions in the inventory for a source grouping, respectively. For the $V_i$ tracers, the emissions are set equal on a ppmC basis. For the initial condition (IC) source grouping, the $N_{IC}$ and $V_{IC}$ tracers are initialized from the UAM initial concentration fields and receive no more mass input after the start of the simulation. For the boundary condition (BC) source grouping, the fluxes of $NO_X$ and VOC entering the UAM from the boundaries are effectively interpreted as emissions of the $N_{BC}$ and $V_{BC}$ tracers at the model boundaries. Unlike emission source groupings, boundary and initial conditions also introduce ozone directly into the UAM. Since there is no way of determining whether the ozone in the boundary and initial conditions was formed under VOC or $NO_X$ limited conditions, this ozone is

divided equally between O3N and O3V tracers. However, subsequent ozone formation within UAM from boundary and initial condition VOCs and $NO_X$ is allocated to O3V and O3N tracers based on whether ozone formation occurred under VOC or $NO_X$ limited conditions (discussed below).

**Deposition**

The $N_i$, $V_i$, $O3N_i$ and $O3V_i$ tracers are deposited at rates determined by the standard UAM deposition calculation on a surface grid cell by grid cell basis. For $NO_X$, the deposition velocity for each tracer $N_i$ [VD( $N_i$)] is set equal to the concentration weighted average of the deposition velocities for NO and $NO_2$:

$$VD(N_i) = \frac{NO * VD(NO) + NO_2 * VD(NO_2)}{NO + NO_2} \quad (1)$$

Similarly, the deposition velocity for each tracer $V_i$ is set equal to the concentration weighted average of the deposition velocities for the CBM-IV VOC species (the concentration weighting is performed on a ppmC basis). The deposition velocity for the O3N and O3V tracers is set equal to the ozone deposition velocity.

**Transport and Diffusion**

The $N_i$, $V_i$, $O3N_i$ and $O3V_i$ tracers are transported and diffused by the standard UAM algorithms. As mentioned above, testing of the Ozone Tool showed that the UAM horizontal advection and diffusion algorithm (Smolarkiewicz, 1983) did not accurately preserve the spatial relationships between ozone reaction tracers and their corresponding UAM species (e.g. between the sum of the O3V and O3N species and UAM O3). The distortion in any one model time-step was small, but the distortion built up over time to unacceptable levels. The discrepancies were identified as arising from the Smolarkiewicz algorithm, and the finding was not surprising in light of the well known limitations of the Smolarkiewicz algorithm Odman et al., 1996; Chock and Winkler, 1994). The preferred solution to this problem would be to use an alternative, more accurate, numerical algorithm to solve the horizontal advection and diffusion. However, a more accurate numerical method would change the predictions for the regular UAM species making the predictions of the Ozone Tool different than standard UAM. Such an outcome was inconsistent with the objectives in developing the Ozone Tool, so an alternative approach was adopted. After completing each horizontal transport operation for the ozone reaction tracers (i.e., advection and diffusion along a single row/column of cells) the ozone reaction tracer concentrations were renormalized to be consistent with the standard UAM concentration fields. The effect of the renormalization is to change slightly the diffusivity of individual tracer species along the row/column. The renormalization is implemented in a single subroutine (RECALIB). If, in the future, a more accurate horizontal advection algorithm is implemented in UAM, the renormalization can be removed by simply removing RECALIB.

**Chemical Change**

The $N_i$ tracer mass in each grid cell at each time step decays according to the chemical change in the UAM predicted $NO_X$ ($\Delta NO_X$) weighted by the tracer contribution to the total of $NO_X$ tracers from all source groupings:

$$N_i = N_i + \Delta NO_X * \frac{N_i}{\Sigma N_i} \quad (2)$$

The $V_i$ tracer mass in each grid cell at each time step decays according to the chemical change in the UAM predicted VOC ($\Delta$VOC) weighted by the tracer contribution to the total of VOC tracers from all source groupings. However, because the reactivity of VOCs from different source groupings can be different, a weighting factor based on the OH-reactivity of each V tracer ($kOH_i$) is also introduced. The $kOH_i$ for each source grouping is calculated at the start of each simulation period (typically one day) by averaging the OH rate constants of the speciated VOC emissions for each source grouping. The V tracer mass in each grid cell at each time step decays at a rate determined by the following equation:

$$V_i = V_i + \Delta VOC * \frac{V_i * kOH_i}{\sum_i (V_i * kOH_i)} \quad (3)$$

The O3N and O3V tracers each source grouping accumulate a weighted fraction of the ozone production/destruction activity ($\Delta O_3$) that occurs in each grid cell at each time step. The process of apportioning $\Delta O_3$ across O3N and O3V tracers occurs as follows:

1. Determine whether the local (grid cell/time step) ozone production process is $NO_X$ or VOC limited. As described in detail below, the determination is based on the ratio of the local $HNO_3$ and $H_2O_2$ production rates. If the $H_2O_2$ /$HNO_3$ production ratio is greater than 1/3 during a time step, then ozone formation is $NO_X$ limited. If this ratio is less than or equal to 1/3, then ozone formation is VOC limited.

2. If $\Delta O_3$ is positive (i.e. ozone is produced) under conditions determined to be:

   (a) $NO_X$ limited

$$O3N_i = O3N_i + \Delta O3 * N_i / \Sigma N_i \quad (4)$$

   (b) VOC limited

$$O3V_i = O3V_i + \Delta O3 * \frac{V_i * kOH_i}{\sum_i (V_i * kOH_i)} \quad (5)$$

3. If $\Delta O_3$ is negative (i.e. ozone is chemically destroyed)

$$O3X_i = O3X_i + \Delta O3 * X_i / \Sigma X_i \quad (6)$$

Where X = N and V

**Distinguishing VOC-Limited from $NO_X$-Limited Ozone Formation**

The classic trajectory model EKMA diagram can be used to distinguish VOC-limited from $NO_X$-limited trajectories and develop a classification based on initial VOC-to-$NO_X$ ratio. However, this approach classifies VOC- or $NO_X$-limited behavior based on response the of the peak ozone, which is the net response of a several hours photochemistry. In reality, many of the trajectories start out VOC-limited and become $NO_X$-limited during the course of the day essentially because the $NO_X$ is depleted more rapidly than the VOC. For the Ozone Tool, a more fundamental indicator of the instantaneous state of ozone formation with regard to VOC- or $NO_X$-limitation is required.

The sensitivity of ozone formation to VOCs and $NO_X$ at any given time is attributable to the fate of radicals. The radical pool is often referred to as odd-hydrogen ($HO_X$) and is most usefully considered as the sum of OH, $HO_2$ and $RO_2$ radicals. When $NO_X$ is plentiful, the main radical termination (i.e., $HO_X$ removal) pathway is nitric acid formation, i.e.:

$$OH + NO_2 (+M) \rightarrow HNO_3 (+M) \quad (7)$$

Under these conditions, ozone formation is limited by the rate at which radicals can be formed, which is generally described as the VOC-limited condition. Thus nitric acid ($HNO_3$) production is indicative of plentiful $NO_X$ and VOC-limited ozone formation.

When $NO_X$ is scarce, radical-radical reactions dominate $HO_X$ removal, e.g.:

$$HO_2 + HO_2 (+M) \rightarrow H_2O_2 + O_2 (+M) \quad (8)$$

$$HO_2 + RO_2 \rightarrow ROOH + O_2 \quad (9)$$

Under these conditions, ozone formation is limited by the availability of NO to react with $HO_2$ and $RO_2$ radicals, which is described as the $NO_X$-limited condition. $HO_2$ and $RO_2$ radicals that do not react with NO participate in peroxide formation. Thus, peroxide formation ($H_2O_2$ = hydrogen

peroxide, or ROOH = organic hydroperoxides) is indicative of scarce $NO_X$ and $NO_X$-limited ozone formation.

Sillman (1995) has exploited this situation to develop useful indicators of VOC vs. $NO_X$ limited ozone formation based on the ratio of peroxide production to nitric acid production. Sillman proposed that the transition between these conditions occurs when:

$$(P_{H2O2} + P_{ROOH}) / P_{HNO3} = 0.5 \quad (10)$$

The production rates of nitric acid ($P_{HNO3}$) and hydrogen peroxide ($P_{H2O2}$) in each UAM grid cell at each time step are readily accessible, but the production rate of organic peroxides ($P_{ROOH}$) is not readily accessible because the CBM-IV mechanism does not explicitly track these species. The balance between $P_{ROOH}$ and $P_{H2O2}$ depends upon the relative production of $HO_2$ and $RO_2$ radicals, and Sillman suggests that it is not highly variable within/across simulations. Accordingly, he proposes that equation (10) is equivalent to a transition point of:

$$P_{H2O2} / P_{HNO3} = 0.35 \quad (11)$$

In other words, when this ratio exceeds 0.35 ozone formation is $NO_X$-limited, and when this ratio is less than 0.35 ozone formation is VOC-limited.

**Evaluation of Sillman's ($P_{H2O2} / P_{HNO3}$) Indicator**

Equation (11) was evaluated as an indicator of VOC vs. $NO_X$-limited ozone formation for several trajectory model scenarios using the CBM-IV mechanism as implemented in the UAM.[2] The ozone concentration for a scenario with an initial VOC/$NO_X$ ratio of 10 (0.3 ppmC of VOC, 30 ppb of $NO_X$) is shown in 2- 1. Also plotted, against the right axis, is the ratio ($P_{H2O2} / P_{HNO3}$).

Sillman's proposed ($P_{H2O2} / P_{HNO3}$) transition point of 0.35 is shown by the dashed line. Before about 12 noon, ($P_{H2O2} / P_{HNO3}$) is less than 0.35 indicating VOC-limited ozone formation, whereas from about 12 noon to 7 p.m. ($P_{H2O2} / P_{HNO3}$) exceeds 0.35 indicating $NO_X$-limited ozone formation. After 7 p.m., ($P_{H2O2} / P_{HNO3}$) falls below 0.35 again, but this is after the ozone peak when ozone is decreasing and the concepts of VOC and $NO_X$-limitation are no longer relevant.

In summary, the ($P_{H2O2} / P_{HNO3}$) indicator suggested a transition from VOC to $NO_X$-limited ozone formation at about noon. To investigate whether this prediction is corroborated by responses to emission controls, the trajectory model scenario was re-run with 30 percent reductions in initial concentrations and emissions of VOC and $NO_X$ (Figure 2-2). Figure 2-2 shows that $NO_X$ controls started to be effective at about noon whereas VOC controls had maximum effect before noon. This finding is even clearer in Figure 2- 3, which shows the difference in ozone (control-base) for the reduced VOC and $NO_X$ cases. Thus, the response of ozone to reducing VOC and $NO_X$ was found to be consistent with the prediction of the ($P_{H2O2} / P_{HNO3}$) indicator.

[2] The scenarios begin at sunrise at 6 a.m. with 10 ppb of $O_3$ plus initial VOCs and $NO_X$. There is no dilution, and 5 percent of the initial VOCs and $NO_X$ are added in each hour as emissions.

The evaluation described above and shown in Figures 2-1 through 2-3 was repeated for two more scenarios with different base VOC/$NO_X$ ratios. The results for a base VOC/$NO_X$ ratio of 20 (0.3 ppmC of VOC, 15 ppb of $NO_X$) are shown in Figure 2-4, and for a base VOC/$NO_X$ ratio of 5 (0.15 ppmC of VOC, 15 ppb of $NO_X$) are shown in Figure 2-5. For a base VOC/$NO_X$ ratio of 20 Figure 2-4a shows that the transition from VOC to $NO_X$-limited ozone formation is predicted to occur at about 9:30 a.m. Figure 2-4b shows that this is confirmed by the response to VOC and $NO_X$ controls. For a base VOC/$NO_X$ ratio of 5, Figure 2-5a shows that ozone formation is predicted to remain VOC-limited throughout the day. Figure 2-5b confirms this by showing no net benefit from $NO_X$ control throughout the day.

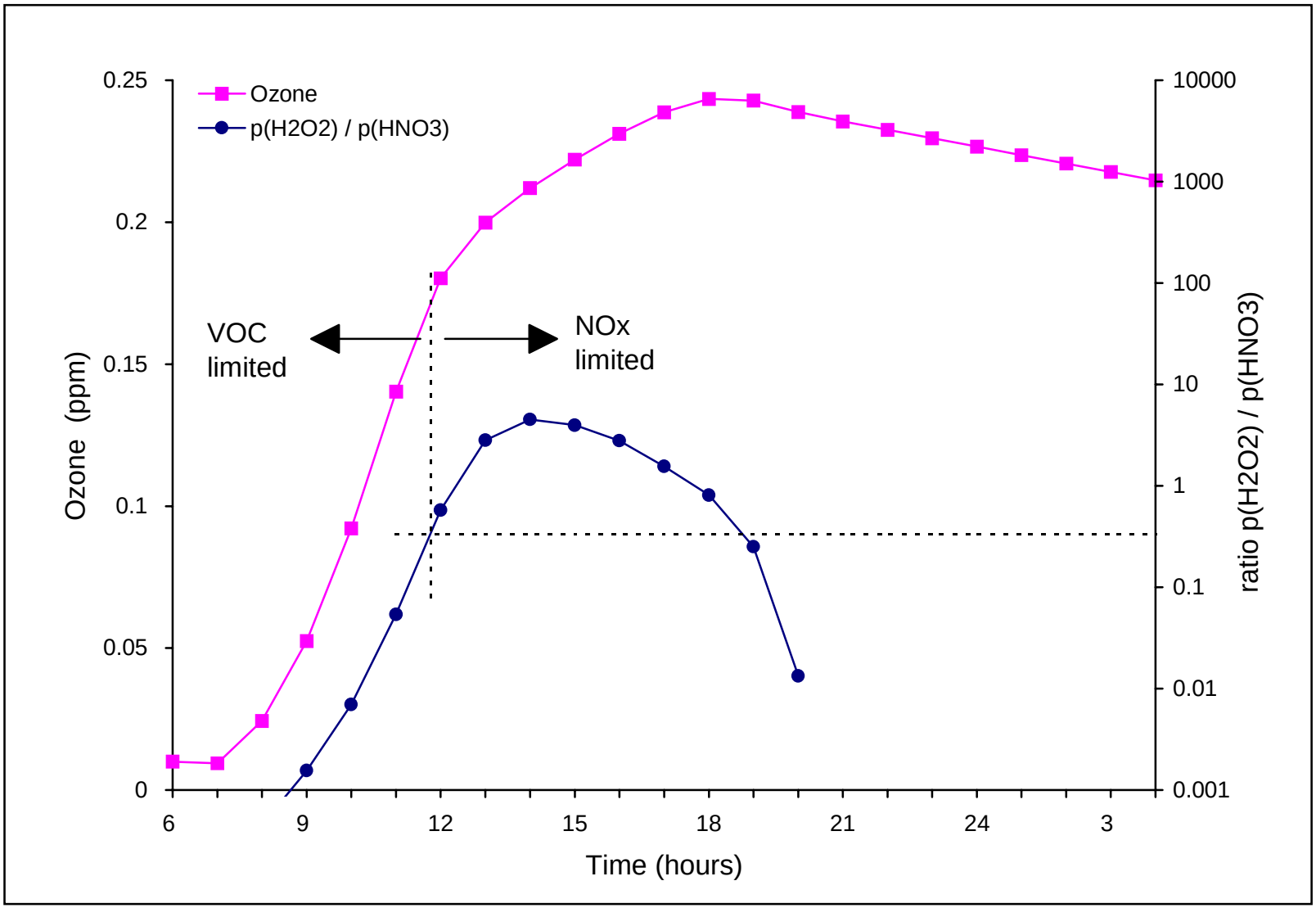



**Figure 2-1**. Box model simulation to evaluate $P_{H202}/P_{HNO3}$ indicator for VOC vs. $NO_X$ limited ozone formation (see text). Ozone is plotted against the left axis, $P_{H202}/P_{HNO3}$ is plotted against the right axis. For PH202/PHNO3 below 0.35 ozone formation is VOC limited. Thus, the transition form VOC to NOx limited ozone formation is predicted to occur about 12 noon. **Initial VOC/$NO_X$ = 10:1.**

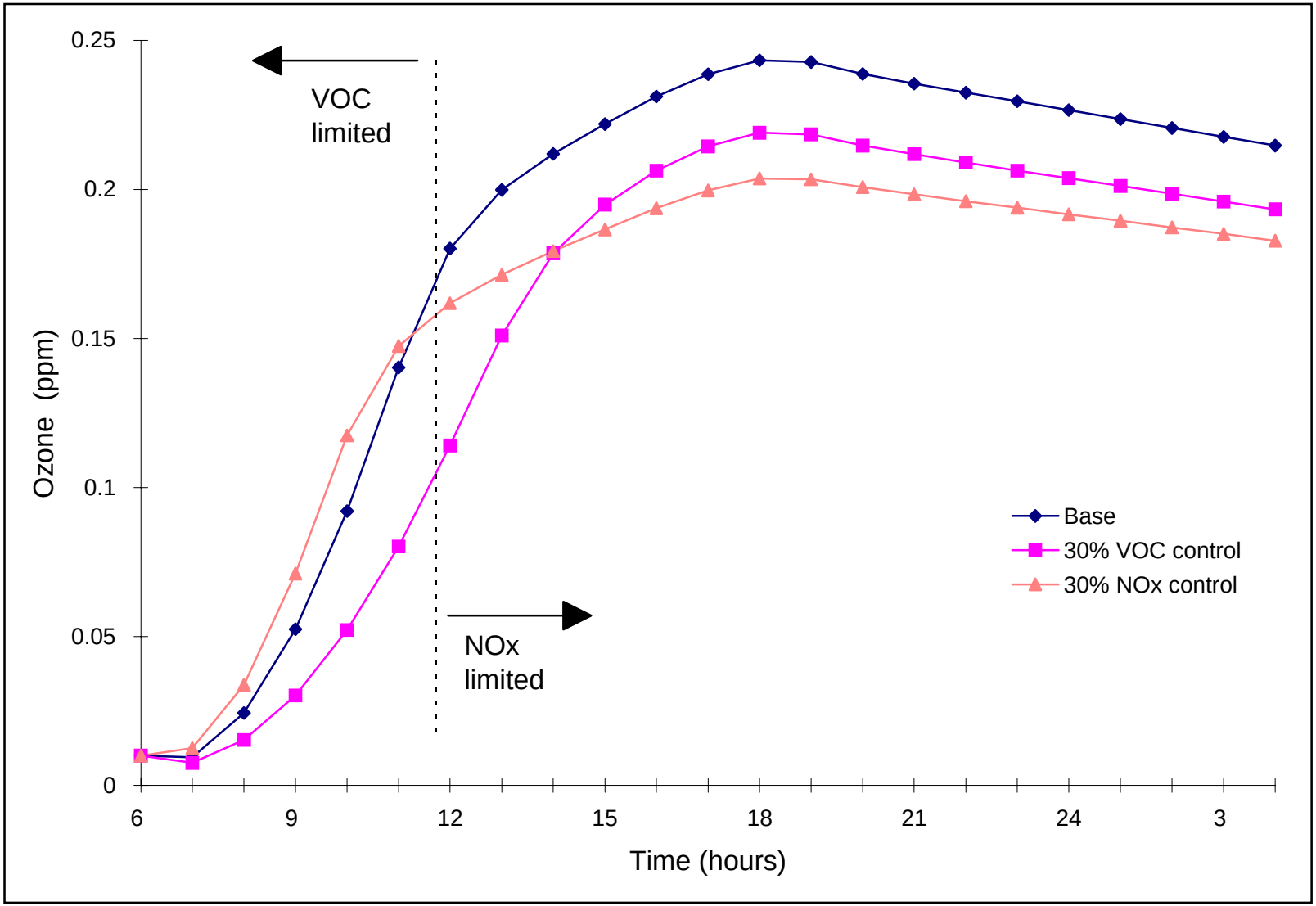



**Figure 2-2.** Effect on ozone of controlling VOC and $NO_X$ by 30 percent for the base scenario shown in Figure 2-1. The vertical dashed line shows the transition form VOC to $NO_X$ limited ozone formation for the base case derived in Figure 2-1. **Initial base case VOC/$NO_X$ = 10:1.**

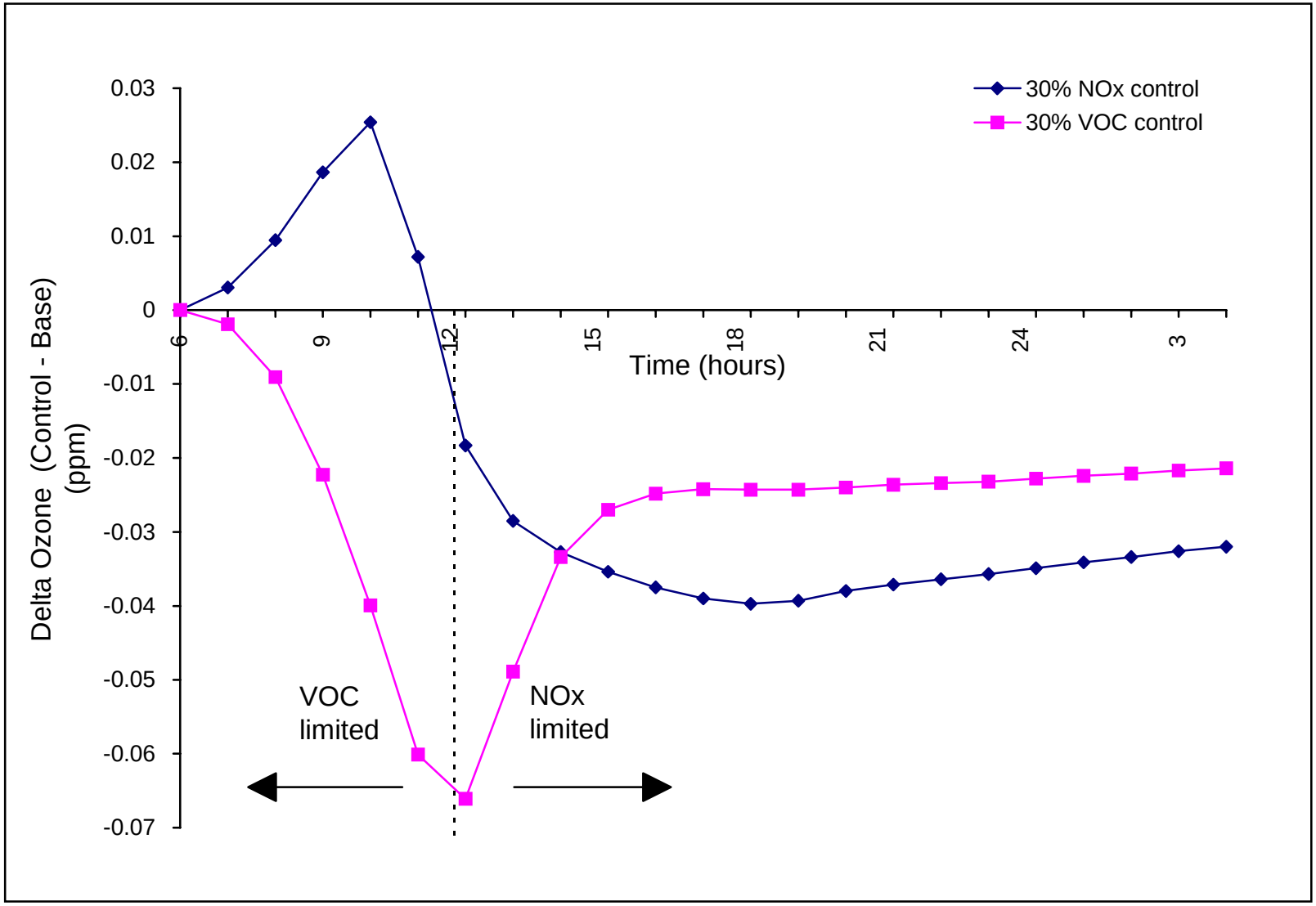



**Figure 2-3.** Change in ozone (control-base) for the VOC and $NO_X$ control scenarios shown in Figure 2-2. The vertical dashed line shows the transition from VOC to $NO_X$ limited ozone formation for the base case derived in Figure 2-1. **Initial base case VOC/$NO_X$ = 10:1.**

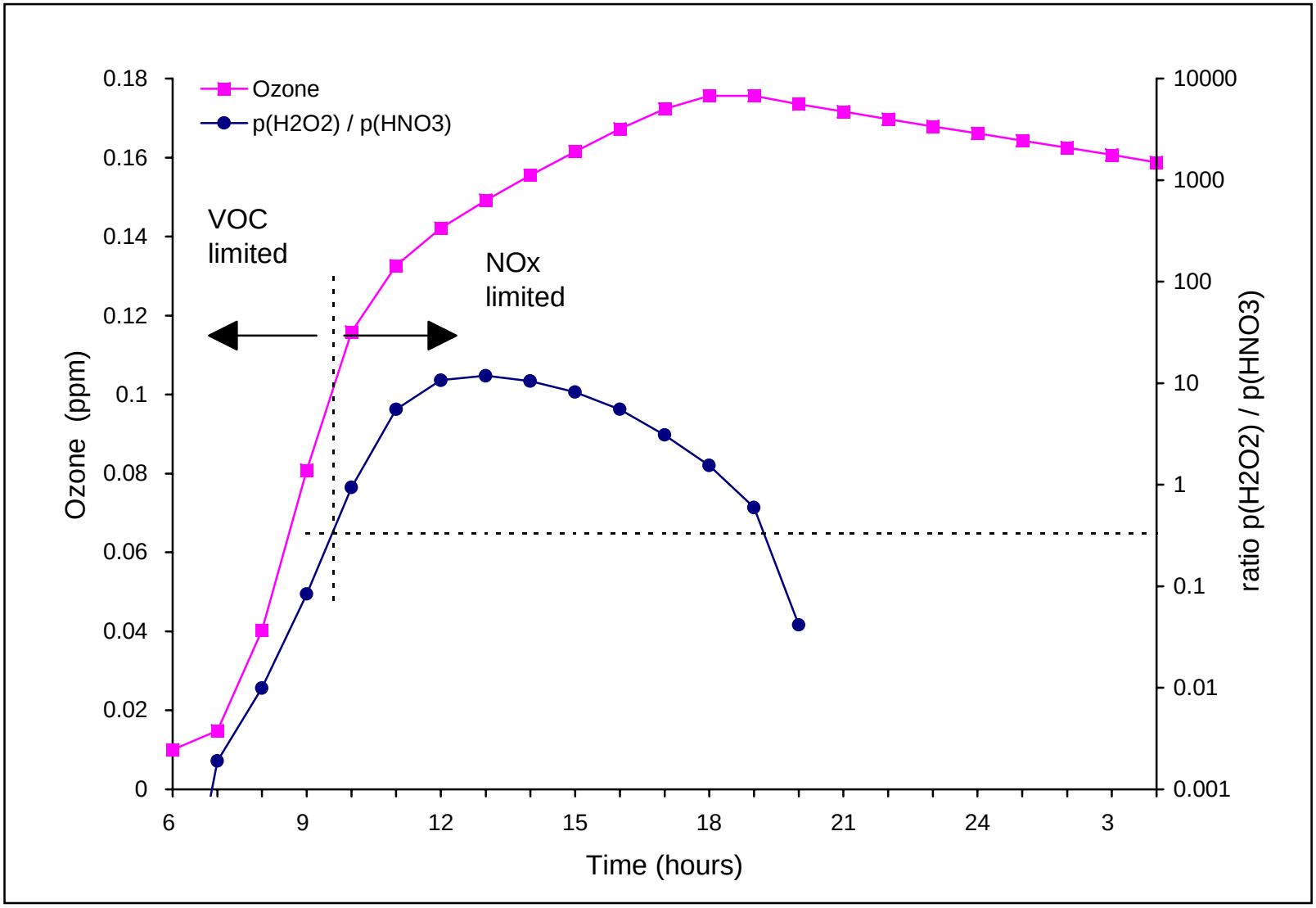



**Figure 2-4a.** As Figure 2-2, but for an **Initial VOC/$NO_X$ = 20:1.**

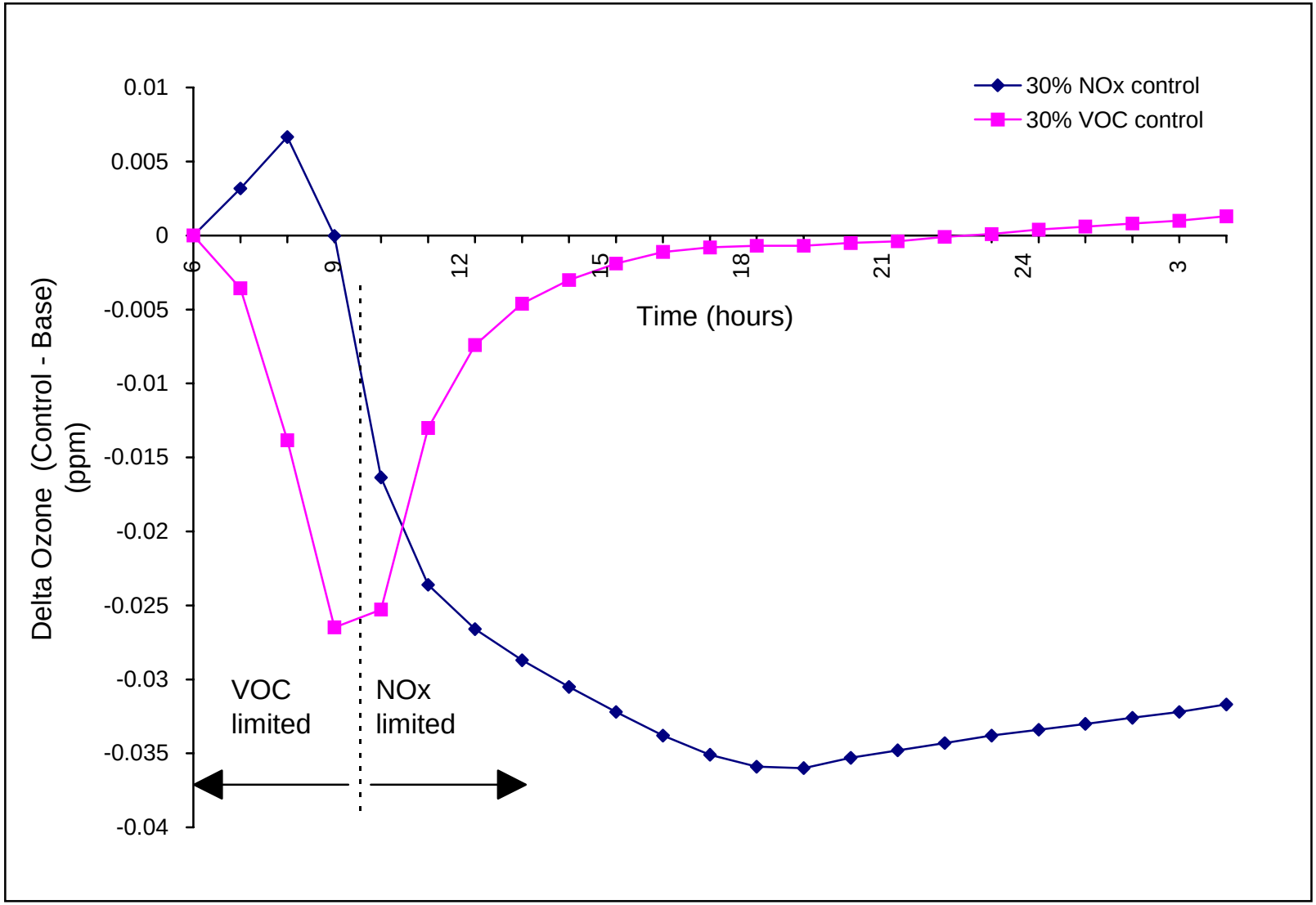



**Figure 2-4b.** As Figure 2-3, but for an **Initial VOC/$NO_X$ + 20:1.**

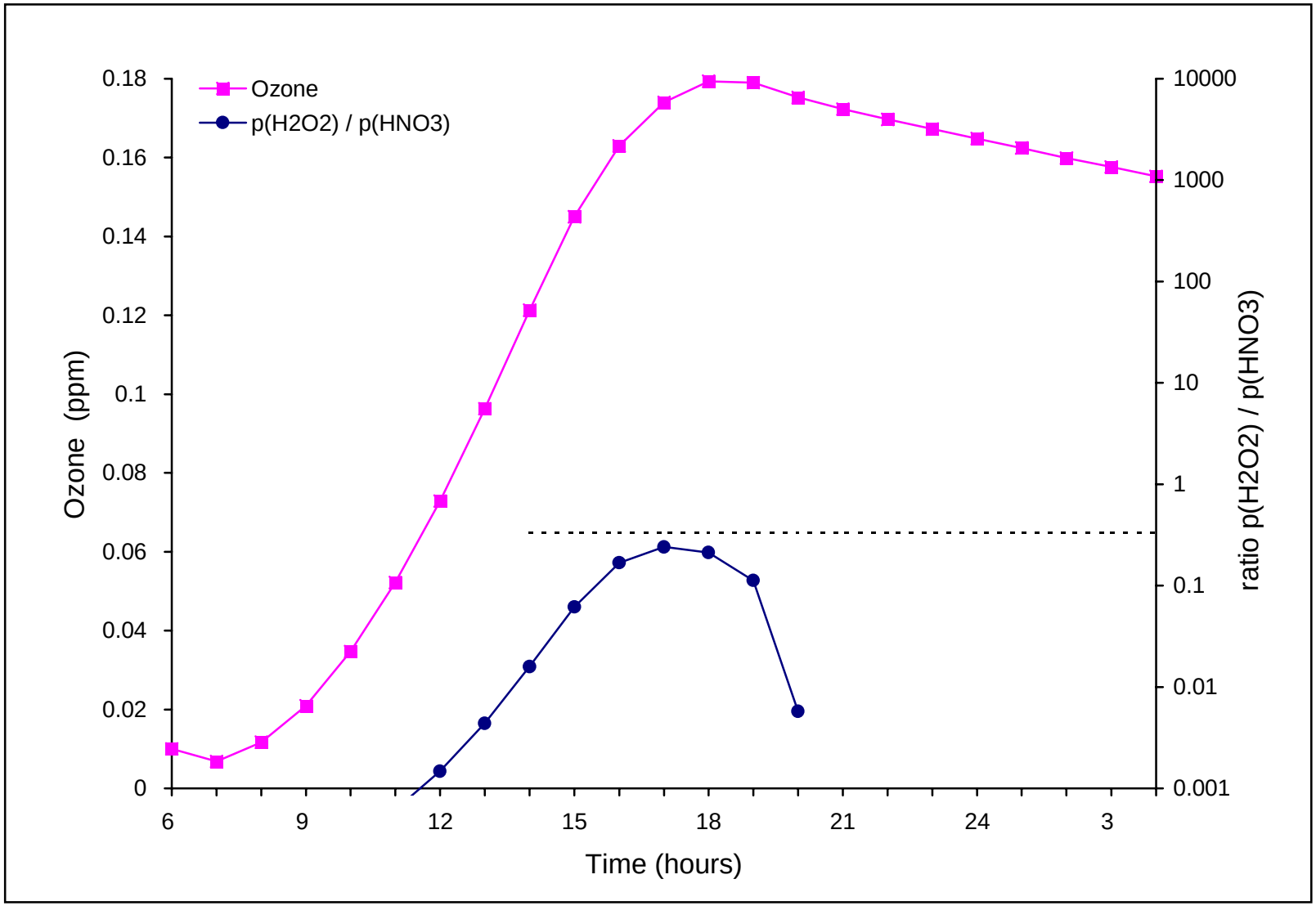



**Figure 2-5a.** As Figure 2-1, but for an **Initial VOC/$NO_X$ = 5:1.**

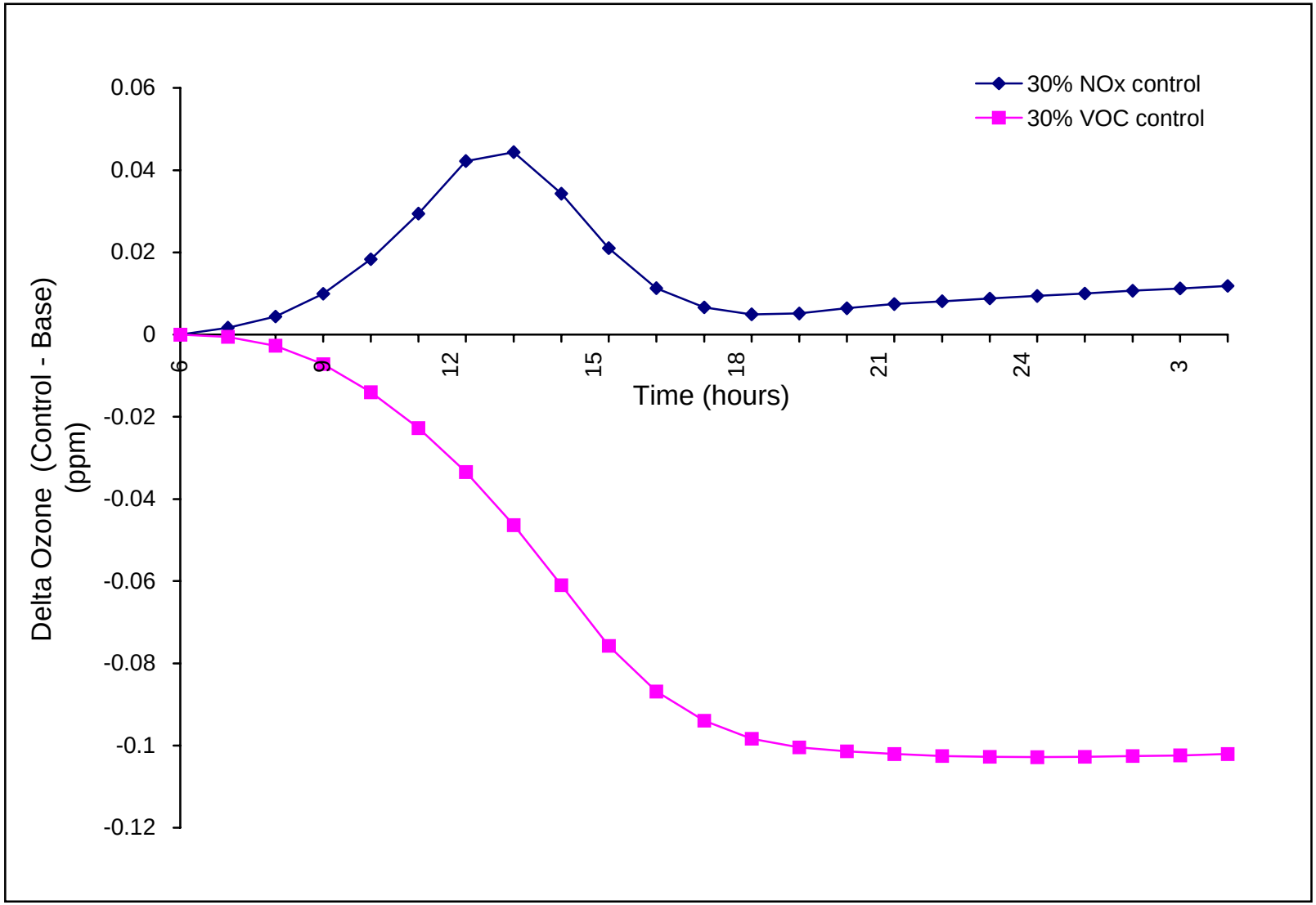



**Figure 2-5b.** As Figure 2-3, but for an **Initial VOC/$NO_X$ = 5:1.**

# 3. CODE STRUCTURE

## Approach

The time splitting technique used in the UAM to solve the ordinary differential equations (ODEs) that describe transport, diffusion, emissions, deposition, and chemical transformation simplified addition of the tracer software to the UAM. Basically, the UAM splits the solution of the atmospheric diffusion/chemistry/deposition ODE into four parts with subroutine calls named STEP1 through STEP4 as follows:

STEP1 - Horizontal advection/diffusion in the x-direction

STEP2 - Horizontal advection/diffusion in the y-direction

STEP3 - Vertical advection/diffusion, emissions, and deposition

STEP4 - Chemical transformation.

New subroutines and subroutine calls were added to UAM to incorporate the new tracer species and apply the steps listed above. The subroutine naming convention in the UAM was followed where possible adding the suffix "PT" to distinguish passive tracer routines (e.g., STEP1PT). Wherever possible the existing UAM code was left intact. The starting point for code development was the UNIX version of the UAM available from EPA and referred to as version 6.22 (available from the EPA via World Wide Web at http://ttnwww.rtpnc.epa.gov/).

The UAM uses an unconventional approach to allocate memory for the many large arrays that are required in a 3-D model. A single large vector (the scratch vector) is declared to block out sufficient memory, and the required arrays are referenced within the scratch vector via pointers. This approach was needed in the past to achieve a kind of dynamic memory re-allocation, but it is no longer necessary. This structure was left in place for all the existing variables used by the UAM and the many new variables required for the tracer software were added as new common blocks.

## Code Flow

The code flow for the Ozone Tool is shown in Figure 3-1. Modified subroutines are shown in bold and entirely new subroutines are shown in bold italics.

## New and Modified Subroutines

The functions of new subroutines and changes to existing subroutines are described below. Routines are listed in the order that they appear in Figure 3-1.

MAIN - Modified by adding a call to subroutine OPENPT.

OPENPT - New routine which reads all of the user options and flags required for the source apportionment algorithm. This is also where all files needed for executing with source apportionment are opened. OPENPT is always called since the first option read is the flag for turning source apportionment on and off. If this option is turned off, the routine returns immediately and the regular model will execute without source apportionment.

AAINIT - Modified by adding calls to all subroutines needed for initializing the source apportionment data structures. The subroutines called include: INITPT, TRSPEC, RDINSTPT, TZEROPT, RESEMPT, RESPTSPT, FILAQPT, CLRBDYPT, FILBDYPT, HDRRCP and HDRWPT. A number of input files are also rewound and an additional call to TZERO has been included. This is done to ensure that all file pointers are at the position expected by the regular model, after source apportionment routines have accessed these files.

CLFILE - Modified by adding a switch which causes an immediate return if the source apportionment flag is turned on. This is done to ensure that data needed by the source apportionment algorithm is still accessible after the file has been processed by the regular model.

INITPT - New routine which just calls routines to set up some of the source apportionment data structures; such as the source region map and the receptor definition data.

RESMAP - New routine which reads the source area map file and stores the data in a gridded array.

RERCP - New routine which reads the receptor definition file and stores the data in common variables.

TRSTAB - New routine which initializes the variables used to identify which of the regular model species will be used by the source apportionment algorithm. The $NO_X$, O3 and VOC species are flagged and the carbon number of each VOC species is assigned.

TRSPEC - New routine which sets up the species names and initializes pointers used to access the various types of tracers in the tracer arrays. Pointers are initialized for both the concentration array and the emissions array.

RDINSTPT - New routine which reads the tracer species instantaneous file for restart simulation days and loads the data into the concentration array. This routine is not called on the startup day of a simulation.

TZEROPT - New routine which reads the headers of the emission files used for source groupings. The array which maps emission species to model species is initialized for each of the emission files. Each file is read until the beginning hour of the simulation is reached.

CLCEWT - New routine which calculates the average reactivity of each of the emissions tracer species. For each source grouping and source region, the appropriate emission file is read for all hours in the simulation period. The average reactivity for the simulation period is calculated as the mass weighted average reactivity of all of the VOC species. Since the reactivity of the NOx tracer species is not used, these values are initialized to zero.

CLCIWT - New routine which calculates the average reactivity of the VOC initial condition tracer species. The initial conditions are read from the AIRQUALITY file provided for the current simulation period. The average reactivity for the simulation period is calculated as the mass weighted average of reactivity of all of the VOC species (including all layers).

CLCBWT - New routine which calculates the average reactivity of the VOC boundary condition tracer species. The boundary conditions are read from the BOUNDARY file for each hour in the simulation period. The average reactivity for the simulation period is calculated as the mass weighted average of reactivity of all of the VOC species (including all layers).

RESEMPT - New routine which reads the area source emissions files (including those for source groupings) and fills the emissions arrays. The NOx tracer emission rates are the sum of emission rates for NO and NO2. The tracer VOC emission rates are the sum of the emission rates of all hydrocarbon species on a mole C basis. If source groupings are requested, the sum of emissions from all source groupings is subtracted from the base emissions to calculate the "leftover" source group. The leftover group is always calculated to provide a check on whether the “use leftover group” flag has been set in a logical way (see Section 4).

RESPTSPT - New routine which reads the point source emissions files (including those for source groupings) and fills the emissions arrays. The NOx tracer emission rates are the sum of emission rates for NO and NO2. The tracer VOC emission rates are the sum of the emission rates of all hydrocarbon species on a mole C basis. If source groupings are requested, the sum of emissions from all source groupings is subtracted from the base emissions to calculate the "leftover" source group. The leftover group is always calculated to provide a check on whether the “use leftover group” flag has been set in a logical way (see Section 4).

FILAQPT - New routine which initializes the tracer concentration array at startup. The initial concentrations are loaded into the IC tracers using the initial conditions already read by the regular model. The NOx tracer concentrations are the sum of concentrations for NO and NO2. The tracer VOC concentrations are the sum of the concentrations of all hydrocarbon species on a ppm C basis. The O3N and O3V tracer concentrations are each half of the initial O3 concentration.

CLRBDYPT - New routine which sets all boundary tracer concentrations to zero. This is necessary since the tracer species are calculated by summing the regular model species.

FILBDYPT - New routine which initializes the boundary tracer species. This is done at the beginning of each hour, after the regular model has read the boundary conditions and loaded the data into the concentration arrays. The tracer concentration arrays are filled at the boundary cells for boundary tracers species only. If the "stratify boundary" option is on, each edge of the boundary and the region top are loaded into separate tracer species.

HDRRCP - New routine which writes the header records to the receptor average concentration file. These data include: simulation duration, receptor definition and tracer species list.

HDRWPT - New routine which writes the header information to the output tracer surface concentration file and the output tracer instantaneous files.

SETUP - Modified by adding calls to the routines which read the emissions files and load the tracer emissions arrays (RESEMPT and RESPTSPT). These routines are called only if the source apportionment algorithm is turned on.

ACCUM - Modified by adding calls to the routines which sum the average concentrations for the tracer species (ADDRCP and PEKRCP). These routines are called only if the source apportionment algorithm is turned on.

ADDRCP - New routine which adds the concentrations for each receptor to the running sum of concentrations. These data will then be averaged over all time steps to calculate hourly average concentrations. For POINT receptor types, a bi-linear interpolation scheme is used to calculate the concentration at the given point. For CELL AVERAGE receptor types, the concentrations over all of the specified cells are averaged before being added to the running sum.

ADVANC - Modified by adding calls to the routines that perform the transport and chemistry for the tracer species. These routines are called only if the source apportionment algorithm is turned on.

STEP1PT - New routine which performs the horizontal advection for the tracer concentrations for each row. This routine was created by making slight modifications to the STEP1 routine.

RECALIB - New routine which re-calibrates the tracer concentrations to be consistent with the regular model. This is necessary because the steep concentration gradients in the tracer concentration fields exacerbate numerical imprecision in the Smolarkiewicz advection scheme.

STEP2PT - New routine which performs the horizontal advection on the tracer concentrations for each column. This routine was created by making slight modifications to the STEP2 routine.

STEP34 - Modified by adding a call to the routine that performs vertical advection and diffusion on the tracer concentrations (STEP3PT). In addition, code has been added which allows for adjustments to tracer concentrations to account for the effects of the chemistry in the regular model (STEP4PT).

STEP3PT - New routine which performs the vertical advection and diffusion of the tracer concentrations. This is also where emissions are injected into the tracer concentration field. This routine was created by making modifications to the STEP3 routine.

STEP4PT - New routine which adjusts the tracer concentrations for the effects of the chemistry being performed in the regular model. The effects of the chemistry algorithm are calculated in the STEP34 routine and passed in the argument list of this routine. The ozone reaction tracer species are adjusted based on the current conditions in the photochemistry (e.g. $NO_X$-limited or VOC-limited). This is also where the decay adjustment to the timing racers is performed.

AVGRCP - New routine which writes the hourly average concentrations at each receptor to the receptor average concentrations file.

INSTPT - New routine which writes the tracer concentration field to the output instantaneous file to be used for restart. The file is rewound and the header is rewritten at each hour. Therefore, the instantaneous concentration file contains only one hour at a time. The odd hours (ending hour) are written to the first output instantaneous file while the even hours are written to the second output instantaneous output file. This routine also writes the average concentrations to the surface tracer file.

***INDICATES ENTIRELY NEW SUBROUTINE***
**INDICATES MODIFIED SUBROUTINE**

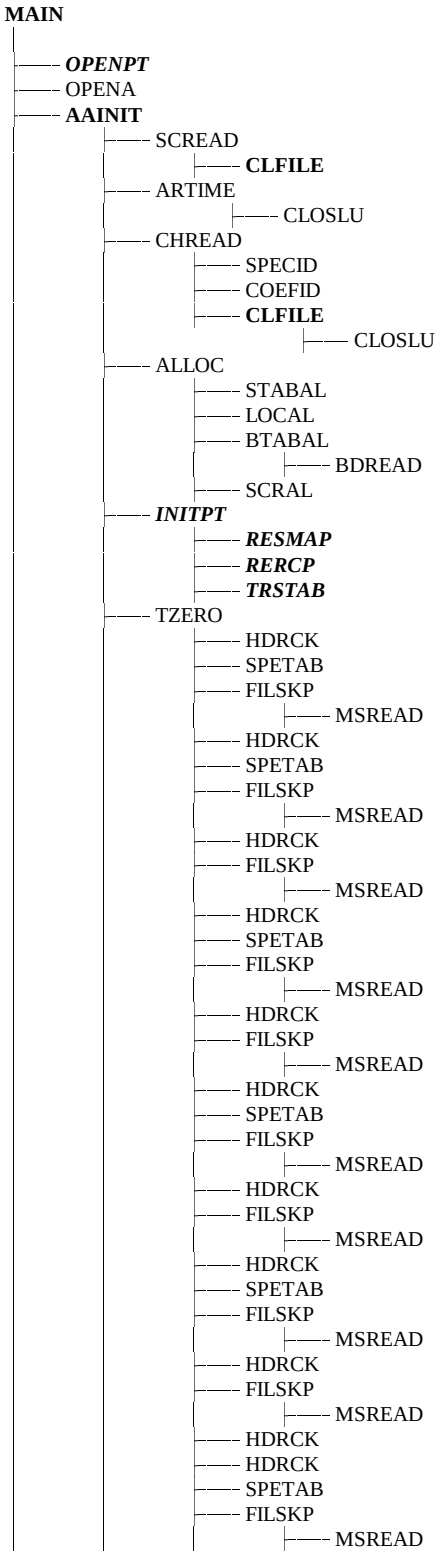



**Figure 3-1.** Code flow diagram for the UAM ozone tool with new and modified subroutines highlighted**.**

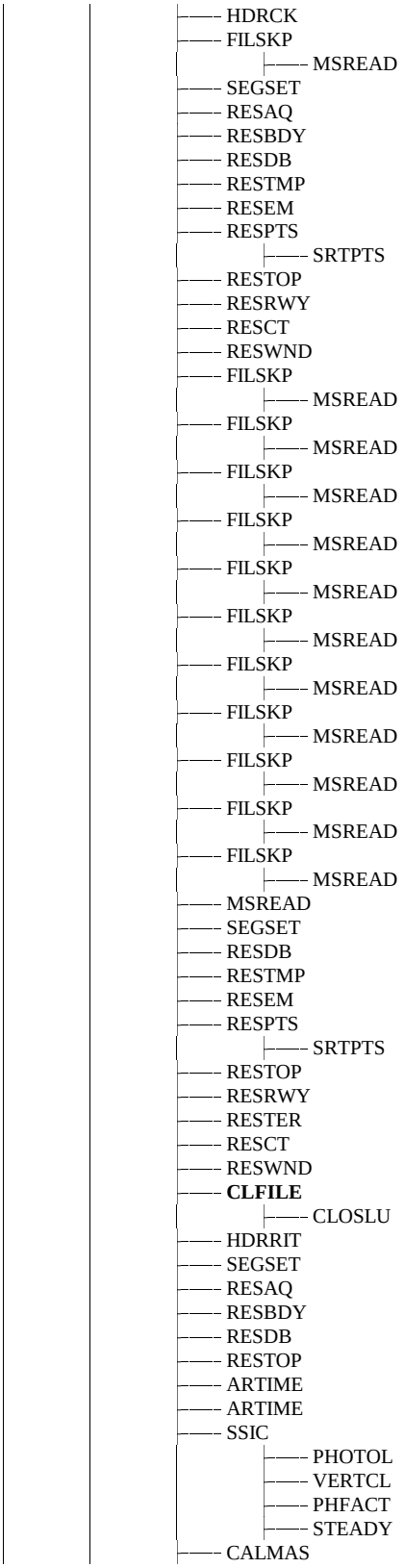



**Figure 3-1.** Continued.

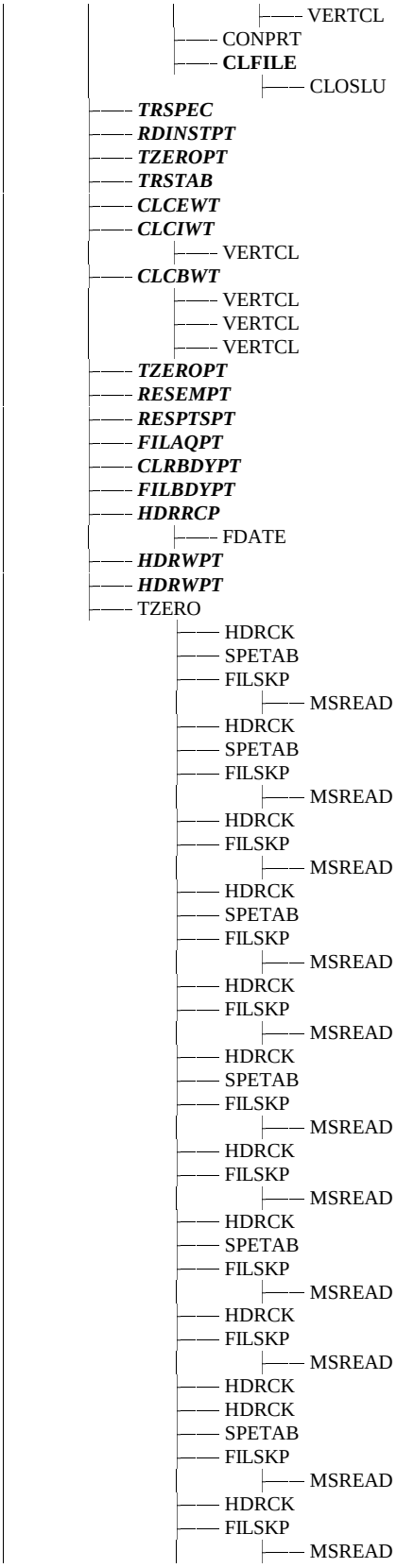



**Figure 3-1.** Continued.

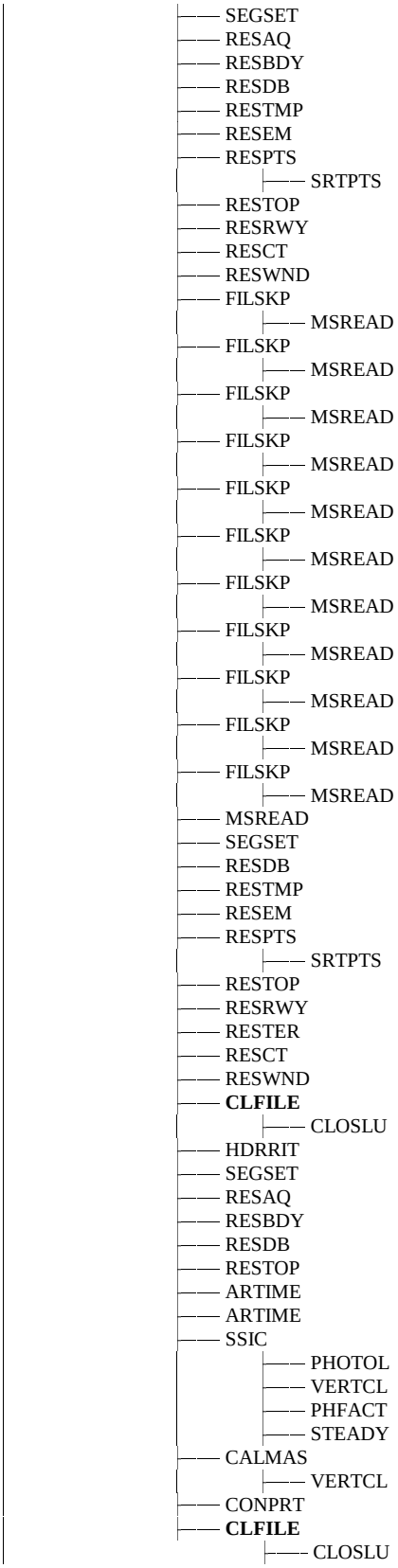



**Figure 3-1.** Continued.

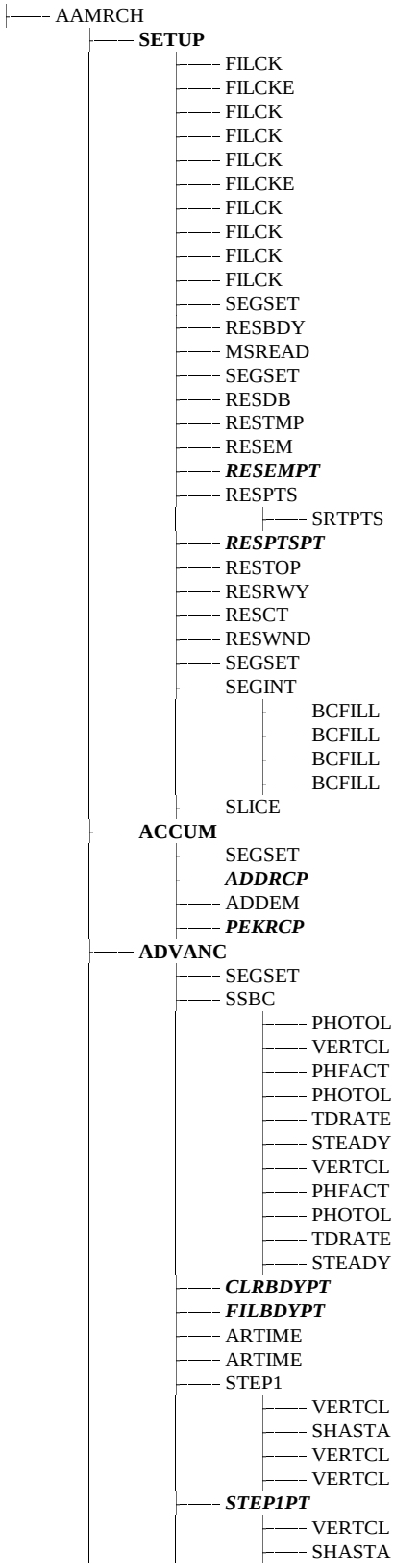



**Figure 3-1.** Continued.

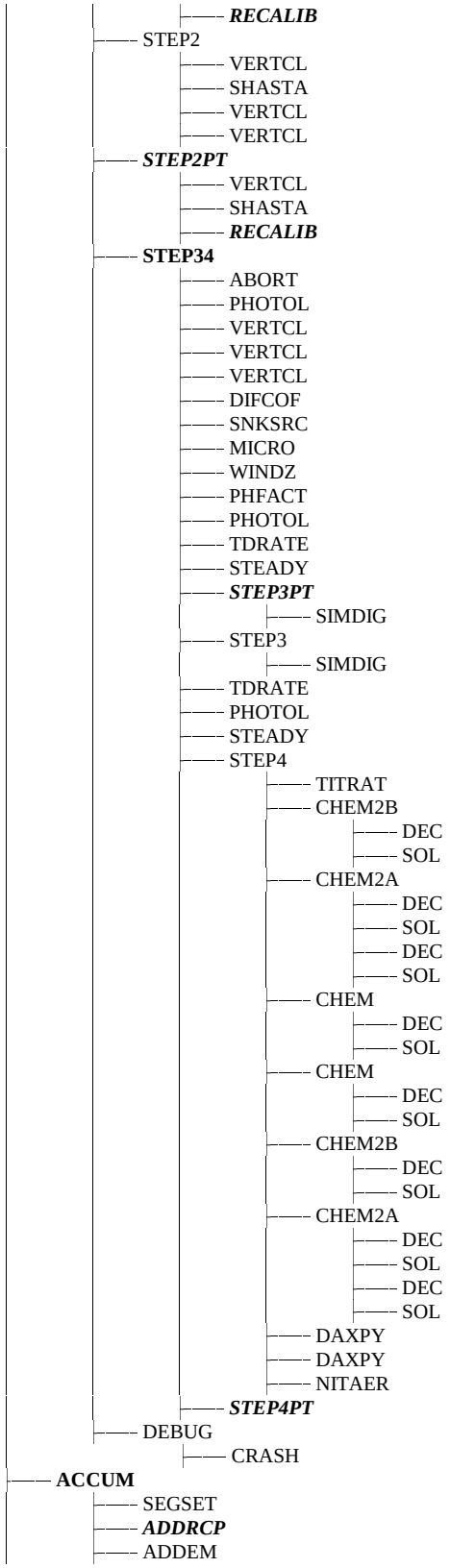



**Figure 3-1.** Continued.

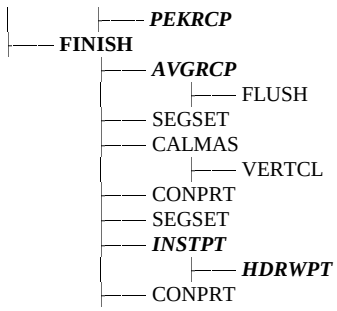



**Figure 3-1.** Concluded.

**Maximum Tracer Species and Memory Requirements**

The total amount of memory used by the Ozone Tool is determined primarily by the total number of tracer species allocated and the size of the modeling domain (number of grid cells). The core model (i.e., without tracers) requires approximately 9 megabytes of memory for a 65 by 50 by 5 grid cell domain. The maximum number of tracer species is set when the code is compiled by the parameter MXTRSP in the "tracer.cmd" include file. For every 100 tracer species allocated the memory requirement increases by 12.3 megabytes. The configuration shown in Figure 3-2 (a section of the "tracer.cmd" file) would allow for 500 tracer species, requiring a total of 71 megabytes of memory to execute.

```
c
c-----------------------------------------------------------------------
c    Parameters for array bounds:
c-----------------------------------------------------------------------
c
c   MXXCEL   I   maximum number of grid cells in the X-direction
c   MXYCEL   I   maximum number of grid cells in the Y-direction
c   MXCELL   I   maximum number of grid cells in domain
c   MXZCEL   I   maximum number of grid cells in the Z-direction
c   MXSIMS   I   maximum number of simulation days
c   NTRSTD   I   number of "standard" tracer species per source region
c   MXTRSP   I   maximum number of total tracer species in simulation
c   MXPNTS   I   maximum number of point sources in elevated file
c
      integer*4 MXXCEL
      integer*4 MXYCEL
      integer*4 MXCELL
      integer*4 MXZCEL
      integer*4 MXSIMS
      integer*4 NTRSTD
      integer*4 MXTRSP
      integer*4 MXPNTS
c
      parameter( MXXCEL = 65 )
      parameter( MXYCEL = 50 )
      parameter( MXCELL = MXXCEL * MXYCEL )
      parameter( MXZCEL =  5 )
      parameter( MXSIMS =  3 )
      parameter( NTRSTD =  4 )
      parameter( MXTRSP = 500 )
      parameter( MXPNTS = 5000 )
```

**Figure 3-2.** Section of the tracer.cmd file showing where the maximum number of tracer species is set (highlighted). In this case, the value is 500 species.

The total number of tracer species needed for a given simulation can be calculated using the following formula:

$$MXTRSP = 2* N_t * N_R* (N_{days} + 1) +4* (1 + N_{BC} + (N_E * N_R) )$$

where,

| | | |
|---|---|---|
| $N_t$ | = | number of timing releases per day |
| $N_{days}$ | = | number of days in the complete simulation |
| $N_{BC}$ | = | 1 if "stratify boundary" is off<br>4 if "stratify boundary" is on |
| $N_E$ | = | number of emission categories |
| $N_R$ | = | number of source regions. |

Thus, the available number of tracer species can be used for any combination of ozone reaction tracer species and timing tracer species that does not exceed the maximum. This allows the user to balance increased spatial, emissions category or temporal resolution within available memory resources at run time (i.e., without needing to recompile the model).

**Options for Format of Binary Input/Output Files**

The UAM reads and writes many 3-D, time resolved files that require significant disk storage. To minimize the storage requirements, these files are in binary formats as documented in the UAM User's Guide (EPA, 1990). Most UNIX workstations use the same binary format (IEEE, big endian). Digital Equipment Corporation (DEC) Alpha workstations use a different format by default. This can be changed by invoking a DEC compiler option "-convert big_endian." However, because of the way the UAM stores some variables (e.g., species names) as real numbers, binary files written on a DEC Alpha workstation with the "convert big_endian" option are not readable by other workstations. Engineers from DEC have provided the UAM user community with a routine to solve this problem (BSWAP), and it is provided with the Ozone Tool source code. DEC Alpha users who wish to exchange binary files with other work stations can compile the Ozone Tool with the Makefile provided for DEC Alpha workstations that calls the BSWAP routine and invokes the compiler option "-convert big_endian."

# 4. RUNNING THE MODEL

## RUN FILES AND USER OPTIONS

Several example run files for the Ozone Tool are shown in Figures 4-1 through 4-4. The format is a command line at the top to execute the model followed by the input parameters and input/output filenames required for the model run. The file names shown in the lower part of Figure 4-1 are the same as for a standard UAM run for the same scenario (see the UAM users guide for details: EPA, 1990) and are not described here. the new input parameters and input/output filenames required for the Ozone Tool are shown in bold. Notice that the information is structured in the following order: flags and parameters come first, input filenames come second and output filenames come last.

The options and file requirements for the Ozone Tool are as follows:

**Passive Tracer**

| | | |
|---|---|---|
| | TRUE | Source apportionment active, additional options and files must be specified. |
| | FALSE | Source apportionment inactive. No source apportionment options/files are specified and the model executes the same as the standard UAM. |

**Simulation Restart**

| | | |
|---|---|---|
| | TRUE | Continuation of a previous run. A "Tracer Initialize" file must be supplied, usually the last "Second Output Inst" file from the previous run. |
| | FALSE | Start of a run. No "Tracer Initialize" supplied. |

**Stratify Boundary**

| | | |
|---|---|---|
| | TRUE | Separate tracer types will be used for the N, S, E, W and Top boundaries. |
| | FALSE | A single tracer type will be used for all 5 boundaries. |

| | | |
|---|---|---|
| **# of Source Regions** | | The number of source areas for the run. The number must be the same as the number of source areas defined in the "Source area mapping" file. |
| **# of Emiss Groups** | | The number of emission groups for the run. Together with the "Use leftover group" flag, this determines the number of pairs emission files that must be supplied below. Additional details are provided below. |
| **Use leftover group** | TRUE | Calculate a 'leftover' emissions group from the difference between the sum of the emission group files and the regular UAM emission files. The model will verify that this difference is not trivially small. If it is trivial, the model run will terminate and the user should consider whether this flag was set in error or the leftover group is too small to be calculated in this way. |

| | |
|---|---|
| FALSE | Do not calculate a 'leftover' emissions group. The model will verify that the sum of the emission group files supplied is the same as the UAM emission files. If it is not the model terminate and the user should consider whether this flag was set in error or a leftover group should be used. |
| **# timing releases** | The number of timing tracer releases per 24 hour period, e.g., 4 means a new release starting every six hours (hours 0, 6, 12 and 18). If the simulation is started in the middle of the day (e.g. at hour 15), the first tracer release is time stamped with the model start time, subsequent releases occur on a schedule as if the start time were at hour zero. The model can be run without timing tracers by specifying zero for this parameter. |
| **Source area mapping** | File defining the source areas defined below. |
| **Receptor definition** | File defining the receptor locations defined below. |
| **Tracer Initialize** | Only required if the simulation restart flag is set to true above. File must contain the instantaneous concentrations of tracers from end of the preceding simulation. Usually, the file is the "Second Output Inst" file from the previous day. |
| **EMISSIONS group 1**<br>**PTSOURCE group 1**<br>**EMISSIONS group 2**<br>**PTSOURCE group 2**<br>**EMISSIONS group N**<br>**PTSOURCE group N** | Zero, one, or several pairs of emission files consistent with the "# of Emiss Groups" and "Use leftover group" options specified above. Details are provided below. |
| **First Output Inst.** | Instantaneous concentration file for tracers at last odd hour completed. File is in UAM instantaneous file binary format. |
| **Second Output Inst.** | Instantaneous concentration file for tracers at last even hour completed. This file would be used to start a run for a continuation day if the end/start time is midnight (usually the case). |
| **Surface Concentrat.** | Hourly average concentration for tracers in surface layer. File is in UAM average file binary format. |
| **Receptor Conc.** | Hourly average tracer concentrations at receptors specified in the "Receptor definition" file. File has an ASCII format compatible with the postprocessing software as described below. |

```
/bin/time ../src/03tool.dec << EOF
Passive Tracer     | TRUE
Simulation Restart | FALSE
Stratify Boundary  | FALSE
# of Source Regions| 17
# of Emiss Groups  | 1
Use leftover group | FALSE
# timing releases  | 2
Source area mapping|../inputs/tracer/area17.map
Receptor definition|../inputs/tracer/receptor.def
First Output Inst. |../output/tracer/inst.tracer.238.1
Second Output Inst.|../output/tracer/inst.tracer.238.2
Surface Concentrat.|../output/tracer/surface.conc.238
Receptor Conc.     |../output/tracer/receptor.conc.238
METSCALARS         7|../inputs/aug87/files.26/metscl.h01.bin
SIMCONTROL         8|../run/sprep.238.bin
CHEMPARAM          9|../inputs/chemparm.panx1.bin
AIRQUALITY        10|../inputs/h01.air
BOUNDARY          11|../inputs/87bas.bnd
DIFFBREAK         12|../inputs/difbrk.h00.826-828.bin
EMISSIONS         13|../inputs/aug87/emiss.1987.26/emiss.dbase1.bin
PTSOURCE          14|../inputs/aug87/emiss.1987.26/ptsrce.dbase1.bin
TEMPERATUR        17|../inputs/aug87/files.26/temper.h01.bin
TOPCONC           43|../inputs/h01.tpc
REGIONTOP         44|../inputs/regntp.h01.826-828.bin
TERRAIN           45|../inputs/terain.65x40.bin
WIND              46|../inputs/aug87/files.26/wind.n72xt.bin
MESSAGES           6|../output/aug87/aout.870826
AVERAGE           41|../output/aug87/avrg.870826
INSTANTANEOUS     42|../output/aug87/inst.870826
DEPOSITION        47|../output/aug87/depn.870826
EOF
```

**Figure 4-1.** The Ozone Tool sample job stream. Lines specific to the Ozone Tool are shown in bold, non-bold lines would be the same for a standard UAM simulation. The options for this run are as follows: passive tracers are active, first day of a simulation (i.e., restart false), single tracer type for all boundaries, 17 source regions, one emission group (i.e., zero additional emission files and no leftover group), and two timing tracer releases per day.

```
/bin/time ../src/03tool.dec << EOF
Passive Tracer      | TRUE
Simulation Restart  | TRUE
Stratify Boundary   | FALSE
# of Source Regions| 17
# of Emiss Groups   | 1
Use leftover group  | FALSE
# timing releases   | 2
Source area mapping|../inputs/tracer/area17.map
Receptor definition|../inputs/tracer/receptor.def
Tracer Initialize  |../output/tracer/inst.tracer.238.2
First Output Inst.  |../output/tracer/inst.tracer.239.1
Second Output Inst.|../output/tracer/inst.tracer.239.2
Surface Concentrat.|../output/tracer/surface.conc.239
Receptor Conc.      |../output/tracer/receptor.conc.239
METSCALARS          7|../inputs/aug87/files.27/metscl.h01.bin
SIMCONTROL          8|../run/sprep.239.bin
CHEMPARAM           9|../inputs/chemparm.panx1.bin
AIRQUALITY         10|../output/aug87/inst.870826
BOUNDARY           11|../inputs/87bas.bnd
DIFFBREAK          12|../inputs/difbrk.h00.826-828.bin
EMISSIONS          13|../inputs/aug87/emiss.1987.27/emiss.dbase1.bin
PTSOURCE           14|../inputs/aug87/emiss.1987.27/ptsrce.dbase1.bin
TEMPERATUR         17|../inputs/aug87/files.27/temper.h01.bin
TOPCONC            43|../inputs/h01.tpc
REGIONTOP          44|../inputs/regntp.h01.826-828.bin
TERRAIN            45|../inputs/terain.65x40.bin
WIND               46|../inputs/aug87/files.27/wind.n72xt.bin
MESSAGES            6|../output/aug87/aout.870827
AVERAGE            41|../output/aug87/avrg.870827
INSTANTANEOUS      42|../output/aug87/inst.870827
DEPOSITION         47|../output/aug87/depn.870827
EOF
```

**Figure 4-2.** The Ozone Tool sample job stream. Options are the same as in Figure 4-1, but in this case the run is a continuation from the run shown in Figure 4-1 and so the restart flag is set to TRUE and a “Tracer Initialize” file is supplied.

```
/bin/time ../src/03tool.dec << EOF
Passive Tracer      | TRUE
Simulation Restart  | TRUE
Stratify Boundary   | FALSE
# of Source Regions| 17
# of Emiss Groups   | 3
Use leftover group  | TRUE
# timing releases   | 2
Source area mapping|../inputs/tracer/area17.map
Receptor definition|../inputs/tracer/receptor.def
Tracer Initialize  |../output/tracer/inst.tracer.238.2
EMISSIONS group 1  |../inputs/aug87/emiss.1987.27/emiss.gp1.bin
PTSOURCE  group 1  |../inputs/aug87/emiss.1987.27/ptsrce.gp1.bin
EMISSIONS group 2  |../inputs/aug87/emiss.1987.27/emiss.gp2.bin
PTSOURCE  group 2  |
First Output Inst. |../output/tracer/inst.tracer.239.1
Second Output Inst.|../output/tracer/inst.tracer.239.2
Surface Concentrat.|../output/tracer/surface.conc.239
Receptor Conc.     |../output/tracer/receptor.conc.239
METSCALARS          7|../inputs/aug87/files.27/metscl.h01.bin
SIMCONTROL          8|../run/sprep.239.bin
CHEMPARAM           9|../inputs/chemparm.panx1.bin
AIRQUALITY         10|../output/aug87/inst.870826
BOUNDARY           11|../inputs/87bas.bnd
DIFFBREAK          12|../inputs/difbrk.h00.826-828.bin
EMISSIONS          13|../inputs/aug87/emiss.1987.27/emiss.dbase1.bin
PTSOURCE           14|../inputs/aug87/emiss.1987.27/ptsrce.dbase1.bin
TEMPERATUR         17|../inputs/aug87/files.27/temper.h01.bin
TOPCONC            43|../inputs/h01.tpc
REGIONTOP          44|../inputs/regntp.h01.826-828.bin
TERRAIN            45|../inputs/terain.65x40.bin
WIND               46|../inputs/aug87/files.27/wind.n72xt.bin
MESSAGES            6|../output/aug87/aout.870827
AVERAGE            41|../output/aug87/avrg.870827
INSTANTANEOUS      42|../output/aug87/inst.870827
DEPOSITION         47|../output/aug87/depn.870827
EOF
```

**Figure 4-3.** The Ozone Tool sample job stream. The options are similar to Figure 4-2, but in this case the run is a continuation day of a run with three emission groups. The three emission groups are defined by supplying two pairs of extra emission files (EMISSIONS group 1; PTSOURCE group 1; EMISSIONS group 2; PTSOURCE group 2) and setting the "Use leftover group" flag to TRUE for the model to calculate the third group internally. The "PTSOURCE group 2" filename is blank because group 2 is a category with no point source emissions (e.g., biogenics).

```
/bin/time ../src/03tool.dec << EOF
Passive Tracer      | TRUE
Simulation Restart  | TRUE
Stratify Boundary   | FALSE
# of Source Regions| 17
# of Emiss Groups   | 3
Use leftover group  | FALSE
# timing releases   | 2
Source area mapping|../inputs/tracer/area17.map
Receptor definition|../inputs/tracer/receptor.def
Tracer Initialize   |../output/tracer/inst.tracer.238.2
EMISSIONS group 1   |../inputs/aug87/emiss.1987.27/emiss.gp1.bin
PTSOURCE  group 1   |../inputs/aug87/emiss.1987.27/ptsrce.gp1.bin
EMISSIONS group 2   |../inputs/aug87/emiss.1987.27/emiss.gp2.bin
PTSOURCE  group 2   |
EMISSIONS group 3   |../inputs/aug87/emiss.1987.27/emiss.gp3.bin
PTSOURCE  group 3   |../inputs/aug87/emiss.1987.27/ptsrce.gp3.bin
First Output Inst.  |../output/tracer/inst.tracer.239.1
Second Output Inst.|../output/tracer/inst.tracer.239.2
Surface Concentrat.|../output/tracer/surface.conc.239
Receptor Conc.      |../output/tracer/receptor.conc.239
METSCALARS          7|../inputs/aug87/files.27/metscl.h01.bin
SIMCONTROL          8|../run/sprep.239.bin
CHEMPARAM           9|../inputs/chemparm.panx1.bin
AIRQUALITY         10|../output/aug87/inst.870826
BOUNDARY           11|../inputs/87bas.bnd
DIFFBREAK          12|../inputs/difbrk.h00.826-828.bin
EMISSIONS          13|../inputs/aug87/emiss.1987.27/emiss.dbase1.bin
PTSOURCE           14|../inputs/aug87/emiss.1987.27/ptsrce.dbase1.bin
TEMPERATUR         17|../inputs/aug87/files.27/temper.h01.bin
TOPCONC            43|../inputs/h01.tpc
REGIONTOP          44|../inputs/regntp.h01.826-828.bin
TERRAIN            45|../inputs/terain.65x40.bin
WIND               46|../inputs/aug87/files.27/wind.n72xt.bin
MESSAGES            6|../output/aug87/aout.870827
AVERAGE            41|../output/aug87/avrg.870827
INSTANTANEOUS      42|../output/aug87/inst.870827
DEPOSITION         47|../output/aug87/depn.870827
EOF
```

**Figure 4-4.** The Ozone Tool sample job stream. The options are equivalent to Figure 4-3 (i.e. a continuation day of a run with three emission groups) but in this case all three emission groups are defined explicitly by supplying extra emission files (EMISSIONS group 1; PTSOURCE group 1; EMISSIONS group 2; PTSOURCE group 2; EMISSIONS group 3; PTSOURCE group 3). Therefore, the "Use leftover group" flag is set to FALSE. The "PTSOURCE group 2" filename is blank because group 2 is a category with no point source emissions (e.g., biogenics).

**Specifying Emission Groups**

The Ozone Tool can apportion ozone and ozone precursor concentrations among several emission categories. To achieve this, the emissions for the separate groups must be supplied as pairs of separate emissions files, one love level file and one point source file for each group. The additional emission files must be in the standard UAM emission file format (EPA, 1990). If the group being separated has no elevated emissions (e.g. biogenics), the point source file name for the group can be left blank. If the emission group being separated has no surface emissions (e.g. a utility), the surface file name for the group can be left blank.

Imagine a case where the emission inventory is split into three groups. Three pairs of emission files could be supplied that together have the same total emissions as the regular UAM emissions files. Alternatively, two pairs of files could be supplied and the third group calculated from the "leftover" emissions (i.e., the regular UAM emissions minus the two groups specified).Both approaches could be useful, depending upon the emissions files available to the user. Accordingly, the Ozone Tool reads an input flag "use leftover group" that can be set true or false. If a leftover group is selected, the model verifies that the group is not too small to calculate within the numerical precision of the computer (this also traps cases where the flag was set true in error). If no leftover group is selected, the model verifies that the total emissions for the groups supplied are equal to the regular UAM emissions i.e., that a leftover group is not needed.

The number of pairs of emission files that need to be supplied for different model configurations is summarized in Table 4-1. Table 4-1 also show how the emissions groups are numbered, which is reflected in the tracer species names (defined below).

**Table 4-1.** Numbers of pairs of emission files (i.e., low level file and point source file) needed for different model configurations.

| Number of Emission Groups | Use Leftover Group | Number of Pairs of Emission Files Needed | Numbering of Emission Groups and Tracer Species |
|---|---|---|---|
| 1 | Not Applicable | 0 | 0 |
| n (n>1) | False | n | 1,2,3,...n |
| | True | n-1 | 1,2,3,...n |

**Running without timing tracers**

The Ozone Tool can be run without timing tracers if the "# timing releases" parameter is set to zero. Source apportionment of ozone and precursors is unaffected by this since these two functions of the model are independent. If timing tracers are omitted, the postprocessing software ("browser") described below will not report estimated release times for precursor emissions, nor will it estimate whether recirculation is likely to have occurred. Users may choose to run without timing tracers in situations where temporal resolution is not required.

Omitting timing tracers reduces the number of tracer species employed and therefore may permit users to select relatively more geographic/emissions category resolution within the same computer memory limitations.

## INPUT FILE FORMATS

The Ozone Tool reads several input files that are in UAM binary format (EPA, 1990). These are the low level emissions file (EMISSIONS group 1, EMISSIONS group 1, etc.) , point source emissions file (PTSOURCE group 1, PTSOURCE group 2, etc.) and the tracer instantaneous concentration file ("Tracer initialize" file).

### Source area mapping

The Ozone Tool can apportion ozone and ozone precursor concentrations among several geographic regions within the modeling domain, as shown in Figure 1-1. The "source area mapping" file identifies which region each surface grid cell is a member of. The format of the file is an array of integer number (i3) corresponding to the UAM domain. Figure 4-5 shows the source area mapping file corresponding to Figure 1-1. Since the UAM domain in Figure 1-1 has 40 rows and 65 columns of cells, the file shown in Figure 4-5 has 40 lines with 65 numbers on each line. The first number (top left) always corresponds to the Northwest corner of the domain.

### Receptor definition

Tracer concentrations for selected receptor locations are output to an ASCII file every hour. The receptors for each model run are defined in the "Receptor definition" input file. An example is shown in Figure 4-6. Three types of receptors are supported:

| | |
|---|---|
| POINT | a point specified in the co-ordinate system of the UAM grid. Concentrations at the point are determined by bi-linear interpolation of the surrounding four surface cells. |
| SINGLE CELL | a single surface cell identified by number. |
| CELL AVERAGE | a group of surface cells identified by number that are averaged together to provide multi-cell average tracer concentrations. |

Each receptor can be identified by a 10 character name. The formats for specifying each receptor type are given in Table 4-2.

# Example Source Area Mapping File

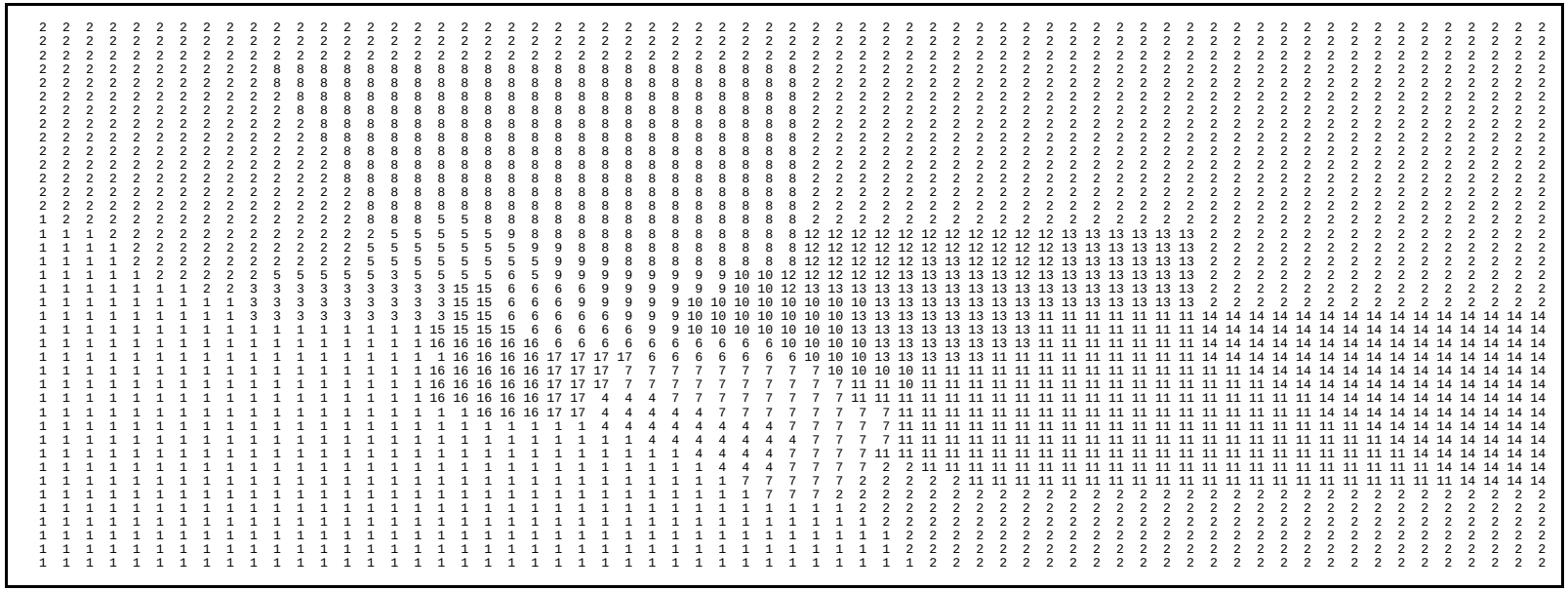


**Figure 4-5.** Example source area mapping file for the domain and source areas shown in Figure 1-1.

**Table 4-2.** Format for the receptor definition file.

| Receptor Type | Line | Columns | Data |
|---|---|---|---|
| POINT | 1 | 1-15 | The word “POINT” |
| | 1 | 21-30 | Receptor name |
| | 1 | 31-40 | X co-ordinate |
| | 1 | 41-50 | Y co-ordinate |
| SINGLE CELL | 1 | 1-15 | The word “SINGLE CELL” |
| | 1 | 21-30 | Receptor name |
| | 1 | 31-40 | X cell number |
| | 1 | 41-50 | Y cell number |
| CELL AVERAGE | 1 | 1-15 | The words “CELL AVERAGE” |
| | 1 | 21-30 | Receptor name |
| | 1 | 31-40 | The number of cells to average (M) |
| | 2-M | 1-10 | X cell number |
| | 2-M | 21-30 | X cell number |

```
POINT              Rubidoux  461.520   3762.040
POINT              Pasadena  396.400   3778.500
POINT              Lennox    373.000   3755.000
SINGLE CELL        Peak        45          18
CELL AVERAGE       Region 10    8
        31        19
        32        19
        33        19
        34        19
        31        18
        32        18
        33        18
        34        18
```

**Figure 4-6**. Example receptor definition file.

## OUTPUT FILE FORMATS

The Ozone Tool writes several output files that are in binary format (EPA, 1990). These are the tracer instantaneous concentration files ("First Output Inst." and "Second Output Inst." files) and the surface tracer average concentration file ("Surface Concentrat." file). In addition, the Ozone Tool writes out tracer concentrations for selected receptor locations to an ASCII file ("Receptor Conc." file). The naming conventions for tracer species and the format of the receptor concentration file are discussed below.

**Timing Tracers**

Inert Tracer **Idddhhrrr**
Decay Companion Tracer **Ddddhhrrr**

**ddd** Julian day, e.g., 240
**hh** Hour tracer release started at, e.g., 12
**rrr** Region tracer released from, i.e., 001, 002, 003, etc

Examples: I24012001, D24100012

**Ozone Reaction Tracers**

Emission Sources **SSSeeerrr**

**SSS** Species type, i.e., NOX, VOC, O3V or O3N
**eee** Emissions group:
Single group, always 000
Multiple groups, 001, 002, etc.
**rrr** Region tracer released from, 001, 002, 003, etc.

Initial/Boundary **SSSeeerrr**

**SSS** Species type, i.e., NOX, VOC, O3V or O3N
**eee** Initial Concentrations: always 000
Boundary Concentrations not stratified by boundary: always 000
Boundary Concentrations stratified by boundary: WST, EST, STH, NTH, TOP indicating boundary of origin
**rrr** IC for Initial Concentrations, BC for Boundary Concentrations

Examples: NOX000015, VOC002015, O3V000IC, O3NTOPBC

**Figure 4-7**. Naming conventions for tracer species.

**Tracer Species Names**

The names of tracer species uniquely identify the information carried by each species and, taken as a group, identify the model configuration in any run. The naming conventions are defined in Figure 4-7. Species names have less than ten characters consistent with UAM convention.

**Receptor Concentration File**

Hourly average tracer concentrations at user specific receptor locations are output to the "receptor concentration" file. The file is in comma delimited ASCII format suitable for importing into a spreadsheet (a spreadsheet postprocessing tool is available to visualize the data in this file, as described below). An example output file is shown if Figure 4-8. Two header lines at the top of the file identify the model version and the date the run was performed. Next, two lines identify the time period covered by the file and the averaging interval (generally one hour, determined by the UAM simulation control file; EPA, 1990). Next, three lines define the model configuration and seven lines specify the numbers of tracer species that result from this configuration. The names of each tracer species are given on six lines ordered by tracer species type: the order in which species are listed here is the same as the order in which tracer concentrations are given later in the file.

The tracer species names are followed by the number of receptors and receptor names. Note that the first receptor (receptor 1) is always the location of the hourly peak ozone. Since the location of the hourly peak varies from hour to hour, the X and Y locations are left blank. Receptors 2 and higher are those specified in the "Receptor definition" file. The tracer concentrations are reported in blocks with a date and time stamp at the head of each block. Within each block, receptors are reported in numerical order. For each receptor, there are six lines of data for the tracer species identified at the heading "Tracer Names". All values are in UAM units of ppm. At the bottom of the data block for each receptor are two lines with three numbers: these are the total tracer $NO_X$, VOC, and ozone (first line) and regular UAM $NO_X$, VOC and ozone (second line).

```
URBAN AIRSHED MODEL, SOURCE APPORTIONMENT VERSION -- 960315 ,
Mon Apr 29 10:37:34 1996                ,

 File Duration  ,     87238,     15.00,     87238,     24.00,
Average Interval ,    1.0000

Number of timing periods     ,         2
Number of source areas       ,        17
Number of emission groupings ,         1
Number of tracer species     ,       144
Number of NOx species        ,        19
Number of VOC species        ,        19
Number of O3N species        ,        19
Number of O3V species        ,        19
Number of INERT TIME species ,        34
Number of DECAY TIME species ,        34

Tracer Names,
NOX000IC ,NOX000BC ,NOX001001,NOX001002,NOX001003,NOX001004,NOX001005 ..
VOC000IC ,VOC000BC ,VOC001001,VOC001002,VOC001003,VOC001004,VOC001005 ..
O3N000IC ,O3N000BC ,O3N001001,O3N001002,O3N001003,O3N001004,O3N001005 ..
O3V000IC ,O3V000BC ,O3V001001,O3V001002,O3V001003,O3V001004,O3V001005 ..
I23815001,I23815002,I23815003,I23815004,I23815005,I23815006,I23815007 ..
D23815001,D23815002,D23815003,D23815004,D23815005,D23815006,D23815007 ..

Number of receptors ,         6
  No,   Name,    Type,    Xloc,      Yloc,
   1, HourlyPeak,    1,          ,          ,
   2, Rubidoux  ,    0,     461.5,     3762.0,
   3, Pasadena  ,    0,     396.4,     3778.5,
   4, Lennox    ,    0,     373.0,     3755.0,
   5, Peak      ,    1,        45,         18,
   6, Region 10 ,    8,        31,         19,
                             32,         19
                             33,         19
                             34,         19,
                             31,         18,
                             32,         18,
                             33,         18,
                             34,         18,

Time Varying Tracer Data,

 Data for Period,     87238,     15.00,     87238,     16.00,
  Receptor,    1,
1.3265E-02, 1.3544E-09, 1.0000E-16, 1.0974E-15, 1.0000E-16, 1.0000E-16 ..
1.2237E-01, 3.3869E-08, 1.0000E-16, 1.6165E-14, 1.0000E-16, 1.0000E-16 ..
8.7304E-02, 1.1926E-08, 1.0000E-16, 1.0000E-16, 1.0000E-16, 1.0000E-16 ..
9.0300E-02, 1.5269E-08, 1.0188E-16, 2.6997E-15, 1.0213E-16, 1.0162E-16 ..
1.0036E-16, 4.0640E-15, 1.0036E-16, 1.0036E-16, 1.0036E-16, 1.0029E-16 ..
1.0000E-16, 3.7563E-15, 1.0000E-16, 1.0000E-16, 1.0000E-16, 1.0000E-16 ..
1.4500E-02, 1.2663E-01, 1.7770E-01,
1.4500E-02, 1.2663E-01, 1.7770E-01,
  Receptor,    2,
(File continues with data for remaining receptors and hours)
```

**Figure 4-8**. Example Receptor Concentration File. Lines ending ".." are truncated to fit the page, and the file would continue with data for additional receptors and hours in the same format.

## POSTPROCESSING

The Ozone Tool outputs hourly average tracer concentrations to two files:

| | |
|---|---|
| Surface Concentration | Hourly average concentration for tracers in surface layer. The file is in UAM average file binary format. |
| Receptor Concentration | Hourly average tracer concentrations at receptors specified in the "Receptor definition" file. The file has an ASCII format compatible with the Receptor Concentration file "browser" described below. |

The tracer concentrations in the "Surface Concentration" file can be displayed using any post-processing software normally used for displaying UAM average file outputs.

### Receptor Concentration file "browser"

The "Receptor Concentration" file contains information for all receptors and all hours within the model run that created the file. A post-processing tool is available to allow the user to "browse" through the information contained in this file and prepare displays like Figure 1-2. The "browser" is a Microsoft Excel Spreadsheet that is controlled by a graphical user interface (GUI) allowing you to rapidly visualize results for any receptor. To use this software, the user must have Microsoft Excel (version 5 or higher). The browser is comprised of three files:

| | |
|---|---|
| O3TOOL.XLS | - browser spreadsheet with displays for monochrome printers |
| O3TCOL.XLS | - browser spreadsheet with color displays |
| ENVIRON.XLA | - library of macro functions called by O3TOOL or O3TCOL |

All three files should be placed in a single directory. To use the browser, open either O3TOOL.XLS or O3TCOL.XLS as you would any Excel spreadsheet.

Instructions for using the browser are given below. The browser is GUI driven (point and click) and easy to use. The following instructions assume some familiarity with Excel.

1. Open Excel and then File/Open o3tool.xls. When the browser is opening you will may be asked if you want to re-establish links, say no. If you say yes, the links will likely fail resulting in warnings that may be safely ignored.

2. Move to the front sheet (controls) of o3tool. Click the "Import File" button at top left and select the data file to be visualized. The selected data file is imported as a second spreadsheet.

3. When the data file is opened, all of the information on the controls sheet is updated for the new file (numbers of tracers, receptors, etc.). To begin viewing the data, click the "Copy Receptor Data for Specified Time" button at top right to select the receptor (by number) and time to view results for. The user must also choose the method for rank ordering source contributions ("Sort by Sum" is a useful default choice). Click on

"OK" to proceed. On the next dialog box, choose how many source areas you want to see results for. About 4 is a good default, this value can be changed later. Click on "OK" to proceed.

4. The browser now finds the data requested, calculates the values needed to plot the bar and pie charts (on the "Calcs" sheet) and moves to the "GraphWork" sheet to view the summary graphs and tables.

5. Use the buttons to the right of the display to change the number of sources, change the hour, or print the graph. The receptor or file can be changed from this page also.

The graphs and tables shown on the "Calcs" sheet are standard Excel graphics that may be customized using Excel commands and features.

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