

DRAFT

Calculation of Reactivity Scales Using Regional Models

By
William P. L. Carter
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Abstract

Detailed procedures and algorithms for deriving measures relative ozone reactivities for volatile organic compounds (VOCs) from results of multi-cell regional model calculations are described. The objective is to provide a standard set of procedures, terminology, and documentation requirements that can be used by different groups and with different models to obtain comparable results. The metrics and procedures described are based on previous work of Carter et al (2003), "Investigation of VOC Reactivity Effects Using Existing Regional Air Quality Model," with additional detail given for applications using more detailed chemical mechanisms. The ozone reactivity metrics described are regional average ozone, regional average ozone over the standard, minimum substitution error, regional maximum incremental reactivity (MIR) and regional MIR to maximum ozone incremental reactivity (MOIR), relative to 1-hour or to 8-hour average daily maximum ozone. An Excel spreadsheet with calculations and macros illustrating the procedures discussed in this document is provided and discussed. Recommended reporting requirements for presentation of VOC reactivity results using regional models is described.

Contents

Background and Objectives	2
Methods and Procedure.....	3
Terms and Concepts	3
Choice of Model, Mechanism, Sensitivities to Calculate, and Quantification Basis	3
Base ROG Specification.....	9
Model Calculations.....	14
Initial Post-Processing.....	17
Daily Maximum 1-Hour O ₃	18
Daily Maximum 8-Hour O ₃	18
Calculation of Reactivity Metrics.....	19
Regional Average Ozone Metric (av).....	21
Regional Average Ozone Over Standard Metric (ovs).....	21
Minimum Substitution Error Metric (mse).....	22
Regional MIR Metric (mir).....	22
Regional MIR to MOIR metric (mm).....	22
Metrics Calculation Algorithm	22
Reactivity Computation for Compounds.....	23
Example Calculation and Macro Spreadsheet	25
Recommended Reporting Requirements	29
References.....	31
Appendix A. Base ROG Compositions and Model Species Assignments.....	33

Background and Objectives

Ground level ozone is formed in a complex series of gas-phase reactions involving the interactions of volatile organic compounds (VOCs) and NO_x in the presence of sunlight. VOCs can differ significantly in their impacts on ozone formation, and taking these differences in ozone “reactivity” into account in VOC regulations may provide a means to achieve ozone reductions in a more cost-effective manner than regulating all reactive VOCs equally. In order to do this, there needs to be some means to quantify relative effects of different types of VOCs on ozone, or ozone reactivity scale. This is complicated by the fact that the effect of VOCs on ozone is not an intrinsic property of the VOC alone, but also depends on the environment in which it is reacting. This includes, but is not necessarily limited to, the levels and emissions of other pollutants present, the length of time they are allowed to react, and physical aspects of the scenario such as dilution, transport, etc. (Carter and Atkinson, 1989; Carter, 1994, RRWG, 1999, and references therein).

The only practical way to represent how VOC reactivities depend on the environment is to calculate their ozone impacts using computer airshed models. Because of computer limitations, most previous comprehensive reactivity scales, including the Maximum Incremental Reactivity (MIR) scale (Carter, 1994) that was incorporated in California Vehicle (CARB, 1993) and aerosol coatings (CARB, 2000) regulations, were calculated using single-cell box or trajectory models. Such models are a highly simplified representation of ambient conditions, and provide no information on how ozone impacts vary over time and space under realistic ambient conditions. In order to represent ambient conditions realistically, and how ozone impacts differ over time and space, it is necessary to use multi-cell grid models.

The Reactivity Research Working Group (RRWG) has been organized to coordinate policy-relevant research related to VOC reactivity. One of the initial research priorities of the RRWG is to investigate how relative reactivity scales can be derived using more realistic multi-cell grid models. As part of an initial investigation of this, Carter et al (2003) utilized a grid model of the Eastern United States to calculate ozone impacts of VOC model species in a condensed chemical mechanism, which varied through time and space within the model domain. A companion study was carried out by Hakami et al (2003), using a similar domain but a different airshed model and a more detailed chemical mechanism. The results of the calculations of Carter et al (2003) were then used to derive a number of different reactivity scales, which differed depending on how ozone impacts were quantified, and the methods to derive single relative ozone impact quantifications from the highly variable impacts calculated for the multiple grid cells of the model. Fourteen different reactivity scales were derived for each different model domain and simulated day, based on two methods to quantify ozone impacts (1-hour and 8-hour daily maximum O_3) and seven methods to derive reactivity scales from the varying impacts throughout the domain. Of these seven methods, two were subsequently judged to be unsatisfactory because of extreme variability or numerical instability. This left five methods to derive reactivity scales for each of the two ozone impact quantifications that are considered to be worthy of further study.

In order to investigate the regional model reactivity metrics developed by Carter et al (2003) using more detailed chemical mechanism, Hanami et al (2004) analyzed the data of Hanami et al (2003) to derive metrics comparable to those of Carter et al (2003), and additional regional model reactivity studies are underway for the EPA. However, these follow-on studies have indicated that duplicating the metrics of Carter et al (2003) is not obvious or straightforward. In calculating the metrics, certain assumptions were made about how to prepare the input data for the ozone sensitivity calculations, how to discriminate in space and time, different averaging approaches in space and time, weighting fine and coarse grid cells, and post-processing of the data to obtain the results in the appropriate units.

Nomenclature employed by different investigators is not always consistent, and the reporting requirements have not been established.

In view of this, the American Chemistry Council (ACC), on behalf of the RRWG, contracted the author to produce a detailed and comprehensive documentation of procedures and algorithms for calculation of reactivity metrics of interest to the RRWG using regional models. The procedures are based on those initially developed by Carter et al (2003), but additional refinement is needed to make them applicable to use of detailed chemical mechanisms and specific chemical compounds, such as employed in the work of Hakami et al (2003, 2004) and future work using detailed mechanisms.

This report assumes that the reader is familiar with the operation of airshed models and previous work on reactivity carried out for the RRWG, specifically the work of Carter et al (2003) and Hamami et al (2003, 2004). Therefore, a detailed background of the concepts, chemical mechanisms, and models employed will not be provided. It is also expected that the procedures, documentation, and examples in this report these will be updated, clarified and modified following review and further input, so the present document should be considered to be preliminary and subject to change.

Methods and Procedure

Terms and Concepts

The concepts and terms are used throughout this report that need to be clearly understood to apply the procedures under discussion are listed and described in Table 1. The purpose of this table is to assure that there is no ambiguity concerning how these terms and concepts are used in this report, which may have somewhat different meanings and uses in other contexts. This table should be read completely before reading the remainder of this document. Other references should be consulted for more details concerning these concepts if they are not familiar to the reader.

Choice of Model, Mechanism, Sensitivities to Calculate, and Quantification Basis

A discussion of the most appropriate models, episodes, and scenario days for use of reactivity assessment is beyond the scope of this report, except to note that it is assumed that a multi-cell grid model is used and that the episode being simulated is such that exceedences of the ozone standard is being simulated. The most appropriate chemical mechanism depends on the model application, and a detailed discussion of this is also beyond the scope of this report. A highly condensed mechanism that adequately represents the range of reactivity characteristics of different types of VOCs may be adequate for the purposes of qualitative assessments of how reactivity scales vary with scenarios and scales, while a more detailed mechanism will probably be needed if impacts of specific chemicals are of interest. In any case, the mechanism should have either explicit representations or well-defined assignments of model species to all classes of VOCs whose reactivities are to be assessed and well-defined assignments of model species to all the VOCs that are in the base ROG mixture

As discussed below, the model simulations need to include at a minimum a simulation of the base case scenario, and simulations sufficient to determine sensitivities to total VOC emissions, total NO_x emissions, model species representing VOCs of interest, and of the base ROG mixture. If a condensed mechanism with a relatively limited number of VOC model species is being used, then the recommended approach is to calculate the sensitivities to all the VOC model species, from which the O₃ sensitivities and reactivities for any VOC compound and for the base ROG mixture can be determined (see, for example, Carter et al, 2003). If a detailed mechanism is being used, perhaps with selected individual compounds

Table 1. Definition of terms and concepts used throughout this report

Term or Concept	Definition and discussion
Chemical compound	Any chemical compound whose ozone impact is of interest (whether directly or because of its contribution to the Base ROG mixture (defined below), regardless of reactivity or EPA exempt status, and regardless of how it is represented in any airshed model. Not to be confused with the “model species” used to represent them in airshed models (discussed below). In order to calculate ozone impact of a chemical compound using this procedure, it is necessary to know how it is represented by the model species in the airshed model being used, and, if ozone impacts are to be quantified on a mass or carbon basis, its molecular weight or carbon number, respectively.
VOC	Any chemical compound whose ozone impact on a VOC reactivity scale is of interest, regardless of reactivity or EPA exempt status, and regardless of how it is represented in any airshed model, other than NO _x . This includes organic compounds included in VOC or TOG anthropogenic or biogenic emissions inventories, and, if applicable, other types of compounds that can promote O ₃ formation in manner similar to VOCs, such as CO, that may be included in inventories separate from VOC or TOG.
NO _x	The sum of NO, NO ₂ and (if applicable) HONO whose emissions are specified in anthropogenic or biogenic NO _x emissions inventories.
Airshed model	The software, methodologies, and scenario-independent databases needed to carry out a model simulation of ozone formation on a regional scale. The chemical mechanism and model species assignment methods is considered to be a part of the model, so if the model software is capable of representing multiple mechanisms, each option with a different mechanism is considered to be a different airshed model in the context of this discussion. The discussion in this report is applicable only to multi-cell Eulerian grid models. Application of trajectory or box models to calculate reactivities is not discussed. The use of model software capable of the Direct Decoupled Method (DDM), or some other method for directly calculating sensitivities of model outputs to changes in model inputs, is recommended but not required.
Model Scenario; Scenario	The geographical domain and time period being simulated by the airshed model and the input datasets that depend on the domain and time period being simulated, such as meteorological and emissions data.
day	A simulated day in the model scenario where simulated ozone impacts are of interest. “Spin-up” days included at the start of the model to remove dependences on initial conditions whose calculations are not of specific interest are not included. To calculate 8-hour average impacts, a full 24 hour day must be simulated plus 7 hours into the next day. In general the simulation will cover more than one simulated day, though in some contexts in the discussion below each simulated day will be treated as if it were a separate scenario. The simulated day depends at midnight in the time zone used for the model inputs and outputs, which usually would be the time zone in the major area of interest in the simulation.
simulated hour; hour	An hour of the simulated day over which a calculated quantity of interest is averaged. Hour 1 refers to the time from midnight to 1 AM in the time zone used

Table 1 (continued)

Term or Concept	Definition and discussion
cell	<p>for specifying model input and output</p> <p>Grid cell in the model domain. In the context of emissions input processing, this refers to all grids in the model domain into which emissions are input, elevated as well as ground level. In the context of processing of output data for O₃ sensitivity information, only ground cells in the portion of the domain where O₃ impacts are of interest are considered.</p>
Base Case Scenario	The model scenario where no changes are made to emissions or other inputs for sensitivity calculation purposes.
Direct sensitivity calculation method	The method of calculating sensitivities to an input parameter (in this case emissions) by conducting separate model calculations with the input parameter modified, then calculating the difference between that and the base case calculation.
DDM (or equivalent) sensitivity calculation method	The method of calculating sensitivities to input parameter by using software such as the Direct Coupled Method (DDM) (Dunker et al, 1980, 2002 and references therein) to calculate derivatives of outputs to inputs as part of the base case simulation by appropriate differentiation of the model equations.
Chemical Mechanism	The part of the airshed model used to represent chemical transformations. This can have varying levels of detail and may or may not have model species added to explicitly represent particular compounds for reactivity calculation purposes. The methodology used to assign model species to chemical compounds is considered to be a part of the chemical mechanism in the context of this discussion.
Model Species	The entities in the chemical mechanism used to represent reactions of emitted compounds. In the context of this discussion, the model species of interest are restricted to those used to represent emissions of VOCs and NO _x (where “VOC” and “NO _x ” are defined as indicated above). Not to be confused with actual compounds. Model species used for reactive intermediates that are not emitted are not considered in this discussion.
Model Species Quantification for Sensitivity Calculations	<p>The method used to quantify changes in emissions of model species when carrying out the calculations of the sensitivities of O₃ to these changes. The three alternatives considered here are carbon, molar, or mass based, as summarized on Table 2. The method determines the units of the initially calculated sensitivity results; i.e., if the carbon method is used the ozone impacts are changes in ozone per fractional change of model species carbon emitted. Note that in this context carbon, mass, or molar quantifications refer to <i>model species</i> carbon, mass, or moles, which may be different than the carbon, mass, or moles of the individual compounds the model species can be used to represent. Note also that the choice of this method does not affect the final reactivity scales results, provided that the post-processing procedures employed are appropriate for the method.</p> <p>Carter et al (2003) used the “carbon” model species quantification method for the sensitivity calculations, and the terminology employed throughout this document is based on this. However, the equations and methods described below are applicable regardless of the method employed, provided that the appropriate set of model species “carbon numbers” (see Table 2) are consistently employed throughout the analysis.</p>

Table 1 (continued)

Term or Concept	Definition and discussion
Model Species “Carbon Number” (relative weight used for model species sensitivity input)	<p>The relative weight of model species used in the model species quantification method employed in the sensitivity calculations, in terms of quantities per mole (see above). The specific meaning of these quantities for each of the approaches is indicated in Table 2. It is called “carbon number” in this document because use of the carbon method, as used by Carter et al (2003), is the preferred approach. However, use of the other approaches are also acceptable, provided that the “carbon number” values appropriate to the approach are consistently employed.</p> <p>Note that these quantities must be positive and nonzero for all model species, and should be of comparable orders of magnitude. Other than this, specific values chosen for these quantities should not affect the final results, provided that they are used consistently and the appropriate procedures are employed.</p>
Inert model species	<p>A model species (or virtual model species if not in the standard mechanism) used to represent emissions of VOC compounds considered to be unreactive. It must have a nonzero (usually unit) carbon number assigned to it. It must be included because it is needed for calculations of sensitivities relative to the base ROG mixture, which may contain compounds considered to be too unreactive to represent by any of the reactive model species in the mechanism.</p>
Explicit model species	<p>A model species that is not normally part of the mechanism or emitted in the base case scenario but that is added for the specific purpose of more accurately calculating the reactivity of particular compounds of interest that are normally represented by lumped model species. (This is not to be confused with model species representing compounds that are already represented explicitly in the mechanism used in the base case calculation, such as formaldehyde and ethene.) The rate constant and mechanistic parameters for this model species should be the recommended measured values or best estimates for the individual compound being represented. Such species should have zero emissions in the base case scenario</p>
Total VOC Emissions	<p>The total emissions flux into a grid cell of model species used to represent compounds in VOC emissions inventories. Does not include emissions of model species used to represent NO_x and CO, but does include emissions of model species used to represent biogenic organic compounds.</p>
Anthropogenic VOC Emissions	<p>The total emissions flux into a grid cell of model species used to represent compounds in anthropogenic VOC emissions inventories. Does not include emissions of model species used to represent NO_x and CO, or emissions of model species used to represent biogenic organic compounds, but can include compounds such as isoprene and terpenes in anthropogenic inventories.</p>
Base ROG Mixture	<p>A standard, model-and-scenario-independent mixture of chemical compounds that is used to represent emissions of non-methane organic compounds from all anthropogenic sources for the purposes of defining a standard for relative reactivity scales. Not to be confused with “Total Anthropogenic Emissions,” which depends on the model scenario used. The same Base ROG mixture should be used in all reactivity assessments in order to place relative reactivities calculated for different models and/or scenarios on the same basis.</p>
Sensitivity	<p>The effect of changing a specific input quantity on the computed concentration of ozone in a ground level cell, given in units of concentration change per relative</p>

Table 1 (continued)

Term or Concept	Definition and discussion
Relative Reactivity	change in the input quantity. The sensitivities that need to be calculated for relative reactivity assessment are sensitivities of ozone to total VOC emissions, total NO _x emissions, emissions of individual model species and emissions of the base ROG mixture. The units of these sensitivities depend on how the model species are input in the sensitivity calculations, as indicated on Table 2.
Relative Reactivity Basis	<p>The amount of additional ozone formed caused by adding a particular chemical compound to the emissions relative to the amount of additional ozone formed caused by adding an equal amount of the base ROG mixture. Depends on the basis for determining “an equal amount,” as indicated below.</p> <p>The units used to determine “an equal amount” of base ROG mixture for the purpose of defining relative reactivities. The options are as follows:</p> <p>“Mass” Ozone impact of the VOC divided by the impact of an equal mass of the base ROG mixture.</p> <p>“Moles” Ozone impact of the VOC divided by the impact of an equal number of moles of compounds in the base ROG mixture.</p> <p>“Carbons” ... Ozone impact of the VOC divided by the impact of an equal number of moles carbon of compounds in the base ROG mixture.</p> <p>Note that these quantifications refer to the mass, moles or moles carbon of the <i>compounds</i> in the base ROG mixture, not the model species used to represent them. Also, mass, moles, or moles carbon include the contributions of any inert species in the base ROG mixture.</p>
Reactivity Metric	A relative reactivity scale (set of relative reactivities for the various compounds for which this can be calculated) derived using a specific procedure as described in the text. Different procedures can be used depending on the relative importances assigned to sensitivities in different types of cells, and since relative as well as absolute sensitivities can vary from cell to cell the relative reactivities will differ depending on what procedure is used.

being represented explicitly using explicit model species added to that mechanism for that purpose (as in the study of Hakami et al, 2003, 2004), it may not be practical calculate sensitivities to all possible VOC species that can be represented in the mechanism. In this case the recommended approach is to directly calculate the sensitivities to the base ROG mixture, rather than deriving it from the sensitivities for its components. The specific procedures for either approach are discussed below.

The approach used by Carter (2004) for calculating box model reactivity scales is to use a lumped mechanism to represent the VOC emissions in the base case scenario and also for calculating the ozone sensitivity for the base ROG, and then add an explicit model species to the mechanism to ozone sensitivities for an individual compound. An analogous approach as applied to a grid model was employed by Hakami et al (2003) in carrying out regional model reactivity assessments for selected compounds represented by the SAPRC-99 detailed mechanism (Carter, 2000), except that multiple explicit model species were added to permit multiple sensitivities to be calculated in a single DDM calculation. In this case, the recommended approach is *not* to use the explicit model species to represent the base case or the components of the base ROG, but to have zero emissions of these model species in

the base case and when the base ROG sensitivity is being calculated. Otherwise, it would be necessary to re-process all the emissions datasets to represent the selected compounds explicitly for each set of compounds whose reactivities are being assessed, which most modelers would prefer to avoid. More significantly, it would result in the base case ozone and the sensitivities to the base ROG depending at least to some extent on the set of compounds whose sensitivities are being calculated, which is not acceptable. Both these problems can be avoided using the recommended procedure of using the lumped mechanism for the base case and the base ROG sensitivity calculations, and using the explicit species only to represent *additional* emissions of individual compounds added for sensitivity purposes.

An additional choice that needs to be made as to how the model species inputs are to be quantified for sensitivity calculation purposes. The three alternative options that could be employed are listed on Table 2. The option chosen should not affect the final results in terms of relative reactivity metrics that are ultimately calculated, but it will determine the units of the sensitivity results coming out of the initial model calculations and therefore the procedures that are needed to convert the results to the desired relative reactivity units (mass, molar, or carbon basis).

In the discussion and the terminology employed below we assume that the carbon quantification method is used for model species in the sensitivity calculations because that is the approach employed by Carter et al (2003). However, the other approaches are equally valid provided they are applied consistently throughout the analysis. The procedures, equations, and algorithms discussed below are applicable regardless of which approach is employed, with the only difference being what the “Carbon Number” (C^{ms}) means and how it is derived, and the units of some of the intermediate sensitivity results. These differences are discussed where applicable below.

Table 2. Alternative quantification methods for model species for sensitivity calculations.

Basis	Description	Meaning of “Carbon Number” (C^{MS}) in discussion below
Carbon	Sensitivities are initially computed on a per-carbon model species basis. This is the approach used by Carter et al (2003) and is used as the basis for the terminology in this approach. Has the advantage that it approximates mass and is well defined for most mechanisms.	Number of carbons assigned to the model species. Must be nonzero (use 1 if no carbons).
Mole	Sensitivities are initially computed on a per-mole basis. This is the approach used by Hakami et al (2003, 2004) for sensitivities to explicit model species. Has the advantage of simplicity for individual compounds but presents conceptual difficulties when computing reactivities for mixtures such as the base ROG.	Has no meaning. Must be 1 for all model species (including the unreactive model species), or C^{ms} can be removed from all the equations and algorithms given below
Mass	Sensitivities are initially computed on a per mass model species basis. Requires assigning a mass to all model species, which is not obvious or well defined in all mechanisms.	Molecular weight assigned to the model species. Must be nonzero.

Base ROG Specification

The quantities of interest in this work are *relative reactivities*, or reactivities relative to some standard base reactive organic gas (ROG) mixture designed to represent total anthropogenic emissions from all sources. In order to use a relative reactivity standard that is consistent across scenarios and episode days, a single standard mixture should be used to represent the base ROG mixture in all calculations, and its reactivities should be calculated based on those for the model species used to represent them in the model simulations. The alternative of using sensitivities to total anthropogenic emissions is not recommended because in general the composition of anthropogenic emissions may vary from scenario to scenario and over space and time in a given scenario. This would result in a standard that is not well defined. Therefore, the recommendation is to use a single mixture as a standard, so a relative reactivity of “1” will mean the same regardless of the scenario.

The composition of the base ROG mixture to serve as the standard for relative reactivity assessment is to some extent a policy decision. However, from a scientific perspective it could be based either on ambient air measurements, such as the base ROG mixture used in the EKMA reactivity scales of Carter (1994), or on total anthropogenic emissions input from some standard airshed scenario, as employed by Carter et al (2003). In either case, the composition needs to be given in terms of mass fractions of actual chemical compounds, with methane, unidentified mass, and nonvolatile mass removed. The compositions of the base ROG mixtures based on those used in the Carter (1994) or Carter et al (2003) studies are given in Table A-1 and Table A-2 in Appendix A. These are given in terms of actual chemical compounds based on the assignments in the current emissions speciation database of Carter (2005). Footnotes to the tables describe the derivations of the compositions in more detail.

In order to calculate the reactivities of the base ROG mixture for a particular model application, it is necessary to determine how this mixture is represented in terms of the model species used in the chemical mechanism employed. The recommended procedure for deriving this for models using the SAPRC-99, CB4, or RADM-2 mechanism is to employ the assignments and software provided with the Carter (2005) emissions speciation database, a discussion of which is beyond the scope of the present document. In any case, consistent speciation and model species assignments should be employed for all model scenarios, with the assignments of the base ROG components being based on how they are represented in the emissions in the base case scenario. In particular, the representation of the components of the base ROG should not depend on the set of compounds or model species whose reactivities are being assessed, and if explicit model species are added to the mechanism to represent reactions of individual compounds more explicitly than they are in the base case simulation, these should *not* be used to represent these compounds in the base ROG. Otherwise, emissions would have to be re-processed for each set of sensitivity calculations and the base ROG sensitivities may vary somewhat depending on which set of compounds are having their reactivities assessed.

The specific procedures to employ when representing and processing for the base ROG are given below. The notation and calculation equations employed are as follows:

Mechanism independent quantities (depends only on the base ROG composition):

c	Index for a chemical compound present in the base ROG
$MF^{ROG}(c)$	Mass fraction of compound c in the base ROG. Mechanism independent. Note that the equations given below require that this be properly normalized, i.e., that $\sum_c MF^{ROG}(c) = 1$.
MW(c)	Molecular weight of chemical compound c.

$nC(c)$ Number of carbons in chemical compound c . (Note that, unlike model species “carbon numbers”, $nC(c)$ is independent of the model species quantification method used for the sensitivity calculations.)

MW^{ROG} Effective molecular weight of the base ROG, i.e., mass per mole of mixture. Given by

$$MW^{ROG} = 1 / \left\{ \sum_c [MF^{ROG}(c)/MW(c)] \right\}$$

nC^{ROG} Effective carbon number (carbons per mole of mixture) of the base ROG. Given by

$$nC^{ROG} = \left\{ \sum_c [MF^{ROG}(c) nC(c) / MW(c)] \right\} MW^{ROG}$$

Mechanism-dependent quantities:

i Index for a model species in the chemical mechanism used in the model, including the model species used to represent unreactive carbon. If no inert model species is used in the model, then a “virtual” model species is added for this purpose.

$Rep(c,i)$ Moles of model species i used to represent one mole of compound c for a particular mechanism in the base case model simulation. In general, for lumped molecule mechanisms such as SAPRC or RADM there may be only one model species where $Rep(c,i)$ is nonzero, but for lumped structure mechanisms such as CB4 there may be more than one model species used to represent a compound.

$MM^{ROG}(i)$ Moles of model species i per gram of base ROG. Given by

$$MM^{ROG}(i) = \sum_c Rep(c,i) MF^{ROG}(c) / MW(c)$$

This is not necessarily the same as $1/MW^{ROG}$ because some mechanisms may use different numbers of moles of model species to represent one mole of compound.

$C^{MS}(i)$ Carbon number or model species weighting for model species i . The meaning of this quantity and how it is derived depends on which model species quantification method is used in the sensitivity calculations, as indicated in Table 2.

The values of C^{MS} to use if the “carbon” method is employed are given in Table 3 for the Carbon Bond mechanism and Table 4 for fixed-parameter SAPRC-99. A different set of carbon assignment could be used, but a consistent set of assignments must be used for any given scenario.

If sensitivities are to be calculated on a per-mole model species basis, then $C^{MS}(i) = 1$ for all model species.

If sensitivities are to be calculated on a per-mass model species basis, then $C^{MS}(i)$ is the molecular weight used for the model species in the model calculation, or some other molecular weight for the types of compounds being represented.

The particular assignments of carbon numbers or molecular weights are not important as long as they are consistent throughout the analysis for a given model scenario.

MWC^{ROG} Grams of base ROG mixture per mole carbon* model species representing the mixture. Given by

$$MWC^{ROG} = 1 / \sum_i C^{ms}(i) MM^{ROG}(i)$$

Note that the unreactive model species (or virtual model species) is included in this sum. Note also that MWC^{ROG} depends on the mechanism because not all mechanisms accurately represent carbon numbers for the mixtures being represented, and MWC^{ROG}

is defined in terms of *model species* carbons.

* If sensitivities are being calculated on a mole model species basis, then this is the mass of the base ROG mixture divided by the total number of moles of model species used to represent it. This is not necessarily the same as MW^{ROG} because not all the compounds may be represented on a mole per mole basis.

If sensitivities are being calculated on a mass model species basis, then this is the number of grams of model species used to represent 1 gram of the base ROG. It will probably be something other than one unless the molecular weights of the lumped model species are adjusted to exactly correspond to those of the compounds in the base ROG they represent. Such adjustment is not necessary.

$FC^{ROG}(i)$ Moles of model species *i* per mole model species carbon* of base ROG. Given by

$$FC^{ROG}(i) = MM^{ROG}(i) MWC^{ROG}$$

* If sensitivities are being calculated on per-mole basis, then this is the mole fraction of model species *i* in the representation of the base ROG.

If sensitivities are being calculated on a mass model species basis, then this is the moles of model species *i* used to represent one gram of model species in the base ROG.

An algorithm that can be used for calculation of MW^{ROG} , nC^{ROG} , MWC^{ROG} and the MM^{ROG} and FC^{ROG} values for any given base ROG mixture and mechanism is as follows:

```

MWROG=0.
nCROG=0.
for c=1 to number_of_compounds
    MWROG = MWROG + (MFROG(c)/MW(c))
    nCROG = nCROG + (MFROG(c)*nC(c)/MW(c))
next c
MWROG = 1./MWROG
nCROG = nCROG * MWROG

TOTMSC=0.
TOTCC=0.
for i=1 to number_of_model_species
    MMROG(i)=0
    for c=1 to number_of_compounds
        MMROG(i)= MMROG(i)+(Rep(c,i)*MFROG(c)/MW(c))
    next c
    TOTMSC = TOTMSC + (CMS(i)*MMROG(i))
next i
MWCROG = 1/TOTMSC
for i=1 to number_of_model_species
    FCROG(i) = MMROG(i)*MWCROG
next i

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This algorithm assumes that $\sum_c MF^{ROG}(c) = 1$. If this cannot be assured, then this total mass needs to be calculated and the “1” in the equation defining MWC^{ROG} should be changed to this total mass.

The values of MW^{ROG} and FC^{ROG} calculated using this procedure are given in in Table 3 for the Carbon Bond mechanism and Table 4 for fixed-parameter SAPRC-99 for the base ROG mixtures given in Table A-1 and Table A-2. Note that because of changes and updates to the speciation database

Table 3. Model species used in the Carbon Bond 4 mechanism, their carbon numbers, and representations of various base ROG mixtures in that mechanism.

Model Species	Model Species Carbons (C ^{MS})	EMITBAS1 [a]			ARBROG94 [b,c]
		Carter et al (2005)	Current [c]	Diff.	
MWC ^{ROG}		17.150	17.150		14.328
MW ^{ROG} [d]		69.36			68.54
NC ^{ROG} [d]		4.044			4.784
FC ^{ROG} (moles/ moles C) x 1000					
PAR	1	547.0	568.2	4%	568.0
OLE	2	20.0	19.7	-1%	13.3
TOL	7	12.0	12.9	7%	13.1
XYL	8	8.0	7.7	-4%	16.4
FORM	1	10.0	10.5	5%	10.0
ALD2	2	19.0	14.3	-32%	24.9
ETH	2	21.0	21.4	2%	13.5
ISOP	5	0.4	0.4	-6%	1.3
MEOH	1	5.0	5.2	4%	-
ETOH	2	21.0	21.3	2%	-
UNR [e]	1	124.0	108.3	-15%	88.8

[a] Mixture used by Carter et al (2003), based on emissions data provided by the EPA (EPA, 1998). See Table A-2.

[b] Mixture used by Carter (1994), based on air quality data. See Table A-1.

[c] Calculated using the Carter (2005) speciation assignments and programs as of 2/21/05.

[d] Mechanism independent

[e] Unreactive model species.

Table 4. Model species used in the condensed version of the SAPRC-99 mechanism, their carbon numbers, and representations of various base ROG mixtures in that mechanism.

Model Species	Model Species Carbons	EMITBAS1 [a]	ARBROG94 [b]
MWC ^{ROG}		15.509	14.912
MW _{ROG} [d]		69.36	68.54
NC ^{ROG} [d]		4.044	4.784
FC ^{ROG} (moles/ moles C) x 1000			
ALK1	2	9.37	17.54
ALK2	3	16.67	24.85
ALK3	4	37.97	27.49
ALK4	5	34.15	35.22
ALK5	8	32.21	18.67
ETHE	2	18.39	14.01
OLE1	5	10.60	11.27
OLE2	5	6.91	12.44
ISOP	5	0.34	1.35
TERP	10	0.66	0.73
ARO1	7	12.10	13.82
ARO2	9	6.50	17.09
HCHO	1	8.88	8.25
CCHO	2	1.97	4.97
RCHO	3	1.46	2.93
BALD	7	-	-
ACET	3	4.24	3.21
MEK	4	2.58	1.14
PRD2	6	1.56	-
MEOH	1	4.71	-
GLY	2	0.10	-
MGLY	3	0.07	-
BACL	4	-	-
PHEN	6	0.48	-
CRES	7	0.33	-
MACR	4	1.03	-
MVK	4	0.14	-
IPRD	5	0.07	-
NROG [d]	1	10.11	2.59

[a] Calculated using the Carter (2005) speciation assignments and programs as of 2/21/05.

[b] Mixture used by Carter et al (2003), based on emissions data provided by the EPA (EPA, 1998). See Table A-2.

[c] Mixture used by Carter (1994), based on air quality data. See Table A-1.

[d] Mechanism independent

assignments made since the base ROG mixture for the Carter et al (2003) study, the current recommended CB4 representation of the base ROG mixture used in that study is somewhat different than that actually employed by Carter et al (2003). Therefore, Table 3 also includes the CB4 species distribution actually used for that base ROG mixture in the Carter et al (2003) study, and the differences between that and the current recommended distribution.

Model Calculations

The input data to the reactivity analysis are provided by airshed model calculations of sensitivities of ground-level O₃ to changes in emissions. The sensitivities can be computed either using the DDM method or by direct calculation by varying the emissions, but should be for the limit of small changes of emissions (i.e., derivatives). Because of the dependence of O₃ on emissions is non-linear and because of numerical uncertainties, the DDM method would in principle yield the most precise and reliable results, and is the preferred approach. However, the principal is the same if the sensitivities are calculated by directly by varying the emissions, as discussed below.

The base calculation is the simulation of the scenario for which the reactivity scale is to be derived. In general, this will be a multi-day simulation with numerous grid cells that may have varying sizes. For the purpose of this reactivity analysis, each day of the simulation is treated as if it is a separate episode, and only ground-level ozone results are used. Data from “spin up” days in the simulation, which are sensitive to initial or boundary conditions, should not be used for reactivity results. The following nomenclature and data are used for the results of the base case simulation:

j	Index a ground-level cell in the model domain where O ₃ is calculated.
N	Number of ground level cells
W(j)	Relative importance of cell j in determining overall reactivity. Determined by policy considerations. For this work, W(j)=1/N if all cells are the same size, or W(j)=A(j) / Σ _j A(j) if the ground-level cells have varying sizes, where A(j) is the ground area covered by the cell. (Unitless)
d	Day of the simulation where O ₃ impacts are of interest.
h	Hour of the simulated day
[O ₃] ^{base} (j,h,d)	Hourly average O ₃ calculated for cell j for hour h for day d. It doesn't matter if it is defined by the beginning or ending time of the hour as long as it is consistent for base case and emissions varying calculations. (Units = concentration)

Note that the hourly average O₃ values for the ground cells, [O₃]^{base}(j,h,d), are the only computed values that are needed from the base case calculation. These are computed as part of the DDM sensitivity calculations if that approach is used.

The episode day is defined as being from midnight to midnight for the time zone used for specifying inputs and outputs of the model calculations, which usually would be the largest population exists in the receptor area of interest in the modeling domain. The averages are associated with the time at the end of the hour, with the first being 0100 (1 AM) and the last being 2400 (12 midnight) on the simulated day in the applicable time zone.

Three or four types of sensitivity calculations with modified emissions (or their equivalents in terms of DDM computations) are needed for VOC reactivity assessment. The following nomenclature and data are used for the input and results of these calculations.

X	The type of emissions that is being varied. For reactivity assessments, it could be either “VOC” for total VOC, “NO _x ” for total NO _x , “MS(i)”, for VOC model species “i”, or “ROG” for the base ROG. See below for a discussion of how these emissions are varied.
t	Time (for emissions input)
$E^{\text{MS}}_{\text{tot}(i,t,j,d)^{\text{base}}}$	Total emissions of model species i from all sources (anthropogenic and biogenic) in the base case scenario at time t in cell j on day d, in units of moles per unit time. Note that in this case “j” refers to all cells into which emissions occur, not just ground-level cells.
$E^{\text{MS}}_{\text{as}(i,t,j,d)^{\text{base}}}$	Total emissions of model species i from anthropogenic sources in the base case scenario at time t in cell j on day d, in units of moles per unit time.
$E^{\text{VOC}}_{\text{tot}(t,j,d)^{\text{base}}}$	Total VOC emissions from all anthropogenic and biogenic sources at time t in cell j on day d, in units of moles carbon* of model species per unit time. Given by: $E^{\text{VOC}}_{\text{tot}(t,j,d)^{\text{base}}} = \sum_i C^{\text{ms}}(i) E^{\text{MS}}_{\text{tot}(i,t,j,d)^{\text{base}}}$ <p>Note that this summation includes emissions of the unreactive model species for the purpose of the calculations discussed here, even if this need not actually be represented in the model.</p>
$E^{\text{VOC}}_{\text{as}(t,j,d)^{\text{base}}}$	Total VOC emissions from all anthropogenic sources at time t in cell j on day d, in units of moles carbon* of model species per unit time. Given by: $E^{\text{VOC}}_{\text{as}(t,j,d)^{\text{base}}} = \sum_i C^{\text{ms}}(i) E^{\text{MS}}_{\text{as}(i,t,j,d)^{\text{base}}}$ <p>Note that this summation includes emissions of the unreactive model species for the purpose of the calculations discussed here, even if this may not actually be represented in the model.</p>
$E^{\text{NO}_x}_{\text{tot}(t,j,d)^{\text{base}}}$	Total NO _x emissions from all sources (anthropogenic and biogenic) at time t in cell j on day d, in the base case scenario, in units of moles nitrogen of model species per unit time
δ	A unitless quantity indicating the extent to which the emissions were changed in the sensitivity calculation. How the change is made depends on “X”, the type of emissions being varied, as indicated below. For DDM calculations, the results are computed for $\lim(\delta) \rightarrow 0$. For sensitivity calculations by difference, δ should be sufficiently large that the emissions change causes results that are greater than numerical uncertainty, but sufficiently small that the results approximate those for arbitrarily small δ. Ideally, if calculation by difference is used, then calculations should be done with at least two different values of δ to determine the limit as $\delta \rightarrow 0$.
$E^{\text{MS}}_{\text{tot}(i,t,j,d,\delta)^{\text{X}}}$	Total emissions of model species i from all sources (anthropogenic and biogenic) at time t in cell j on day d, in units of moles per unit time, in the sensitivity calculation where the sensitivity to emissions type “X” is being determined. Given by $E^{\text{MS}}_{\text{tot}(i,t,j,d,\delta)^{\text{VOC}}} = (1+\delta) E^{\text{MS}}_{\text{tot}(i,t,j,d)^{\text{base}}}$ <p>for calculating sensitivity to total VOC, or by $E^{\text{MS}}_{\text{tot}(i,t,j,d,\delta)^{\text{MS}(i)}} = E^{\text{MS}}_{\text{tot}(i,t,j,d)^{\text{base}}} + \delta E^{\text{VOC}}_{\text{as}(t,j,d)^{\text{base}}} / C^{\text{ms}}(i)$ </p>

$$E^{MS_{tot}(i',t,j,d,\delta)^{MS(i)}} = E^{MS_{tot}(i',t,j,d)^{base}} \text{ (if } i' \neq i \text{)}$$

for calculating sensitivity to model species i , $MS(i)$, or by

$$E^{MS_{tot}(i,t,j,d,\delta)^{ROG}} = E^{MS_{tot}(i,t,j,d)^{base}} + \delta FC^{ROG}(i) E^{VOC_{as}(t,j,d)^{base}}$$

for calculating sensitivity to the base ROG mixture (if needed), or by

$$E^{MS_{tot}(i,t,j,d,\delta)^{NO_x}} = E^{MS_{tot}(i,t,j,d)^{base}}$$

for calculating sensitivity to total NO_x .

$E^{NO_x_{tot}(t,j,d,\delta)^X}$ Total NO_x emissions from all sources (anthropogenic and biogenic) at time t in cell j on day d , in units of moles nitrogen of model species per unit time in the sensitivity calculation where the sensitivity to emissions type “X” is being determined. Given by

$$E^{NO_x_{tot}(t,j,d,\delta)^{NO_x}} = (1 + \delta) E^{NO_x_{tot}(t,j,d)^{base}}$$

for calculating sensitivity to total NO_x , and by

$$E^{NO_x_{tot}(t,j,d,\delta)^X} = E^{NO_x_{tot}(t,j,d)^{base}}$$

otherwise. Note that the speciation of NO_x (e.g., fraction of NO , NO_2 and $HONO$ if applicable) is not changed.

$[O_3]^X(j,h,d,\delta)$ Hourly average O_3 calculated for cell j for hour h for day d for the sensitivity calculation on emissions type “X” varied by δ . (Units = concentration)

$S^X(j,h,d)$ Hourly average sensitivity of O_3 in cell at hour h on day d in cell j to changes in X. Computed by

$$S^X(j,h,d) = \lim(\delta \rightarrow 0) \{ [O_3]^X(j,h,d,\delta) - [O_3]^{base}(j,h,d) \} / \delta$$

in sensitivity calculations by difference. In DDM calculations, the $S^X(j,h,d)$ are obtained from hourly averages of the corresponding calculated instantaneous sensitivities. (Note that the derivative of the average is the same as the average of the derivative.) (Units = concentration per fractional emissions change, on a per-carbon* basis for VOC, $MS(i)$ and ROG, and on a per-nitrogen basis for NO_x .)

* If molar or mass quantification of model species is used in the sensitivity calculation is used, the units are moles or grams of model species, rather than moles carbon.

In the first type of sensitivity calculation ($X=VOC$), the emissions of all VOCs, both biogenic and anthropogenic, is increased by a factor of $(1+\delta)$. The same factor increase is applied to all VOC sources at all times and locations in the modeling domain, so there is no change in relative temporal or spatial distribution of VOC emissions. Initial or boundary VOC levels are not changed. Note that the $S^{VOC}(j,h,d)$ data are only needed for computing MIR or MOIR-to-MIR scales, so if these scales are not needed then these need not be calculated.

In the second type of sensitivity calculation ($X=NO_x$), the NO_x emissions from all sources (biogenic and anthropogenic) are increased by a factor of $(1+\delta)$. The same factor increase is applied to all NO_x sources, and there is no change in relative temporal or spatial distribution of NO_x emissions. Initial or boundary NO_x levels are not changed. As with $S^{VOC}(j,h,d)$, the $S^{NO_x}(j,h,d)$ data are only needed for computing MIR or MOIR-to-MIR scales.

The third type of sensitivity calculation consists of a separate calculation for each reactive VOC model species of interest ($X=MS(i)$, where $MS(i)$ is model species “i”). In this calculation, total carbon (or total molar or mass, depending on the model species sensitivity quantification method) emissions from

all anthropogenic VOC sources increased by a factor of $(1+\delta)$ by adding the necessary amount of model species (i) to cause this increase. Emissions of other model species are not affected. The increased emissions have the same temporal and spatial distribution as the total of anthropogenic emissions. The amount of MS(i) added as a function of time and space depends only on the total amount of anthropogenic VOC carbons emitted at that time and location, not on the speciation of those emissions. The way this is calculated is shown above.

The base ROG sensitivity also needs to be calculated. If the sensitivities for all the non-inert model species needed to represent the base ROG are already being calculated, then the sensitivity to the base ROG is given by

$$S^{\text{ROG}}(j,h,d) = \sum_i FC^{\text{ROG}}(i) C^{\text{ms}}(i) S^{\text{MS}(i)}(j,h,d)$$

and it need not be calculated explicitly. (Note that the sensitivity to the inert model species is by definition zero, so it need not be included in the summation.) If the sensitivities are not being calculated for all the non-inert model species used to represent the base ROG, then it needs to be calculated explicitly. In this calculation, total carbon emissions from all anthropogenic VOC sources increased by a factor of $(1+\delta)$ by adding the necessary amount of the model species mixture representing the base ROG to cause this increase. The way this is calculated is shown above. The increased emissions have the same temporal and spatial distribution as the total of anthropogenic emissions., and will depend only on the total amount of anthropogenic VOC carbons emitted at that time and location, not on the speciation of those emissions.

To summarize, the output from the DDM or base case and sensitivity calculations consist of arrays of $d, j, h, W(j)$ (if applicable), $[O_3]^{\text{base}}(j,h,d)$, and $S^X(j,h,d)$, for $X=(\text{VOC}, \text{NO}_x, \text{ROG}, \text{and MS}(i))$ for each model species whose sensitivity is calculated). Generally, separate files are used for each day.

Initial Post-Processing

The initial post-processing reduces the data to a single O_3 value and set of sensitivity values for each ground-level cell for each simulated day and each type of O_3 quantification method. For this work, the O_3 quantification methods used are daily maximum 1-hour average and daily maximum 8-hour average. Separate post-processing is done for each of these two methods, as discussed below. The nomenclature used is as follows:

- $h1(j,d)$ Hour h where $[O_3]^{\text{base}}(j,h,d)$ has the highest value for a given ground level cell j and simulated day d . If two or more hours of the day have exactly the same O_3 in a cell, then this is the first hour with that maximum O_3 .
- $[O_3]^{\text{max},1}(j,d)$ Daily maximum 1-hour average O_3 in cell j on day d . Given by

$$[O_3]^{\text{max},1}(j,d) = [O_3]^{\text{base}}(j,h1,d)$$
- $S^{X,1}(j,d)$ Sensitivity of the daily maximum 1-hour average O_3 to X . Given by

$$S^{X,1}(j,d) = S^X(j,h1,d)$$
- $h8(j,d)$ Hour $h8$ where $\sum_{h=0..7} [O_3]^{\text{base}}(j,h8+h,d)$ has the highest value for a given ground level cell j and simulated start day d . Note that if $h8+h>24$ then $[O_3]^{\text{base}}(j,h8+h,d)$ is given by $[O_3]^{\text{base}}(j,h8+h-24,d+1)$. Note also that this cannot be computed for the last day of the simulation. If more than one hour in a day has the exact same value of this sum, then the first such hour is used.

- $[O_3]^{\max,8}(j,d)$ Daily maximum 8-hour average O_3 in cell j on day d . Given by

$$[O_3]^{\max,8}(j,d) = \sum_{h=0..7} [O_3]^{\text{base}}(j,h8+h,d) / 8$$
Note that if $h8+h > 24$ then $[O_3]^{\text{base}}(j,h8+h,d)$ is given by $[O_3]^{\text{base}}(j,h8+h-24,d+1)$.
- $S^{X,8}(j,d)$ Sensitivity of the daily maximum 8-hour average O_3 to X . Given by

$$S^{X,8}(j,d) = \{ \sum_{h=0..7} S^X(j,h8+h,d) \} / 8$$
Note that if $h8+h > 24$ then $S^X(j,h8+h,d)$ is given by $S^X(j,h8+h-24,d+1)$.
- $S^{\text{Mi},1}(j,d)$ Same as $S^{X,1}(j,d)$ or $S^{X,8}(j,d)$, respectively, where “X” refers to model species i .
- $S^{\text{Mi},8}(j,d)$

Daily Maximum 1-Hour O_3 .

For each ground level cell, j , and simulated day d , the hour $h1$ is found where $[O_3]^{\text{base}}(j,h,d)$ has the highest value. The sensitivities given for that hour are taken as the sensitivities for the 1-hour maximum O_3 . The algorithm is as follows:

```

for d=1 to number_of_days
  for j=1 to number_of_cells
    h1=1
     $[O_3]^{\max,1}(j,d) = [O_3]^{\text{base}}(j,1,d)$ 
    for h=2 to 24
      if  $[O_3]^{\text{base}}(j,h,d) > [O_3]^{\max,1}(j,d)$  then
        h1=h
         $[O_3]^{\max,1}(j,d) = [O_3]^{\text{base}}(j,h,d)$ 
      endif
    next h
    for X = 1 to number_of_sensitivities
       $S^{X,1}(j,d) = S^X(j,h1,d)$ 
    next X
  next j
next d

```

This yields a dataset consisting of an array of daily maximum 1-hour average O_3 concentrations and sensitivities of this to total VOC, NO_x , and to each VOC model species for each ground level cell for each day of interest in the simulation.

Daily Maximum 8-Hour O_3

For each ground level cell, j , and simulated day d , except for the last day, the hour $h8$ is found where the average of this and the seven subsequent hourly average values of $[O_3]^{\text{base}}(j,h,d)$ has the highest value. The average of the sensitivities given for those 8 hours are taken as the sensitivities for the 8-hour maximum O_3 . The algorithm is as follows:

```

dimension o3tmp(7+number_of_days*24)
dimension SensTmp(number_of_sensitivities, 7+number_of_days*24)
for j=1 to number_of_cells
  h=0
  d=1
  for hh=1 to 7+(number_of_days-1)*24
    h=h+1

```

```

    if h>24 then
        h=1
        d=d+1
    endif
    O3tmp(hh)= [O3]base(j,h,d)
    for X = 1 to number_of_sensitivities
        SensTmp(X,hh)= SX(j,h,d)
    next X
next hh
for hh=1 to (number_of_days-1)*24
    for h=1 to 7
        o3tmp(hh)=o3tmp(hh)+ o3tmp(hh+h)
    next h
next hh
for d=1 to number_of_days-1
    h0=24*(d-1)
    h8=h0+1
    [O3]max,8(j,d) = O3tmp(h0+1)
    for h=2 to 24
        if O3tmp(h0+h) > [O3]max,8(j,d) then
            h8=h0+h
            [O3]max,8(j,d) = O3tmp(h8)
        endif
    next h
    [O3]max,8(j,d) = [O3]max,8(j,d)/8
    for X=1 to number_of_sensitivities
        SX,8(j,d)=SensTmp(X,h8)
        for hh=h8+1 to h8+7
            SX,8(j,d)= SX,8(j,d)+ SensTmp(X,hh)
        next hh
        SX,8(j,d)= SX,8(j,d)/8
    next X
next d
next j

```

Note that this algorithm assumes that d=1 means the first day for which reactivities are to be calculated, which in general will not be the first day of the simulation because of the need for “spinup” days to remove the effects of initial conditions. Note also that the daily maximum 8-hour average O₃ reactivities cannot be calculated for the last day because of the need for data past midnight of that day in order to calculate data on the same basis of the previous days.

This procedure yields a dataset consisting of an array of daily maximum 8-hour average O₃ concentrations and sensitivities of this to total VOC, NO_x, and to each VOC model species for each ground level cell for each day of interest in the simulation except for the last day.

Calculation of Reactivity Metrics

The above procedures give absolute reactivities for each cell and episode day of interest, either relative to 1-hour or 8-hour daily maximum ozone. The procedures below are used to derive a single reactivity metric or scale from the data in all the ground level cells for each episode day. The procedure is the same regardless of whether daily maximum 1-hour average or daily maximum 8-hour average reactivities are being considered, so in the discussion below we will omit the indications of the averaging time. The nomenclature and definition of terms employed is given below.

j	Index a ground-level cell in the model domain where O ₃ is calculated.
N	Number of ground level cells
d	Day of the simulation where O ₃ impacts are of interest.
i	Index for model species for which reactivities are to be calculated
S ^{VOC} (j,d)	Sensitivity of the maximum 1-hour or 8-hour daily average O ₃ to total VOC emissions for cell j on day d. Given by S ^{X,1} (j,d) or S ^{X,8} (j,d), where X = total VOC.
S ^{NOx} (j,d)	Sensitivity of the maximum 1-hour or 8-hour daily average O ₃ to total NO _x emissions for cell j on day d. Given by S ^{X,1} (j,d) or S ^{X,8} (j,d), where X = total NO _x .
S ^{ROG} (j,d)	Sensitivity of the maximum 1-hour or 8-hour daily average O ₃ to emissions of the base ROG mixture for cell j on day d. Given by S ^{X,1} (j,d) or S ^{X,8} (j,d), where X = base ROG.
S(i,j,d)	Sensitivity of the maximum 1-hour or 8-hour daily average O ₃ to emissions of the model species i for cell j on day d. Given by S ^{X,1} (j,d) or S ^{X,8} (j,d), where X = MS(i).
j ^{MIR} (d)	Index of cell where S ^{VOC} (j,d) has the maximum value for day d, for all the cells where S ^{NOX} (j,d) are negative.
[O ₃] ^{max} (j,d)	The daily maximum 1-hour or 8-hour average O ₃ for cell j and day d. Given by [O ₃] ^{max,1} (j,d) or [O ₃] ^{max,8} (j,d).
W(j)	Relative importance of cell j in determining overall reactivity. Determined by policy considerations. For this work, W(j)=1/N if all cells are the same size, or W(j)=A(j) / Σ _j A(j) if the ground-level cells have varying sizes, where A(j) is the ground area covered by the cell. (Unitless)
[O ₃] ^{std}	The ozone exceedences standard concentration for the averaging method being used. Currently 0.12 ppm for 1-hour averages and 0.08 ppm for 8-hour averages.
{logical expression}	Equals 1 if the logical expression is true or zero if it is false. For example, {[O ₃] ^{max} (j,d) > [O ₃] ^{std} } is 1 if the maximum O ₃ in cell j on day d exceeds the O ₃ standard for the averaging period used and is 0 if it does not.
s	Refers to the type of relative reactivity scale, as discussed below.
RR(i,s,d)	The relative reactivity for model species i for scale s for day d. The expression used to calculate it depends on the scale being used, as discussed below. Note that these values depend on the quantification method used for model species in the sensitivity calculations, i.e., how the C ^{MS} quantities are specified, as indicated on Table 2.

Carter et al (2003) considered a total of seven methods to derive global reactivity scales or metrics from the distribution of the reactivities in the various cells in the episode day. However, use of the regional maximum ozone metric is not recommended because it can reflect sensitivities in regions that are insensitive to VOC emissions, and the use of the “minimum substitution error method 2” method is not recommended because it can be numerically unstable. The remaining five metrics, which are recommended for consideration, are summarized in Table 5. The methods for calculating their relative reactivities are discussed below.

Regional Average Ozone Metric (av)

This metric reflects the effects of the VOCs on ozone formation in all locations, weighting ozone at all locations equally, or based on some criterion that is independent of the calculation results. Relative reactivities in this scale, $RR(i,av,d)$, are given by

$$RR(i,av,d) = \sum_j W(j) * S(i,j,d) / \sum_j W(j) * S^{ROG}(j,d)$$

As indicated above, $W(j)$ is the weight the data in the cell is given to the reactivity total. If the objective is to weigh all locations equally, then $W(j)$ would be 1 if all cells were of the same size, or would be proportional to the surface area of the cell if not. The regional average O_3 metrics given by Carter et al (2003) used $W(j)=1$ because domains with different grid size were treated separately. It may be desirable not to include cells over water or unpopulated areas in the averages, in which case the excluded cells could be given $W(j)$ of zero. However, all ground-level cells were counted when this metric was calculated by Carter et al (2003).

Regional Average Ozone Over Standard Metric (ovs)

This metric reflects the effects of the VOCs on ozone formation in locations where the ozone standard for the particular averaging method is exceeded. Relative reactivities in this scale, $RR(i,ovs,d)$, are given by

$$RR(i,ovs,d) = \sum_j W(j) * \{ [O_3]^{max}(j,d) > [O_3]^{std} \} * S(i,j,d) / \sum_j W(j) * \{ [O_3]^{max}(j,d) > [O_3]^{std} \} * S^{ROG}(j,d)$$

Table 5. Summary of alternative global reactivity metrics examined in this report

Code	Designation	Description
av	Regional Average Ozone	Average of incremental reactivities (absolute O_3 impacts) throughout the entire domain. Same as effect of the VOC on the domain-wide average ozone.
ovs	Regional Average O_3 Over the Standard	Average of incremental reactivities (absolute O_3 impacts) for all grid cells where the ozone levels exceeds the specified standard (120 ppb for daily 1-hour maximum, 80 ppb for daily 8-hour maximum).
mse	Minimum Substitution Error	Relative reactivity that minimizes the change in ozone (substitution error) resulting from reactivity-based substitutions. Two alternative methods were examined by Carter et al (2003), but the preferred method is that based on substitutions of the base ROG for the model species, because the other method does not give stable results for model species whose reactivities are distributed around zero.
mir	Regional Maximum Incremental Reactivity	Relative reactivity in the cell with highest sensitivity to total VOC emissions of those where NO_x emissions have a negative impact on ozone.
mm	Regional MIR to MOIR	Average of incremental reactivities (absolute O_3 impacts) for all grid cells where NO_x emissions have a negative impact on O_3 formation. Note that these cells represent MIR to MOIR conditions according to the definition of Carter (1994a).

To be derived on consistent basis with the regional average metrics, the same weights, $W(j)$, should be used. Note that this metric approaches the regional average O_3 metric as $[O_3]^{std} \rightarrow 0$. This metric is not defined if there are no cells where O_3 exceeds the standard.

Minimum Substitution Error Metric (mse)

This metric is defined as the set of relative reactivities that minimize the sum of squares change in O_3 that results when the VOC whose relative reactivity is being assessed (test VOC) is removed and replacing by the base ROG by a factor equal to the amount of test VOC removed times the test VOC's relative reactivity. It is given by

$$RR(i,mse,d) = \sum_j W(j) * S(i,j,d) * S^{ROG}(i,j,d) / \sum_j W(j) * S^{ROG}(i,j,d) * S^{ROG}(j,d)$$

Note that this is the same as the slope of a least squares fit line, forced through zero, of plots of $S(i,j,d)$ vs. $S^{ROG}(j,d)$.

Regional MIR Metric (mir)

This metric is defined as the relative reactivities at the cell where O_3 is the most sensitive to total VOC emissions. Regions with high sensitivities to VOC emissions tend to have highly negative sensitivities to NO_x , but to avoid anomalous situations an additional requirement is added that the cell used to define the MIR metric also have negative sensitivity of O_3 to NO_x . It is given by

$$RR(i,mir,d) = S(i,j^{MIR},d) / S^{ROG}(j^{MIR},d)$$

where j^{MIR} is the cell j where $S^{VOC}(j,d)$ has the highest value of those where $S^{NOx}(j,d) < 0$. Note that this is not truly a global metric because it depends on the sensitivity at only a single point. However, as discussed by Carter et al (2003) the reactivities for this metric tend to be reasonably consistent because they reflect a relatively consistent set of chemical conditions.

Regional MIR to MOIR metric (mm)

This metric reflects the effects of VOCs on O_3 formation in cells whose reactivity characteristics make them particularly sensitive to changes in VOC emissions, and where NO_x control results in increased formation of O_3 . These are defined as cells where the sensitivity of the daily maximum O_3 to NO_x is negative while the sensitivity to total VOCs is positive. The reactivity in this metric is given by:

$$RR(i,mm,d) = \sum_j W(j) * MIRtoMOIR(j,d) * S(i,j,d) / \sum_j W(j) * MM(j,d) * S^{ROG}(j,d)$$

where $MIRtoMOIR(j,d) = \{S^{VOC}(j,d) > 0 \text{ and } S^{NOx}(j,d) < 0\}$

This metric is not defined if there are no cells where $S^{VOC}(j,d) > 0$ and $S^{NOx}(j,d) < 0$.

Metrics Calculation Algorithm

The algorithm for calculation of the metrics discussed above is given below. Since the same procedure is used regardless of averaging time, the indication of the averaging time is omitted in the nomenclature employed. Therefore, the procedure is run twice, once for reactivities relative to the daily maximum 8-hour average O_3 , and once for the daily maximum 8-hour averages.

```
for d=1 to number_of_days
  SumROGav=0
  SumROGovs=0
```

```

SumROGmm=0
SumROGmse=0
MaxSVOC=0.0
for j = 1 to number_of_cells
  SumROGav=SumROGav+(W(j)*SROG(j,d))
  if [O3]max(j,d) > [O3]std then
    SumROGOvs=SumROGOvs+(W(j)*SROG(j,d))
  endif
  if SNOx(j,d) < 0 and SVOC(j,d) > 0 then
    SumROGmm=SumROGmm+(W(j)*SROG(j,d))
  endif
  SumROGmse=SumROGmse+(W(j)*(SROG(j,d)^2))
  if (SVOC(j,d) > MaxSVOC) and (SNOx(j,d) < 0) then
    jMIR=j
    MaxSVOC= sVOC(j,d)
  endif
endif
next j
SROGMIR=SROG(jMIR,d)
for i = 1 to number_of_model_species
  Sumav=0
  Sumovs=0
  Summm=0
  Summse=0
  for j = 1 to number_of_cells
    Sumav=Sumav+(W(j)*S(i,j,d))
    if [O3]max(j,d) > [O3]std then
      Sumovs=Sumovs+(W(j)*S(i,j,d))
    endif
    if SNOx(j,d) < 0 and SVOC(j,d) > 0 then
      Summm=Summm+(W(j)*S(i,j,d))
    endif
    Summse=Summse+(W(j)*S(i,j,d)*SROG(j,d))
  next j
  RR(i,av,d)=Sumav/SumROGav
  RR(i,ovs,d)=Sumovs/SumROGOvs
  RR(i,mm,d)=Summm/SumROGmm
  RR(i,mse,d)=Summse/SumROGmse
  RR(i,mir,d)=S(i,jMIR,d)/SROGMIR
next i
next d

```

Reactivity Computation for Compounds

The procedures discussed above give the ozone reactivities of the model species relative to that of the base ROG mixture on a per-carbon, per mole, or per gram model species basis, depending on how changes in model species emissions were quantified in the sensitivity calculations. These need to be placed on a per mass, per mole, or per carbon basis in terms of actual chemical compounds, which in general may be different than the corresponding quantities in terms of model species. The nomenclature and conversion procedures used are given below:

- m Index for a particular type of reactivity metric (e.g., av, ovs, mse, mir or mm for 1-hour or 8-hour averages)
- i Index for a model species whose reactivity was calculated as describe above

c	Index for chemical compound whose reactivity is of interest
$C^{MS}(i)$	Carbon number for model species i. Depends on the quantification method used for model species in the sensitivity calculations, as indicated in Table 2. If the carbon basis quantification is used, these values are given in Table 3 for the Carbon Bond mechanism and Table 4 for SAPRC-99.
MW(c)	Molecular weight of chemical compound c
nC(c)	Carbon number of compound c. Needed only if relative reactivities of compounds are to be computed on a carbon basis. Not to be confused with model species “carbon number”, which may not be carbon numbers at all if molar or mass or mass quantifications are used for model species in the sensitivity calculations.
MW^{ROG}	Effective molecular weight of the base ROG, calculated as indicated in the discussion of the base ROG, above (Mechanism independent)
nC^{ROG}	Effective carbon number (carbons per mole of mixture) of the base ROG, calculated as indicated in the discussion of the base ROG, above. (Mechanism independent)
MWC^{ROG}	Grams of base ROG mixture per mole carbon* model species representing the mixture, calculated as indicated in the discussion of the base ROG, above.
$Rep^{test}(c,i)$	Moles of model species i used to represent compound c for a particular mechanism when carrying out the ozone sensitivity calculation for this compound. These may not necessarily be the same as the Rep(c,i) values used when computing the model species for the base ROG if separate explicit model species are added to represent the compounds in a more explicit manner than the way they are represented in the base case simulation.
RR(i,m,d)	Relative reactivity of model species i for day d with metric m on a carbon basis (or molar basis if calculated with $C^{MS}(i)=1$ for all i, or mass basis if calculated with $C^{MS}(i)=$ model species molecular weight – see Table 2), derived as discussed in the previous sections. Same as RR(i,av,d) for m=av, etc, derived as discussed above.
$RR^{mol}(i,m,d)$	Relative reactivity of model species i for day d with metric m on a molar basis, in terms of the actual chemical compounds in the base ROG. Given by $RR^{mol}(i,m,d) = C^{MS}(i) RR(i,m,d) MWC^{ROG} / MW^{ROG}$ <p>Note that MW^{ROG} / MWC^{ROG} is the effective carbon number for the base ROG, and division by this is necessary to convert the base ROG sensitivity from moles carbon, moles, or mass model species basis to a molar basis for actual chemical compounds.</p>
$CRR^{mol}(c,m,d)$	Relative reactivity of compound c for day d with metric m on a molar basis. Given by $CRR^{mol}(c,m,d) = \sum_i Rep(c,i) RR^{mol}(i,m,d)$
$CRR^{mas}(c,m,d)$	Relative reactivity of compound c for day d with metric m on a mass basis. Given by $CRR^{mas}(c,m,d) = CRR^{mol}(c,m,d) MW^{ROG} / MW(c)$ <p>or</p> $CRR^{mas}(c,m,d) = \left\{ \sum_i Rep(c,i) C(i) RR(i,m,d) \right\} MWC^{ROG} / MW(c)$
$CRR^C(c,m,d)$	Relative reactivity of compound c for day d with metric m on a carbon basis. Given by $CRR^C(c,m,d) = CRR^{mol}(c,m,d) nC^{ROG} / nC(c)$ <p>Note that this is not necessarily the same as RR(i,m,d) even if the compound is explicitly represented by model species i and the carbon quantification is used for model species for sensitivity calculations, since the number of carbons in the base</p>

ROG may not exactly be represented by the carbon numbers in the model species used to represent it.

- * If molar or mass quantification of model species is used in the sensitivity calculation is used, the units are moles of model species or grams of model species, rather than moles carbon.

It is the set of quantities $CRR^{mol}(c,m,d)$, $CRR^{mas}(c,m,d)$ or $CRR^C(c,m,d)$ that are of specific interest for most applications. The algorithm for the calculation of these quantities is given below:

```
for d=1 to number_of_days
  for i = 1 to number_of_model_species
     $RR^{mol}(i,m,d) = C^{MS}(i) * RR(i,m,d) * MW^{ROG} / MW^{ROG}$ 
  next i
  for c = 1 to number_of_compounds
     $CRR^{mol}(c,m,d) = 0.$ 
    for i = 1 to number_of_model_species
       $CRR^{mol}(c,m,d) = CRR^{mol}(c,m,d) + (Rep^{test}(c,i) * RR^{mol}(i,m,d))$ 
    next i
     $CRR^{mas}(c,m,d) = CRR^{mol}(c,m,d) * MW^{ROG} / MW(c)$ 
     $CRR^C(c,m,d) = CRR^{mol}(c,m,d) * nC^{ROG} / nC(c)$ 
  next c
next d
```

If a single reactivity metric is desired for a multi-day scenario (or a set of different scenario-days if more than one scenario is being combined, then simple averages of these quantities can be used.

Example Calculation and Macro Spreadsheet

Examples of the calculation procedures and discussed in the previous section have been implemented and tested in an Excel spreadsheet “ShowCalc.xls,” which is distributed with this document (available at <http://www.cert.ucr.edu/~carter/RRWG>). Worksheets are given to illustrate calculation of daily 1-hour and 8-hour average maximum O₃ concentrations and their corresponding sensitivity coefficients, processing for a base ROG mixture, calculation of reactivity metrics for model species from sensitivity data in individual cells, and calculations of relative reactivities of chemical compounds in various units.

For each sheet, results of calculations are shown both using spreadsheet formulas and the algorithms discussed above, and the results using the two methods are compared. On each worksheet, example input data provided with the spreadsheet are shown in uncolored font, input data calculated from formulas on other worksheets are shown in green font, data calculated using spreadsheet formulas are shown in blue font, and data calculated by macros are in purple font. Percentage differences between results calculated using spreadsheet formulas and the macros are shown for all the macro-calculated results, and the agreements are seen to be within the numerical precision of the calculations (about 1 part in 10¹⁴). (An “ok” in a difference display indicates that the numbers are exactly the same, and the fractional difference is given in scientific notation otherwise.) Comments and labels are provided where appropriate to indicate the input and output data being shown.

Each worksheet has a control button that executes a macro to calculate the results appropriate to the worksheet. There is a separate macro to process the data in each worksheet. The macros are written in

Excel Visual Basic, which is the general format used in the algorithms given in the previous section. The names used for the variables and arrays are the same as those in algorithms given above, except that superscripts cannot be shown. Each macro has three sections, as follows. (1) The initialization section declares the arrays used and loads the input data into the appropriate arrays and variables from the input data in the corresponding spreadsheet. (2) The calculation section consists of code pasted directly from the algorithms given in the previous sections, with the only editing being for formatting and to make some symbols acceptable to the software. The code is duplicated exactly in order to use the macros as a means to debug the code in the report. (3) The output section outputs the results into the appropriate locations in the spreadsheet for the macro calculation results. As indicated above, those macro-calculated results are all indicated using purple font.

The five worksheets in the spreadsheet file and their corresponding macros illustrate the basic types of calculations and data processing steps discussed above, except for the preparation of the input data for modeling, which is highly model-dependent. These are each described below.

The “Daily Max O3 Calc” sheet provides an example of how to calculate daily 1-hour and 8-hour average ozone concentrations and their corresponding sensitivity values from the hourly average data that are output by the model. The example input includes ozone data from a box model calculation and an arbitrarily-derived set of numbers representing hypothetical sensitivity data for a single input parameter for each hour of a hypothetical three-day simulation. (The “sensitivity” numbers are actually concatenations of the day and hour number and not actual sensitivities, but this is sufficient for illustrative purposes, and assures that each hourly value is unique.) These are given in the first four columns, along with the day and hour number. The next two columns contain formulas calculating the 8-hour averages starting at that hour. An “#N/A” indicates that the 8-hour average could not be computed because sufficient data are not available. (Results for Day 3 8-hour averages are not given for this reason.) The spreadsheet-calculated results show the maximum 1-hour and 8-hour average ozone values for each day, the hour of the ozone maximum (determined by finding the match between the max and the array of hourly values in the input 1-hour or calculated 8-hour columns), and the 1-hour or 8-hour average ozone for those hours. The macro calculations of the maximum O₃ and corresponding sensitivities are given below that, and the differences between the spreadsheet and macro-calculated values are given below that. The macro and spreadsheet values can be seen to agree exactly in all cases.

The “Base ROG Processing” sheet provides an example of processing the “EPAEMIT1” base ROG mixture for the Carbon Bond mechanism, as shown on Table A-2. Note that the Carbon Bond mechanism assignments are taken from the current version of the Carter (2005) speciation database, which are slightly different than those used in the base ROG processing for the Carter et al (2003) reactivity study. The results shown on this sheet will be the same as those on Table 3 under the “Current” column for the EPAEMIT1 mixture, which as indicated there are slightly different than those used by Carter et al (2003). However, using the values calculated using the current assignments is appropriate for illustrative and testing purposes, as discussed further below.

The bottom table on this sheet has six sets of columns providing input data for the components of the base ROG. The first column is the identification code used for the compound in the current Carter (2005) speciation database, and the last column gives the name of the compound. These are given for information purposes only and are not used in the calculations. The second and third column gives the molecular weight and carbon number of the compound, and the fourth column gives the mass fraction of the compound in the base ROG, i.e. MF^{ROG}. The next 11 columns give the current Carbon Bond model species assignments for these compounds in the Carter (2005) speciation database, which are also shown on Table A-2. The names of the CB4 species and their corresponding carbon numbers are shown in their corresponding columns near the top of the worksheet. These are the input data used in the calculations.

The spreadsheet calculations of the MM^{ROG} , MWC^{ROG} , MW^{ROG} , nC^{ROG} , and FC^{ROG} are shown on the table on the sheet immediately under the model species name and carbon number, and the macro calculations of these values are shown on the table under that, and the differences are shown under that. The macro results agree with the spreadsheet calculations within the numerical precision of the calculations in all cases.

The “Model Species Reactivity Calc” sheet gives the daily 1-hour maximum O_3 concentrations and the corresponding sensitivity parameters for each of the 4602 grid cells in the CAMx model simulations of the CRC-NARSTO modeling database for the July 7-15, 1995 episode for July 14 and the 64K grid cells from Carter et al (2003). The first 15 columns in the bottom table give the grid row and column numbers (not used in the calculation), daily maximum 1-hour average O_3 in the grid cells, and the corresponding DDM-calculated sensitivity parameters for total VOC, total NO_x , and the CB4 model species for which sensitivity values were calculated. (Ethane and CO is excluded because these data are not needed for the computation of the base ROG reactivity). Sensitivities were not calculated for ISOP and MEOH model species, but it is necessary to have values of these in order to compute the base ROG reactivity because they are used to represent some of the compounds the base ROG mixture used in this example. Therefore, for the purposes of this example calculation, zero values are entered for the sensitivities of these model species. The next column gives the base ROG sensitivity for each of the cells, calculated from the sensitivities for the model species for those cells, and the FC^{ROG} and C^{MS} values taken from the “Base ROG Processing” sheet, which are given on the table above in the corresponding columns of the model species. The next two columns give logical values (0 for false and 1 for true) for whether the ozone in the cell exceeds the O_3 standard of 0.12 ppm and whether the cell represents MIR to MOIR conditions (total NO_x sensitivity less than 0 and total VOC sensitivity greater than zero). In order to avoid bogging down use of the spreadsheet with multiple calculations in the 4602 cells, only the first row of data in these columns have the actual spreadsheet calculation formula, the remainder are given as values only. To recalculate these if changes are made (such as, for example, changing the base ROG composition or the ozone standard), copy the cells with the calculation to the cells below it for the other grid cells.

Above these data on the bottom table is a column of calculated data giving the sensitivities for the MIR cell, i.e., the cell with the highest total VOC sensitivity. The value for total VOC sensitivity is determined by simply finding the maximum in the columns below it. The other values are determined by finding the index of the row where the total VOC sensitivity matches this maximum, and using the spreadsheet “offset” function to get the data for the other sensitivities. Note that this spreadsheet calculation does not check to assure that the sensitivity to total NO_x is negative, though strictly speaking this is a part of the recommended procedure. However, this is rarely if ever expected to be the case in most realistic scenarios, and is not the case for this episode day, as shown in the “ NO_x ” column for this MIR row. This check is made in the macro calculation, as indicated in the corresponding algorithm given in the “Metrics Calculation Algorithm” section above.

The table above the input data and base ROG composition data tables give the spreadsheet calculation results for the model species relative reactivities for the five metrics described above. The data in the “ROG” column to the right of this table give averages or summations for the base ROG that are needed in the relative reactivity calculations, where applicable. The table above this gives the corresponding values calculated by the macro, with tables to the side showing the differences between the macro and spreadsheet calculated values. In all cases the agreement is better than 1 part in 10^{15} .

The “Carter et al (2003) Rct'y Calc” is the same as the above except that it uses the base ROG composition (FC^{ROG}) values that were given by Carter et al (2003), so the model species reactivity results can be directly compared with those given by Carter et al (2003) (see Table 3 and the associated discussion). The only difference is the FC^{ROG} values are those from Carter et al (2003) and the table giving the macro-calculated model species relative reactivities are replaced by a table giving the values

given by Carter et al (2003) for this episode day and grid size domain. The agreement can be seen to be 2% or better, with the differences attributed at least in part to roundoff error. The format of the display of the differences is modified to be more appropriate for differences of this magnitude.

The “Compound Reactivity Calc” sheet shows how the mass, molar, or carbon-based relative reactivity values are calculated for all the compounds in the base ROG mixture for a selected metric. The metric chosen is the “Minimum Substitution Error” metric for maximum 1-hour average O₃, but the procedures are the same regardless of which metric is used. The input data use the base ROG information derived from the “Base ROG Processing” sheet and the model species reactivity data derived from the “Model Species Reactivity Calc” sheet for the selected metric. The table at the top of the sheet shows the MW^{ROG}, nC^{ROG}, MWC^{ROG} parameters and the model species relative reactivities that were derived from those sheets.

The bottom table contains the compound name, molecular weight, carbon numbers, and Carbon Bond model species representations used for the compounds in the base ROG mixture, which are the same as those given on the “Base ROG Processing” sheet. (Note that the model species representations used for calculating compound reactivities could be different if explicit model species are added to the mechanism to represent the compounds. This could actually be done for ethane since its reactivity was calculated by Carter et al (2003), but it was not done in this example for reasons that will be evident below.) The next three columns give the spreadsheet calculations for the molar, mass-based, and carbon-based relative reactivities for all the compounds, the three columns after that show these values calculated using the macro, and the three columns after that show the differences between these methods. In all cases the calculations agreed exactly.

Additional data and calculations are included on this spreadsheet in order to provide an additional test of the relative reactivity calculation procedures and results. In particular, if the relative reactivities of all the compounds in the base ROG mixture are calculated using the exact same set of model species as used to represent them in the base ROG, then the sum of the relative reactivities of the compounds in the base ROG, weighed by their contributions to the base ROG, should equal 1. This is because the relative reactivities of the compounds is defined as their impact in the particular metric with respect to this base ROG, and reactivities of mixtures are sums of the reactivities of the components times their relative contributions. In particular if the calculations were done correctly, then

$$\begin{aligned}\sum_c \text{MF}^{\text{ROG}}(c) \text{CRR}^{\text{mas}}(c,m,d) &= 1 \\ \sum_c \text{MoIF}^{\text{ROG}}(c) \text{CRR}^{\text{mol}}(c,m,d) &= 1 \\ \text{and} \quad \sum_c \text{CF}^{\text{ROG}}(c) \text{CRR}^{\text{C}}(c,m,d) &= 1\end{aligned}$$

where MoIF^{ROG}(c) and CF^{ROG}(c) are the mole fraction and carbon fraction of compound c in the base ROG, respectively. (This would not necessarily be the case if explicit or other special model species were added to more accurately calculate sensitivities of any compound in the base ROG, which is why we did not use the explicitly calculated reactivity for ethane in this example.) To conduct this test, the MF^{ROG}, MoIF^{ROG} and CF^{ROG} are added to the table in this sheet, where the MF^{ROG} data are the same as in the “Base ROG Processing” sheet, and the MoIF^{ROG} and CF^{ROG} values are calculated from this using

$$\begin{aligned}\text{MoIF}^{\text{ROG}}(c) &= \{ \text{MF}^{\text{ROG}}(c) / \text{MW}(c) \} / \{ \sum_{c'} \text{MF}^{\text{ROG}}(c') / \text{MW}(c') \} = \text{MF}^{\text{ROG}}(c) \text{MW}^{\text{ROG}} / \text{MW}(c) \\ \text{CF}^{\text{ROG}}(c) &= \text{MoIF}^{\text{ROG}}(c) \text{nC}(c) / \{ \sum_{c'} \text{nC}(c') \text{MoIF}^{\text{ROG}}(c') \} = \text{MoIF}^{\text{ROG}}(c) \text{nC}(c) / \text{nC}^{\text{ROG}}\end{aligned}$$

The summations using the equations above are given at the bottom of the table with the compounds in the columns with the spreadsheet calculated values of the corresponding version of CRR. The sums were found to be one to within 1 part in 10¹⁴.

Recommended Reporting Requirements

In order for the results of any reactivity assessment to be useful for research and policy applications, it is important that sufficient information be provided that the results can be replicated, and that the underlying assumptions, choices, methods, terminology, and scientific and be adequately documented. Given below is a summary of what propose as *minimum* reporting requirements when present results of reactivity scale calculations using regional models. It is important to recognize that the list may not be fully comprehensive and additional information may be appropriate, depending on the objective of the work and the intended use for the data.

1. Specification of the modeling software employed, references to its documentation, and specification of the options and version employed. Any documentation referenced should be publicly available, preferable on a publicly accessible internet site. If modifications or enhancements were made to the software since the time of its available documentation, these should be adequately described. If the DDM method or other special software features are used to calculate sensitivities, references to the scientific and mathematical should be provided or given if that information is not in the literature or a publicly accessible report.
2. Specification of the modeling database employed, including the domain, episode days, emissions and meteorological databases, boundary conditions. It is particularly important that the source of emissions inventory be clearly specified. The information provided, together with the software, version, and options described above, must be sufficient so other could duplicate the base case calculation. If the episode has been modeled using the same database and software in a previous study and the database is adequately documented in a publicly available report, then reference to that report should be sufficient to satisfy this requirement. If the referenced report describes more than one episode or database, the one used in this work should be unambiguously indicated.
3. Specification of the chemical mechanism for the base case simulation. Although specification of the base case chemical mechanism is part of point 1, above, it is particularly important that the mechanism be adequately documented for reactivity calculations. Therefore a reference should made directly to the source or documentation of the mechanism, and not indirectly through a reference to the model documentation as a whole. A complete listing of the mechanism, including information used for deriving photolysis rates, should be provided if the mechanism is not exactly the same as in the reference documentation.
4. Specification and documentation for any modifications made to the base case mechanism for the purpose of reactivity assessments. If the model species whose sensitivities are being calculated are the same as those used in the base mechanism, then this should be so stated. If explicit model species are added for more accurate calculation for individual compounds (e.g., ethane in the case of the study of Carter et al, 2003 and the various explicitly represented VOCs calculated by Hakami et al, 2003), then the mechanisms used for those species should be listed or documented.
5. Specification of exactly how the sensitivity calculations were carried out. If the direct sensitivity calculation method was used, then the amounts that the emissions inputs were varied, the time and space distributions, and how the variations depended on the base case emissions should be clearly specified. If a DDM or similar type of software is employed, then the DDM input specifications should be described in such a way that the direct sensitivity calculation input that would give the same results (assuming linearity) is evident. The specification of the sensitivity calculation inputs should make it clear what the units are for the sensitivity coefficients that are being calculated.

6. The model species quantification method for sensitivity calculations should be made clear as part of the specifications for point 5, above. If the carbon or mass model species quantification method is used, then the carbon numbers or molecular weights used for each of the model species (the $C^{MS}(i)$ values) should be given for each model species (whether lumped or explicit) for which sensitivities are calculated. If the molar model species quantification method is employed, and reference is made to this document as to the methods and terminology employed, the documentation should state that C^{MS} values of 1 were used for all model species.
7. The cells whose sensitivities are used for deriving the reactivity metrics, and their relative importance values, $W(j)$. For example, if all ground-level cells in the domain are used and the cells are either weighted equally or on a ground area basis if they are different sizes, this should be so stated. If any part of the domain, such as cells over water or outside a region of interest, are excluded, then this should be stated. This should be specified sufficiently so that anyone attempting to duplicate the calculation will know how to derive $W(j)$ for all cells in the domain.
8. The composition of the base ROG mixture employed as the relative reactivity standard, in terms of both actual chemical compounds and the model species used to represent them in the base ROG sensitivity calculation, should be specified. The mapping of model species to all the compounds in the base ROG that yields the distribution of model species used to represent it in the base ROG sensitivity calculations should also be included, since this provides necessary documentation for the model representation of this mixture. If the base ROG composition and model species representations are exactly the same as given in this document or a previous publicly-available report or article, then reference to a document giving this information should be sufficient. It is recommended that only model species used in the base simulation be used to represent the base ROG mixture when calculating its sensitivity, but if a different procedure is employed this should be clearly stated and justified.
9. The model species used to represent each of the compounds whose reactivities are being specified should be stated specified. If they are represented by explicit model species, then it is sufficient to state this. If they are represented by an explicit model species for another compound (i.e, using the “lumped molecule” representation), then this should be stated. In the latter case the documentation should clearly indicate that differences in molecular weight and carbon number, if any, are properly taken into account in computing mass or carbon based relative reactivities.
10. The calculation methods used to derive the reactivity metrics should be clearly documented, preferably in reference to the procedures discussed in this report. If any procedures differ from those discussed here, the differences should be documented and the anticipated effect on the results should be documented. It should be clearly stated whether the base ROG sensitivity was calculated directly or derived from sensitivities for the model species used to represent it.
11. The units of any results that are presented that have units should be specified, and it should be clearly indicated whether relative reactivity results are on a mass, molar, or carbon basis.

If the calculated reactivity scales are to be used for regulatory applications, all the input files, software, scripts, and output files should be archived so the results can be duplicated exactly, even if (and especially if) at a later date if the software or data are updated or modified. Information should be provided concerning the machine, operating system, etc. so that the calculations should be run using the input and program source files provided. The archive and information needed to duplicate the calculations should be provided to the regulatory agency that is using the reactivity scale, and the agency should make these available to the public on request.

Note that reference citations are an acceptable means to provide the information in most cases, provided that the reference cited is publicly available and the citations is made that is unambiguous as to which version or method is used if the cited reference describes more than one version or method. References cited to document the chemical mechanism and the representation of the base ROG and the test VOCs whose reactivities are being calculated should be primary references and not provide this information only through reference citations.

It may not be practical to provide all this information when the study is being written up as an executive summary or for publication in a scientific journal or other medium where there are significant space limitations. In this case, the information that is not in the shorter article should be in an addendum or appendix or in a publicly available report. If a detailed report is cited it should be available on a public FTP or web site, where the information and applicable data can be downloaded without password requirements or other restrictions.

References

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Appendix A. Base ROG Compositions and Model Species Assignments

Table A-1. Composition of the ARBROG94 base ROG mixture derived from ambient air data, based on that used to calculate the EKMA Reactivity scales of Carter (1994).

Profile ID = ARBROG94 [a]				
Database ID [a]	Weight Fraction	Description	Lumped Model Species Representation	
			SAPRC-99	CB4
C78-78-4	7.64e-2	2-methyl-butane	ALK4	5 PAR
C106-97-8	7.33e-2	n-butane	ALK3	4 PAR
C108-88-3	5.94e-2	toluene	ARO1	TOL
C74-98-6	4.35e-2	propane	ALK2	1.5 PAR + 1.5 UNR
C74-84-0	3.54e-2	ethane	ALK1	0.4 PAR + 1.6 UNR
C75-28-5	3.20e-2	2-methylpropane; isobutane	ALK3	4 PAR
C109-66-0	3.09e-2	n-pentane	ALK4	5 PAR
C74-85-1	2.64e-2	ethylene	ETHE	ETH
C107-83-5	2.17e-2	2-methylpentane	ALK4	6 PAR
C124-18-5	1.83e-2	n-decane	ALK5	7 PAR + 3 UNR
C71-43-2	1.80e-2	benzene	0.295 ARO1	PAR + 5 UNR
C74-86-2	1.77e-2	acetylene	ALK2	PAR + UNR
C50-00-0	1.66e-2	formaldehyde	HCHO	FORM
C108-38-3	1.62e-2	m-xylene	ARO2	XYL
C106-42-3	1.62e-2	p-xylene	ARO2	XYL
C589-43-5	1.61e-2	2,4-dimethylhexane	ALK5	8 PAR
C96-14-0	1.56e-2	3-methylpentane	ALK4	6 PAR
C592-41-6	1.51e-2	1-hexene	OLE1	4 PAR + OLE
C75-07-0	1.47e-2	acetaldehyde	CCHO	ALD2
C95-47-6	1.35e-2	o-xylene	ARO2	XYL
C526-73-8	1.29e-2	1,2,3-trimethylbenzene	ARO2	PAR + XYL
C108-67-8	1.26e-2	1,3,5-trimethylbenzene	ARO2	PAR + XYL
C589-34-4	1.25e-2	3-methylhexane	ALK5	7 PAR
C67-64-1	1.25e-2	acetone	ACET	3 PAR
C108-08-7	1.15e-2	2,4-dimethylpentane	ALK4	7 PAR
C100-41-4	9.46e-3	ethylbenzene	ARO1	PAR + TOL
C96-37-7	9.44e-3	methylcyclopentane	ALK4	6 PAR
C115-07-1	9.35e-3	propylene	OLE1	PAR + OLE
C142-82-5	8.40e-3	n-heptane	ALK5	7 PAR
C592-76-7	8.13e-3	1-heptene	OLE1	5 PAR + OLE
C592-27-8	8.04e-3	2-methylheptane	ALK5	8 PAR
C589-53-7	8.04e-3	4-methylheptane	ALK5	8 PAR
C110-54-3	7.94e-3	n-hexane	ALK4	6 PAR
C565-59-3	7.82e-3	2,3-dimethylpentane	ALK5	7 PAR
C646-04-8	7.76e-3	trans-2-pentene	OLE2	PAR + 2 ALD2
C627-20-3	7.76e-3	cis-2-pentene	OLE2	PAR + 2 ALD2
C2213-23-2	7.65e-3	2,4-dimethylheptane	ALK5	9 PAR
C622-96-8	6.91e-3	p-ethyltoluene	ARO2	PAR + XYL
C620-14-4	6.91e-3	m-ethyltoluene	ARO2	PAR + XYL
C611-14-3	6.91e-3	o-ethyltoluene	ARO2	PAR + XYL
C111-84-2	6.65e-3	n-nonane	ALK5	7 PAR + 2 UNR

Table A-1 (continued)

C95-63-6	6.59e-3	1,2,4-trimethylbenzene	ARO2	PAR + XYL
C79-29-8	6.46e-3	2,3-dimethylbutane	ALK4	6 PAR
C78-79-5	6.17e-3	isoprene	ISOP	ISOP
C109-67-1	6.08e-3	1-pentene	OLE1	3 PAR + OLE
C111-65-9	5.90e-3	n-octane	ALK5	7 PAR + UNR
C78-93-3	5.52e-3	methyl ethyl ketone (mek) (2-butanone)	MEK	4 PAR
C66-25-1	5.12e-3	hexanal (hexanaldehyde)	RCHO	4 PAR + ALD2
C106-98-9	5.05e-3	1-butene	OLE1	2 PAR + OLE
C108-87-2	4.81e-3	methylcyclohexane	ALK5	7 PAR
C80-56-8	4.81e-3	a-pinene	TERP	6 PAR + 0.5 OLE + 1.5 ALD2
C624-64-6	4.77e-3	trans-2-butene	OLE2	2 ALD2
C124-11-8	4.58e-3	1-nonene	OLE1	7 PAR + OLE
C563-46-2	4.49e-3	2-methyl-1-butene	OLE2	4 PAR + FORM
C115-11-7	4.49e-3	2-methylpropene (isobutene)	OLE2	3 PAR + FORM
C103-65-1	4.36e-3	n-propylbenzene	ARO1	2 PAR + TOL
C110-82-7	4.02e-3	cyclohexane	ALK5	6 PAR
C98-83-9	3.94e-3	a-methylstyrene	OLE2	OLE + TOL
C112-40-3	3.88e-3	n-dodecane	ALK5	8 PAR + 4 UNR
C590-18-1	3.83e-3	cis-2-butene	OLE2	2 ALD2
C3221-61-2	3.82e-3	2-methyloctane	ALK5	9 PAR
C2216-34-4	3.82e-3	4-methyloctane	ALK5	9 PAR
C591-76-4	3.65e-3	2-methylhexane	ALK5	7 PAR
C99-87-6	3.60e-3	1-methyl-4-isopropylbenzene	ARO2	2 PAR + XYL
C535-77-3	3.60e-3	1-methyl-3-isopropylbenzene	ARO2	2 PAR + XYL
C135-01-3	3.60e-3	1,2-diethylbenzene (ortho)	ARO2	2 PAR + XYL
C105-05-5	3.60e-3	1,4-diethylbenzene (para)	ARO2	2 PAR + XYL
C287-92-3	3.46e-3	cyclopentane	ALK4	5 PAR
C590-86-3	3.21e-3	isovaleraldehyde (3-methylbutanal)	RCHO	3 PAR + ALD2
C110-62-3	3.21e-3	n-pentanal (n-valeraldehyde)	RCHO	3 PAR + ALD2
S2-91087	3.09e-3	3-methyl-5-ethylheptane	ALK5	10 PAR
C871-83-0	3.09e-3	2-methylnonane	ALK5	7 PAR + 3 UNR
C2051-30-1	3.09e-3	2,6-dimethyloctane	ALK5	10 PAR
C20278-85-7	3.09e-3	2,3,5-trimethylheptane	ALK5	10 PAR
C15869-89-3	3.09e-3	2,5-dimethyloctane	ALK5	10 PAR
C14686-14-7	2.99e-3	trans-3-heptene	OLE2	3 PAR + 2 ALD2
C7688-21-3	2.94e-3	cis-2-hexene	OLE2	2 PAR + 2 ALD2
C4050-45-7	2.94e-3	trans-2-hexene	OLE2	2 PAR + 2 ALD2
C123-38-6	2.84e-3	propionaldehyde	RCHO	PAR + ALD2
C75-83-2	2.78e-3	2,2-dimethylbutane	ALK3	5 PAR + UNR
C513-35-9	2.52e-3	2-methyl-2-butene	OLE2	3 PAR + ALD2
C934-80-5	2.50e-3	1,2-dimethyl-4-ethylbenzene	ARO2	2 PAR + XYL
C934-74-7	2.50e-3	1,3-dimethyl-5-ethylbenzene	ARO2	2 PAR + XYL
C933-98-2	2.50e-3	1,2-dimethyl-3-ethylbenzene	ARO2	2 PAR + XYL
C874-41-9	2.50e-3	1,3-dimethyl-4-ethylbenzene	ARO2	2 PAR + XYL
C2870-04-4	2.50e-3	1,3-dimethyl-2-ethylbenzene	ARO2	2 PAR + XYL
C1758-88-9	2.50e-3	1,4-dimethyl-2-ethylbenzene	ARO2	2 PAR + XYL
C106-99-0	2.34e-3	1,3-butadiene	OLE2	2 OLE
C538-68-1	2.25e-3	n-pentylbenzene	ARO1	4 PAR + TOL
C29316-05-0	2.25e-3	s-pentylbenzene	ARO1	4 PAR + TOL
C1196-58-3	2.25e-3	3-phenylpentane	ARO1	4 PAR + TOL

Table A-1 (continued)

C135-98-8	2.15e-3	(1-methylpropyl)benzene (sec-butyl benzene)	ARO1	3 PAR + TOL
C821-95-4	2.06e-3	1-undecene	OLE1	9 PAR + OLE
C101823-01-2	2.06e-3	trans-4-methyl-2-decene	OLE2	7 PAR + 2 ALD2
C17312-53-7	1.94e-3	3,6-Dimethyl Decane	ALK5	8 PAR + 4 UNR
C111-66-0	1.87e-3	1-octene	OLE1	6 PAR + OLE
C13466-78-9	1.82e-3	3-carene	TERP	6 PAR + 0.5 OLE + 1.5 ALD2
C1120-21-4	1.80e-3	n-undecane	ALK5	8 PAR + 3 UNR
C14850-23-8	1.68e-3	trans-4-octene	OLE2	3 PAR + 2 ALD2 + UNR
C27831-13-6	1.67e-3	1,2-dimethyl-4-ethenyl benzene	OLE2	PAR + OLE + TOL
C2039-89-6	1.67e-3	1,4-dimethyl-2-ethenyl benzene	OLE2	PAR + OLE + TOL
C98-82-8	1.60e-3	cumene (isopropyl benzene)	ARO1	2 PAR + TOL
C563-45-1	1.59e-3	3-methyl-1-butene	OLE1	3 PAR + OLE
C123-72-8	1.56e-3	butyraldehyde	RCHO	2 PAR + ALD2
C1678-91-7	1.40e-3	ethylcyclohexane	ALK5	8 PAR
C95-93-2	1.31e-3	1,2,4,5-tetramethylbenzene	ARO2	2 PAR + XYL
C527-53-7	1.31e-3	1,2,3,5-tetramethylbenzene	ARO2	2 PAR + XYL
C488-23-3	1.31e-3	1,2,3,4-tetramethylbenzene	ARO2	2 PAR + XYL
C100-52-7	1.21e-3	benzaldehyde	NROG	7 UNR
C110-83-8	1.00e-3	cyclohexene	OLE2	2 PAR + 2 ALD2
C1632-70-8	9.70e-4	5-methylundecane	ALK5	8 PAR + 4 UNR
C1002-43-3	9.70e-4	3-methylundecane	ALK5	8 PAR + 4 UNR
C872-05-9	9.35e-4	1-decene	OLE1	8 PAR + OLE
C17302-28-2	9.00e-4	2,6-dimethylnonane	ALK5	8 PAR + 3 UNR
C98-06-6	8.50e-4	t-butylbenzene	ARO1	2 PAR + TOL + UNR
C538-93-2	8.50e-4	(2-methylpropyl)benzene	ARO1	3 PAR + TOL
C3982-64-7	4.94e-4	1,3-dimethyl-5-propylbenzene	ARO2	3 PAR + XYL
C16021-20-8	4.94e-4	1-ethyl-2-propylbenzene	ARO2	3 PAR + XYL
C1595-04-6	4.94e-4	1-methyl-3-butylbenzene	ARO2	3 PAR + XYL
C13732-80-4	4.94e-4	1,2-diethyl-4-methylbenzene	ARO2	3 PAR + XYL
C2847-72-5	4.50e-4	4-methyldecane	ALK5	8 PAR + 3 UNR
C13151-34-3	4.50e-4	3-methyldecane	ALK5	8 PAR + 3 UNR
S2-91058	3.58e-4	trans-2,2-trimethyl-3-heptene	OLE2	5 PAR + 2 ALD2
C6434-77-1	3.58e-4	cis-2-nonene	OLE2	5 PAR + 2 ALD2
C3074-64-4	3.58e-4	2,3-dimethyl-2-heptene	OLE2	5 PAR + 2 ALD2
C20063-92-7	3.58e-4	trans-3-nonene	OLE2	5 PAR + 2 ALD2
C16993-86-5	3.58e-4	2-methyl-2-octene	OLE2	5 PAR + 2 ALD2
C10405-85-3	3.58e-4	Trans-4-Nonene	OLE2	5 PAR + 2 ALD2
S2-91120	3.30e-4	1-methyl-4-n-pentylbenzene	ARO2	4 PAR + XYL
C99-62-7	3.30e-4	1,3-isodipropylbenzene	ARO2	4 PAR + XYL
C98-19-1	3.30e-4	1-(1,1-dimethylethyl)-3,5-dimethylbenzene	ARO2	3 PAR + XYL + UNR
C877-44-1	3.30e-4	1,2,4-triethylbenzene	ARO2	4 PAR + XYL
C102-25-0	3.30e-4	1,3,5-triethylbenzene	ARO2	4 PAR + XYL
C100-18-5	3.30e-4	1,2-isodipropylbenzene	ARO2	4 PAR + XYL
C694-35-9	3.20e-4	3-ethylcyclopentene	OLE2	3 PAR + 2 ALD2
C28823-42-9	3.20e-4	3-methyl-2,4-hexadiene	OLE2	3 PAR + 2 ALD2
C2146-38-5	3.20e-4	1-ethyl cyclopentene	OLE2	5 PAR + OLE
C1541-23-7	3.20e-4	1,5-heptadiene	OLE2	3 PAR + 2 ALD2
C1077-16-3	2.70e-4	n-hexylbenzene	ARO1	5 PAR + TOL
C629-50-5	1.89e-4	n-tridecane	ALK5	9 PAR + 4 UNR
C59643-70-8	1.87e-4	3,4-Diethyl-2-Hexene (E)	OLE2	3 PAR + 2 ALD2 + 3 UNR

Table A-1 (continued)

C4485-13-6	1.87e-4	4-propyl-3-heptene	OLE2	6 PAR + 2 ALD2
C19781-18-1	1.87e-4	2,3-dimethyl-2-octene	OLE2	6 PAR + 2 ALD2
C19780-61-1	1.87e-4	3-ethyl-2-methyl-2-heptene	OLE2	6 PAR + 2 ALD2
C19398-89-1	1.87e-4	Trans-4-Decene	OLE2	3 PAR + 2 ALD2 + 3 UNR
C822-50-4	1.40e-4	trans-1-2-dimethylcyclopentane	ALK5	7 PAR
C2452-99-5	1.40e-4	1,2-dimethylcyclopentane	ALK5	7 PAR
C1640-89-7	1.40e-4	ethylcyclopentane	ALK5	7 PAR
C1638-26-2	1.40e-4	1,1-dimethylcyclopentane	ALK5	7 PAR
C1192-18-3	1.40e-4	cis-1-2-dimethylcyclopentane	ALK5	7 PAR
S2-43252	3.15e-5	2,2,5-triethylheptane	ALK5	13 PAR
C17453-93-9	3.15e-5	5-Methyl Dodecane	ALK5	9 PAR + 4 UNR
C17312-57-1	3.15e-5	3-Methyl Dodecane	ALK5	9 PAR + 4 UNR
C17301-28-9	3.15e-5	3,6-Dimethyl Undecane	ALK5	9 PAR + 4 UNR
C17301-23-4	3.15e-5	2,6-dimethylundecane	ALK5	13 PAR
C14638-54-1	3.15e-5	2,4,6,8-Tetramethyl Nonane	ALK5	9 PAR + 4 UNR

- [a] Designation of the profile in the Carter (2005) emissions speciation and profile database. The Composition is based on the mixture used by Carter (1994, 2000) to calculate reactivity scales using EKMA models. The mixture was originally specified in terms of SAPRC detailed model species. Those model species that referred to mixtures were assigned to individual chemical compounds using the mixture assignments in the emissions speciation database of Carter (2005) as of 7/7/04.
- [b] Categorization codes for the compounds used in the Carter (2005) emissions speciation database. Codes starting with "C" are based on the CAS number of the compound. Codes starting with "S" are used for compounds whose CAS numbers are unknown.

Table A-2. Composition of the EPAEMIT1 base ROG mixture derived from emissions data, based on total emissions profile provided by the EPA in 1998. [a]

<u>Profile ID = EMITBAS1 [a]</u>				
Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C64-17-5	5.73e-2	ethyl alcohol	ALK3	ETOH
C67-63-0	4.86e-2	isopropyl alcohol	ALK4	3 PAR
C108-88-3	4.21e-2	toluene	ARO1	TOL
C74-85-1	3.33e-2	ethylene	ETHE	ETH
C106-97-8	3.24e-2	n-butane	ALK3	4 PAR
C109-66-0	2.83e-2	n-pentane	ALK4	5 PAR
C71-43-2	2.21e-2	benzene	0.295	PAR + 5 UNR
			ARO1	
C142-82-5	1.91e-2	n-heptane	ALK5	7 PAR
C74-98-6	1.85e-2	propane	ALK2	1.5 PAR + 1.5 UNR
C110-54-3	1.78e-2	n-hexane	ALK4	6 PAR
C78-78-4	1.74e-2	2-methyl-butane	ALK4	5 PAR
C50-00-0	1.72e-2	formaldehyde	HCHO	FORM
C75-28-5	1.72e-2	2-methylpropane; isobutane	ALK3	4 PAR
C67-64-1	1.59e-2	acetone	ACET	3 PAR
C71-36-3	1.40e-2	n-butyl alcohol	ALK5	4 PAR
C74-84-0	1.23e-2	ethane	ALK1	0.4 PAR + 1.6 UNR
C123-86-4	1.21e-2	n-butyl acetate	ALK4	5 PAR + UNR
C78-93-3	1.18e-2	methyl ethyl ketone (mek) (2-butanone)	MEK	4 PAR
C109-87-5	1.14e-2	dimethoxymethane (methylal)	ALK4	3 PAR
C115-07-1	1.14e-2	propylene	OLE1	PAR + OLE
C95-47-6	1.13e-2	o-xylene	ARO2	XYL
C127-18-4	1.13e-2	perchloroethylene	ALK1	2 UNR
C111-46-6	1.06e-2	diethylene glycol (2,2'-oxybisethanol)	ALK5	4 PAR
C108-38-3	1.05e-2	m-xylene	ARO2	XYL
C100-41-4	9.92e-3	ethylbenzene	ARO1	PAR + TOL
C67-56-1	9.72e-3	methyl alcohol	MEOH	MEOH
C106-42-3	9.27e-3	p-xylene	ARO2	XYL
C100-42-5	8.67e-3	styrene	OLE2	0.5 OLE + TOL
C108-87-2	8.60e-3	methylcyclohexane	ALK5	7 PAR
C108-21-4	8.22e-3	isopropyl acetate	ALK3	4 PAR + UNR
C74-86-2	8.10e-3	acetylene	ALK2	PAR + UNR
C110-82-7	6.81e-3	cyclohexane	ALK5	6 PAR
C115-10-6	6.44e-3	dimethyl ether	ALK3	2 PAR
C141-78-6	6.06e-3	ethyl acetate	ALK2	3 PAR + UNR
C106-98-9	6.04e-3	1-butene	OLE1	2 PAR + OLE
C79-20-9	5.97e-3	methyl acetate	ALK2	2 PAR + UNR
C109-67-1	5.87e-3	1-pentene	OLE1	3 PAR + OLE
C77-68-9	5.80e-3	3-Hydroxy-2,2,4-Trimethylpentyl-1-Isobutyrate	ALK5	7 PAR + 5 UNR
C18491-15-1	5.80e-3	1-Hydroxy-2,2,4-Trimethylpentyl-3-Isobutyrate	ALK5	7 PAR + 5 UNR
C111-65-9	5.62e-3	n-octane	ALK5	7 PAR + UNR
C75-07-0	5.59e-3	acetaldehyde	CCHO	ALD2
C57-55-6	5.46e-3	propylene glycol	ALK5	3 PAR
C75-09-2	5.46e-3	dichloromethane {methylene chloride}	ALK1	UNR

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C109-60-4	5.20e-3	propyl acetate	ALK3	4 PAR + UNR
C107-41-5	4.68e-3	hexylene glycol (2-methylpentane-2,4-diol)	ALK5	6 PAR
C111-90-0	4.63e-3	carbitol {degee} {2-(2-ethoxyethoxy)ethanol}	ALK5	6 PAR
C124-18-5	4.47e-3	n-decane	ALK5	7 PAR + 3 UNR
C106-99-0	4.32e-3	1,3-butadiene	OLE2	2 OLE
C75-21-8	4.28e-3	ethylene oxide	NROG	PAR + UNR
C68-12-2	4.21e-3	dimethyl formamide	ALK5	2 PAR + UNR
C110-80-5	4.14e-3	2-ethoxyethanol {cellosolve} {egee}	ALK5	4 PAR
C111-15-9	4.12e-3	2-ethoxyethyl acetate {cellosolve acetate}	ALK5	5 PAR + UNR
C111-76-2	4.07e-3	butyl cellosolve {2-butoxyethanol} {egbe}	ALK5	6 PAR
C96-14-0	4.07e-3	3-methylpentane	ALK4	6 PAR
C108-90-7	3.87e-3	chlorobenzene	0.295 ARO1	PAR + 5 UNR
C62-53-3	3.79e-3	aniline {aminobenzene}	0.295 ARO1	0.75 XYL
C107-02-8	3.71e-3	acrolein (2-propenal)	MACR	0.5 OLE + ALD2
C64-19-7	3.55e-3	acetic acid	ALK2	PAR + UNR
C108-10-1	3.50e-3	methyl isobutyl ketone	PRD2	6 PAR
C107-13-1	3.45e-3	acrylonitrile	ALK5	PAR + OLE
C106-46-7	3.31e-3	p-dichlorobenzene	0.295 ARO1	PAR + 5 UNR
C124-09-4	3.27e-3	hexamethylenediamine	ALK5	4 PAR + ALD2
C589-43-5	3.26e-3	2,4-dimethylhexane	ALK5	8 PAR
C420-56-4	3.23e-3	trimethylfluorosilane	NROG	2 PAR + UNR
C96-37-7	3.07e-3	methylcyclopentane	ALK4	6 PAR
C80-56-8	3.05e-3	a-pinene	TERP	6 PAR + 0.5 OLE + 1.5 ALD2
C79-29-8	2.98e-3	2,3-dimethylbutane	ALK4	6 PAR
C1120-21-4	2.92e-3	n-undecane	ALK5	8 PAR + 3 UNR
C110-43-0	2.91e-3	methyl amyl ketone	PRD2	7 PAR
C108-95-2	2.91e-3	phenol (carbolic acid)	PHEN	PAR + 5 UNR
C79-01-6	2.88e-3	trichloroethylene (tce)	ALK3	ETH
C104-51-8	2.82e-3	n-butylbenzene	ARO1	3 PAR + TOL
C71-55-6	2.79e-3	1,1,1-trichloroethane	NROG	2 UNR
C107-83-5	2.79e-3	2-methylpentane	ALK4	6 PAR
C107-06-2	2.73e-3	ethylene dichloride	ALK1	2 UNR
C107-21-1	2.59e-3	ethylene glycol	ALK5	2 PAR
C108-05-4	2.56e-3	vinyl acetate	OLE1	PAR + OLE + UNR
C75-83-2	2.56e-3	2,2-dimethylbutane	ALK3	5 PAR + UNR
C75-69-4	2.55e-3	trichlorofluoromethane	NROG	UNR
C56-23-5	2.47e-3	carbon tetrachloride	NROG	UNR
C60-29-7	2.45e-3	ethyl ether	ALK5	4 PAR
C584-84-9	2.44e-3	2,4-toluene diisocyanate {tdi}	NROG	TOL + 2 UNR
C110-98-5	2.44e-3	diisopropylene glycol; 1,1'-oxydipropan-2-ol	ALK5	2 PAR + 2 ALD2
C80-62-6	2.43e-3	methyl methacrylate	OLE2	2 PAR + OLE + UNR
C74-95-3	2.41e-3	methylene bromide	NROG	UNR
C123-38-6	2.39e-3	propionaldehyde	RCHO	PAR + ALD2

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C75-01-4	2.39e-3	vinyl chloride	ALK4	ETH
C98-82-8	2.23e-3	cumene (isopropyl benzene)	ARO1	2 PAR + TOL
C2452-99-5	2.21e-3	1,2-dimethylcyclopentane	ALK5	7 PAR
C95-50-1	2.19e-3	o-dichlorobenzene	0.295 ARO1	PAR + 5 UNR
C108-08-7	2.15e-3	2,4-dimethylpentane	ALK4	7 PAR
C625-54-7	2.12e-3	ethyl isopropyl ether	ALK5	5 PAR
C111-84-2	2.12e-3	n-nonane	ALK5	7 PAR + 2 UNR
C1640-89-7	2.05e-3	ethylcyclopentane	ALK5	7 PAR
C7379-12-6	2.04e-3	2-methyl-3-hexanone	PRD2	7 PAR
C112-40-3	2.04e-3	n-dodecane	ALK5	8 PAR + 4 UNR
C108-94-1	2.02e-3	cyclohexanone	PRD2	6 PAR
C98-01-1	2.01e-3	2-furfural	ARO1	PAR + OLE + ALD2
C127-91-3	1.99e-3	b-pinene	TERP	8 PAR + OLE
C140-88-5	1.96e-3	ethyl acrylate	OLE1	2 PAR + OLE + UNR
C1638-26-2	1.94e-3	1,1-dimethylcyclopentane	ALK5	7 PAR
C123-72-8	1.91e-3	butyraldehyde	RCHO	2 PAR + ALD2
C75-56-9	1.90e-3	propylene oxide	ALK2	2 PAR + UNR
C67-66-3	1.90e-3	chloroform	NROG	UNR
C589-34-4	1.90e-3	3-methylhexane	ALK5	7 PAR
C646-04-8	1.90e-3	trans-2-pentene	OLE2	PAR + 2 ALD2
C76-16-4	1.90e-3	hexafluoroethane {f-116}	NROG	2 UNR
C563-46-2	1.86e-3	2-methyl-1-butene	OLE2	4 PAR + FORM
C112-41-4	1.86e-3	1-Dodecene	OLE1	10 PAR + OLE
C112-34-5	1.86e-3	2-(2-butoxyethoxy)ethanol {butyl carbitol}	ALK5	8 PAR
C95-63-6	1.84e-3	1,2,4-trimethylbenzene	ARO2	PAR + XYL
C108-93-0	1.82e-3	cyclohexanol	ALK5	6 PAR
C142-29-0	1.80e-3	cyclopentene	OLE2	PAR + 2 ALD2
C71-23-8	1.70e-3	n-propyl alcohol	ALK4	3 PAR
C78-84-2	1.67e-3	isobutyraldehyde	RCHO	2 PAR + ALD2
C75-65-0	1.67e-3	tert-butyl alcohol	ALK2	3 PAR + UNR
C79-10-7	1.67e-3	acrylic acid	OLE1	OLE + UNR
C78-83-1	1.67e-3	isobutyl alcohol	ALK5	4 PAR
C822-50-4	1.67e-3	trans-1-2-dimethylcyclopentane	ALK5	7 PAR
C1192-18-3	1.67e-3	cis-1-2-dimethylcyclopentane	ALK5	7 PAR
C109201-63-0	1.65e-3	butyl isopropyl phthalate	ARO1	8 PAR + 7 UNR
C76-13-1	1.64e-3	trichlorotrifluoroethane-f113	NROG	2 UNR
C141-32-2	1.64e-3	n-butyl acrylate	OLE1	4 PAR + OLE + UNR
C141-43-5	1.63e-3	ethanolamine	ALK5	ALD2
C75-00-3	1.63e-3	ethyl chloride	ALK2	2 UNR
C593-67-9	1.63e-3	Ethylene amine	OLE1	ALD2
C106-93-4	1.63e-3	ethylene dibromide	ALK1	2 UNR
C75-71-8	1.60e-3	dichlorodifluoromethane (f-12)	NROG	UNR
C64-18-6	1.59e-3	formic acid	ALK2	UNR
C624-64-6	1.57e-3	trans-2-butene	OLE2	2 ALD2

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C78-92-2	1.57e-3	sec-butyl alcohol	ALK5	4 PAR
C591-76-4	1.57e-3	2-methylhexane	ALK5	7 PAR
C106-89-8	1.56e-3	epichlorohydrin	ALK5	3 PAR
C100-44-7	1.56e-3	benzyl chloride	0.295	TOL
			ARO1	
C513-35-9	1.55e-3	2-methyl-2-butene	OLE2	3 PAR + ALD2
C126-99-8	1.54e-3	chloroprene (2-chloro-1,3-butadiene)	ALK4	2 OLE
C124-04-9	1.52e-3	adipic acid	ALK5	4 PAR + 2 UNR
C619-99-8	1.52e-3	3-ethylhexane	ALK5	8 PAR
C78-79-5	1.51e-3	isoprene	ISOP	ISOP
C590-19-2	1.48e-3	1,2-butadiene {methylallene}	OLE1	PAR + 1.5 OLE
C504-60-9	1.48e-3	piperylene {1,3-pentadiene} (mixed isomers)	OLE2	PAR + 2 OLE
C79-09-4	1.48e-3	propionic acid	ALK2	2 PAR + UNR
C108-67-8	1.47e-3	1,3,5-trimethylbenzene	ARO2	PAR + XYL
C111-77-3	1.45e-3	methyl carbitol {2-(2-methoxyethoxy)ethanol} {degme}	ALK5	5 PAR
C109-86-4	1.45e-3	2-methoxyethanol {methyl cellosolve} {egme}	ALK5	3 PAR
C97-85-8	1.45e-3	isobutyl isobutyrate	ALK4	7 PAR + UNR
C75-46-7	1.41e-3	trifluoromethane (f-23)	NROG	UNR
C96-33-3	1.41e-3	methyl acrylate	OLE1	PAR + OLE + UNR
C106-63-8	1.41e-3	isobutyl acrylate {2-propenoic acid}	OLE1	4 PAR + OLE + UNR
C91-20-3	1.40e-3	naphthalene	ARO2	2 PAR + XYL
C108-24-7	1.38e-3	acetic anhydride	NROG	2 PAR + 2 UNR
C541-05-9	1.36e-3	hexamethylcyclotrisiloxane	NROG	6 PAR
C79-00-5	1.32e-3	1,1,2-trichloroethane	ALK1	2 UNR
C84-74-2	1.31e-3	dibutyl phthalate	ARO1	9 PAR + 7 UNR
C627-20-3	1.29e-3	cis-2-pentene	OLE2	PAR + 2 ALD2
C540-84-1	1.27e-3	2,2,4-trimethylpentane	ALK4	7 PAR + UNR
C1678-91-7	1.24e-3	ethylcyclohexane	ALK5	8 PAR
C61168-10-3	1.24e-3	1-nonene-4-one	MVK	7 PAR + OLE
C1634-04-4	1.24e-3	methyl t-butyl ether (mtbe)	ALK3	4 PAR + UNR
C98-95-3	1.23e-3	nitrobenzene	0.295	PAR + 5 UNR
			ARO1	
C75-08-1	1.23e-3	ethyl mercaptan	ALK5	2 PAR
C526-73-8	1.20e-3	1,2,3-trimethylbenzene	ARO2	PAR + XYL
C629-62-9	1.19e-3	n-pentadecane	ALK5	10 PAR + 5 UNR
C103-65-1	1.09e-3	n-propylbenzene	ARO1	2 PAR + TOL
C136-60-7	1.09e-3	n-butyl benzoate	ARO1	5 PAR + 6 UNR
C107-31-3	1.07e-3	methyl formate	ALK1	PAR + UNR
C620-14-4	1.07e-3	m-ethyltoluene	ARO2	PAR + XYL
C75-15-0	1.06e-3	carbon disulfide	NROG	PAR
C592-27-8	1.03e-3	2-methylheptane	ALK5	8 PAR
C85-44-9	1.03e-3	phthalic anhydride	ARO1	PAR + 7 UNR
C638-04-0	1.00e-3	cis-1,3-dimethylcyclohexane	ALK5	8 PAR
C17302-28-2	9.47e-4	2,6-dimethylnonane	ALK5	8 PAR + 3 UNR
C109-69-3	9.05e-4	1-chlorobutane	ALK3	4 PAR
C26730-16-5	8.51e-4	6-Methyl Tetradecane	ALK5	10 PAR + 5 UNR

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C18435-22-8	8.51e-4	3-Methyl Tetradecane	ALK5	10 PAR + 5 UNR
C13286-72-1	8.51e-4	3,9-Diethyl Undecane	ALK5	15 PAR
C15869-89-3	8.39e-4	2,5-dimethyloctane	ALK5	10 PAR
C590-18-1	8.35e-4	cis-2-butene	OLE2	2 ALD2
C2216-34-4	8.13e-4	4-methyloctane	ALK5	9 PAR
C629-50-5	7.95e-4	n-tridecane	ALK5	9 PAR + 4 UNR
C2207-03-6	7.92e-4	trans-1,3-dimethylcyclohexane	ALK5	8 PAR
C611-14-3	7.90e-4	o-ethyltoluene	ARO2	PAR + XYL
C98-83-9	7.85e-4	a-methylstyrene	OLE2	OLE + TOL
C637-50-3	7.85e-4	b-methylstyrene	OLE2	OLE + TOL
C3221-61-2	7.75e-4	2-methyloctane	ALK5	9 PAR
C2216-33-3	7.61e-4	3-methyloctane	ALK5	9 PAR
C75-45-6	7.56e-4	chlorodifluoromethane (f-22)	NROG	UNR
C2207-04-7	7.47e-4	trans-1,4-dimethylcyclohexane	ALK5	8 PAR
C2847-72-5	7.34e-4	4-methyldecane	ALK5	8 PAR + 3 UNR
C103-71-9	7.33e-4	phenyl isocyanate	0.295 ARO1	PAR + 6 UNR
C15869-85-9	7.31e-4	5-methylnonane	ALK5	10 PAR
C287-92-3	7.31e-4	cyclopentane	ALK4	5 PAR
C622-96-8	7.27e-4	p-ethyltoluene	ARO2	PAR + XYL
C14720-74-2	7.18e-4	2,2,4-trimethylheptane	ALK5	10 PAR
C5881-17-4	6.99e-4	3-ethyloctane	ALK5	10 PAR
C565-59-3	6.70e-4	2,3-dimethylpentane	ALK5	7 PAR
C15869-93-9	6.41e-4	3,5-dimethyloctane	ALK5	10 PAR
C95-48-7	6.41e-4	o-cresol (2-methyl-benzenol)	CRES	TOL
C108-39-4	6.41e-4	m-cresol (3-methyl-benzenol)	CRES	TOL
C106-44-5	6.41e-4	p-cresol (4-methyl-benzenol)	CRES	TOL
Sx-015	6.31e-4	2,3,4-trimethyl-5-propylheptane	ALK5	17 PAR
C1560-92-5	6.31e-4	2-methylheptadecane	ALK5	17 PAR
C3178-29-8	6.11e-4	4-Propyl Heptane	ALK5	10 PAR
C19398-77-7	6.11e-4	3,4-Diethyl Hexane	ALK5	7 PAR + 3 UNR
C100-18-5	6.10e-4	1,2-isodipropylbenzene	ARO2	4 PAR + XYL
C2207-01-4	6.07e-4	cis-1,2-dimethylcyclohexane	ALK5	8 PAR
C592-41-6	5.99e-4	1-hexene	OLE1	4 PAR + OLE
C124-17-4	5.93e-4	diethylene glycol butyl ether acetate {2-2-(butoxyethoxy)ethylacetate}	ALK5	9 PAR + UNR
C1569-02-4	5.77e-4	1-ethoxy-2-propanol	ALK5	5 PAR
C629-59-4	5.71e-4	n-tetradecane	ALK5	10 PAR + 4 UNR
C6975-98-0	5.61e-4	2-methyldecane	ALK5	11 PAR
C13151-34-3	5.51e-4	3-methyldecane	ALK5	8 PAR + 3 UNR
C589-81-1	5.35e-4	3-methylheptane	ALK5	8 PAR
C556-67-2	5.11e-4	octamethylcyclotetrasiloxane	NROG	8 PAR
C592-13-2	4.93e-4	2,5-dimethylhexane	ALK5	8 PAR
C3074-75-7	4.91e-4	2-methyl-4-ethylhexane	ALK5	9 PAR
C871-83-0	4.85e-4	2-methylnonane	ALK5	7 PAR + 3 UNR
C99-62-7	4.84e-4	1,3-isodipropylbenzene	ARO2	4 PAR + XYL
C3074-71-3	4.79e-4	2,3-dimethylheptane	ALK5	9 PAR
C4032-86-4	4.71e-4	3,3-dimethylheptane	ALK5	9 PAR

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C577-55-9	4.71e-4	1,4-isodipropylbenzene	ARO2	4 PAR + XYL
C5989-27-5	4.69e-4	d-limonene	TERP	4 PAR + OLE + 2 ALD2
C110-63-4	4.68e-4	1,4-butanediol	ALK5	4 PAR
C4074-46-8	4.66e-4	4-methyl-2-propyl-phenol	CRES	3 PAR + TOL
C3073-66-3	4.57e-4	1,1,3-trimethylcyclohexane	ALK5	9 PAR
C565-75-3	4.56e-4	2,3,4-trimethylpentane	ALK5	8 PAR
C6876-23-9	4.49e-4	trans-1,2-dimethylcyclohexane	ALK5	8 PAR
C921-47-1	4.46e-4	2,3,4-trimethylhexane	ALK5	9 PAR
C141-93-5	4.42e-4	1,3-diethylbenzene (meta)	ARO2	2 PAR + XYL
C7045-71-8	4.41e-4	2-methylundecane {isododecane}	ALK5	12 PAR
C544-76-3	4.34e-4	hexadecane	ALK5	11 PAR + 5 UNR
C590-73-8	4.23e-4	2,2-dimethylhexane	ALK4	7 PAR + UNR
C624-29-3	4.23e-4	cis-1,4-dimethylcyclohexane	ALK5	8 PAR
C100-52-7	4.07e-4	benzaldehyde	NROG	7 UNR
Sx-016	4.05e-4	3,4,8-trimethyl-5-propyldodecane	ALK5	18 PAR
C6418-44-6	4.05e-4	3-methylheptadecane	ALK5	18 PAR
C6236-88-0	3.99e-4	trans 1-methyl-4-ethylcyclohexane	ALK5	9 PAR
C1679-00-1	3.99e-4	1,4-Diethyl-Cyclohexane	ALK5	7 PAR + 3 UNR
C104-76-7	3.98e-4	2-ethyl-1-hexanol	ALK5	8 PAR
C1678-99-5	3.92e-4	1,3-Diethyl-Cyclohexane	ALK5	10 PAR
C13150-81-7	3.88e-4	2,6-dimethyldecane	ALK5	12 PAR
C135-01-3	3.77e-4	1,2-diethylbenzene (ortho)	ARO2	2 PAR + XYL
C17312-53-7	3.73e-4	3,6-Dimethyl Decane	ALK5	8 PAR + 4 UNR
C609-26-7	3.71e-4	2-methyl-3-ethylpentane	ALK5	8 PAR
C6165-40-8	3.68e-4	7-Methyl Pentadecane	ALK5	11 PAR + 5 UNR
C2882-96-4	3.68e-4	3-Methyl Pentadecane	ALK5	11 PAR + 5 UNR
C175032-36-7	3.68e-4	4,8-Dimethyl Tetradecane	ALK5	11 PAR + 5 UNR
C82144-67-0	3.64e-4	3,7-Dimethyl Dodecane	ALK5	10 PAR + 4 UNR
C6418-41-3	3.64e-4	3-Methyl Tridecane	ALK5	10 PAR + 4 UNR
C6224-52-8	3.64e-4	3,8-Diethyl Decane	ALK5	14 PAR
C13287-21-3	3.64e-4	6-Methyl Tridecane	ALK5	10 PAR + 4 UNR
C2051-30-1	3.61e-4	2,6-dimethyloctane	ALK5	10 PAR
C107-22-2	3.60e-4	glyoxal	GLY	PAR + FORM
C17301-94-9	3.58e-4	4-methylnonane	ALK5	7 PAR + 3 UNR
C463-58-1	3.53e-4	carbonyl sulfide	NROG	UNR
C589-53-7	3.50e-4	4-methylheptane	ALK5	8 PAR
C560-21-4	3.49e-4	2,3,3-trimethylpentane	ALK5	7 PAR + UNR
C6443-92-1	3.49e-4	cis-2-heptene	OLE2	3 PAR + 2 ALD2
C625-65-0	3.49e-4	2,4-dimethyl-2-pentene	OLE2	3 PAR + 2 ALD2
C592-76-7	3.49e-4	1-heptene	OLE1	5 PAR + OLE
C10574-37-5	3.49e-4	2,3-dimethyl-2-pentene	OLE2	3 PAR + 2 ALD2
C14686-14-7	3.43e-4	trans-3-heptene	OLE2	3 PAR + 2 ALD2
C24910-63-2	3.43e-4	3,4-dimethyl-2-pentene	OLE2	3 PAR + 2 ALD2
C37027-60-4	3.38e-4	3-Butoxy-1-butene	OLE1	6 PAR + OLE
C4516-69-2	3.37e-4	1,1,3-trimethylcyclopentane	ALK5	8 PAR
C7688-21-3	3.32e-4	cis-2-hexene	OLE2	2 PAR + 2 ALD2
C34522-19-5	3.31e-4	trans 1-methyl-3-propyl cyclohexane	ALK5	10 PAR

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C17302-27-1	3.30e-4	2,5-dimethylnonane	ALK5	11 PAR
C17085-96-0	3.29e-4	3-ethyldecane	ALK5	12 PAR
C496-11-7	3.28e-4	indan	ARO2	PAR + XYL
C563-45-1	3.27e-4	3-methyl-1-butene	OLE1	3 PAR + OLE
C108-31-6	3.27e-4	maleic anhydride	OLE2	2 OLE
C2815-58-9	3.27e-4	1,2,4-trimethylcyclopentene	OLE2	4 PAR + 2 ALD2
C15890-40-1	3.22e-4	cis-1,trans-2,3-trimethylcyclopentane	ALK5	8 PAR
C4170-30-3	3.20e-4	crotonaldehyde	IPRD	OLE + ALD2
Sx-007	3.16e-4	2,8-dimethyl-5-ethyloctane	ALK5	12 PAR
C123-42-2	3.11e-4	diacetone alcohol (4-hydroxy-4-methyl-2-pentanone)	MEK	6 PAR
C78-98-8	3.08e-4	methyl glyoxal	MGLY	FORM + ALD2
C925-54-2	3.07e-4	2-methyl-hexanal	RCHO	5 PAR + ALD2
C1678-80-4	3.07e-4	trans,trans-1,2,4-trimethylcyclohexane	ALK5	9 PAR
C131-11-3	3.03e-4	dimethyl phthalate	ARO1	3 PAR + 7 UNR
C98-06-6	3.03e-4	t-butylbenzene	ARO1	2 PAR + TOL + UNR
C62238-33-9	3.03e-4	1-Ethyl-2-Propyl Cyclohexane	ALK5	11 PAR
S2-99079	3.00e-4	cis,trans-1,2,4-trimethylcyclohexane	ALK5	9 PAR
C1678-93-9	2.96e-4	butylcyclohexane	ALK5	10 PAR
C2216-30-0	2.92e-4	2,5-dimethylheptane	ALK5	9 PAR
C91-57-6	2.85e-4	2-methylnaphthalene	ARO2	3 PAR + XYL
C562-49-2	2.85e-4	3,3-dimethylpentane	ALK3	6 PAR + UNR
C767-58-8	2.79e-4	1-methyl indan	ARO2	2 PAR + XYL
C90-12-0	2.75e-4	1-methyl naphthalene	ARO2	2 PAR + XYL + UNR
S2-99044	2.72e-4	6-ethyl-2-methyloctane	ALK5	11 PAR
C590-66-9	2.67e-4	1,1-dimethylcyclohexane	ALK5	8 PAR
C4926-90-3	2.66e-4	1-methyl-1-ethylcyclohexane	ALK5	9 PAR
C1002-43-3	2.65e-4	3-methylundecane	ALK5	8 PAR + 4 UNR
C4050-45-7	2.63e-4	trans-2-hexene	OLE2	2 PAR + 2 ALD2
S2-99051	2.62e-4	3-ethyl-3-methyloctane	ALK5	11 PAR
C872-05-9	2.61e-4	1-decene	OLE1	8 PAR + OLE
C527-53-7	2.59e-4	1,2,3,5-tetramethylbenzene	ARO2	2 PAR + XYL
C3525-27-7	2.55e-4	3-ethyl -1-heptene	OLE1	7 PAR + OLE
C617-78-7	2.55e-4	3-ethylpentane	ALK4	7 PAR
C464-06-2	2.55e-4	2,2,3-trimethylbutane	ALK4	6 PAR + UNR
C7094-26-0	2.47e-4	1,1,2-trimethylcyclohexane	ALK5	9 PAR
C123-04-6	2.44e-4	3-(chloromethyl)-heptane	ALK4	8 PAR
C13151-35-4	2.38e-4	5-methyldecane	ALK5	11 PAR
C674-76-0	2.32e-4	4-methyl-trans-2-pentene	OLE2	2 PAR + 2 ALD2
C75-72-9	2.32e-4	chlorotrifluoromethane (f-13)	NROG	UNR
C7667-60-9	2.29e-4	cis-1,trans-2,trans-4-trimethylcyclohexane	ALK5	9 PAR
C74-87-3	2.28e-4	methyl chloride	NROG	UNR
C20278-85-7	2.28e-4	2,3,5-trimethylheptane	ALK5	10 PAR
C85-01-8	2.26e-4	phenanthrene	ARO2	6 PAR + XYL
C4259-00-1	2.25e-4	1,1,2-trimethylcyclopentane	ALK5	8 PAR
C547-63-7	2.25e-4	methyl isobutyrate	ALK3	5 PAR
C815-24-7	2.25e-4	2,2,4,4-tetramethyl-3-pentanone	PRD2	9 PAR

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
S2-91087	2.23e-4	3-methyl-5-ethylheptane	ALK5	10 PAR
C105-05-5	2.22e-4	1,4-diethylbenzene (para)	ARO2	2 PAR + XYL
C17301-23-4	2.17e-4	2,6-dimethylundecane	ALK5	13 PAR
C2213-23-2	2.14e-4	2,4-dimethylheptane	ALK5	9 PAR
C1678-92-8	2.13e-4	propylcyclohexane	ALK5	9 PAR
C1632-70-8	2.11e-4	5-methylundecane	ALK5	8 PAR + 4 UNR
C15869-92-8	2.10e-4	3,4-dimethyloctane	ALK5	10 PAR
C538-93-2	2.07e-4	(2-methylpropyl)benzene	ARO1	3 PAR + TOL
C2870-04-4	2.06e-4	1,3-dimethyl-2-ethylbenzene	ARO2	2 PAR + XYL
C5911-04-6	2.03e-4	3-methylnonane	ALK5	7 PAR + 3 UNR
C65-85-0	1.98e-4	benzoic acid	ARO1	PAR + 6 UNR
C535-77-3	1.95e-4	1-methyl-3-isopropylbenzene	ARO2	2 PAR + XYL
C17301-28-9	1.94e-4	3,6-Dimethyl Undecane	ALK5	9 PAR + 4 UNR
C930-90-5	1.94e-4	trans-2-ethylmethylcyclopentane	ALK5	8 PAR
C1758-88-9	1.94e-4	1,4-dimethyl-2-ethylbenzene	ARO2	2 PAR + XYL
C1072-05-5	1.93e-4	2,6-dimethylheptane	ALK5	9 PAR
C696-29-7	1.92e-4	isopropylcyclohexane (2-methylethyl cyclohexane)	ALK5	9 PAR
C17453-93-9	1.83e-4	5-Methyl Dodecane	ALK5	9 PAR + 4 UNR
C17312-57-1	1.83e-4	3-Methyl Dodecane	ALK5	9 PAR + 4 UNR
C625-27-4	1.82e-4	2-methyl-2-pentene	OLE2	4 PAR + ALD2
C581-42-0	1.80e-4	2,6-dimethyl naphthalene	ARO2	4 PAR + XYL
C571-58-4	1.80e-4	1.4-dimethylnaphthalene	ARO2	4 PAR + XYL
S2-43252	1.79e-4	2,2,5-triethylheptane	ALK5	13 PAR
C14638-54-1	1.79e-4	2,4,6,8-Tetramethyl Nonane	ALK5	9 PAR + 4 UNR
C939-27-5	1.79e-4	2-ethylnaphthalene	ARO2	4 PAR + XYL
C100-61-8	1.78e-4	4-methylaniline	0.295 ARO1	TOL
C7146-60-3	1.77e-4	2,3-dimethyloctane	ALK5	10 PAR
C1795-27-3	1.75e-4	cis-1,cis-3,5-trimethylcyclohexane	ALK5	9 PAR
C2613-69-6	1.71e-4	cis-1,cis-2,3-trimethylcyclopentane	ALK5	8 PAR
S2-99075	1.70e-4	trans,cis-1,2,4-trimethylcyclohexane	ALK5	9 PAR
C95-93-2	1.69e-4	1,2,4,5-tetramethylbenzene	ARO2	2 PAR + XYL
C3522-94-9	1.64e-4	2,2,5-trimethylhexane	ALK4	8 PAR + UNR
S2-99076	1.60e-4	trans,trans-1,3,5-trimethylcyclohexane	ALK5	9 PAR
C110-83-8	1.58e-4	cyclohexene	OLE2	2 PAR + 2 ALD2
C75-73-0	1.58e-4	tetrafluoromethane {carbon tetrafluoride} {r 14}	NROG	UNR
C693-89-0	1.55e-4	1-methylcyclopentene	OLE2	2 PAR + 2 ALD2
C629-78-7	1.55e-4	n-heptadecane	ALK5	11 PAR + 6 UNR
C538-68-1	1.55e-4	n-pentylbenzene	ARO1	4 PAR + TOL
C7525-62-4	1.53e-4	m-ethyl styrene	OLE2	PAR + OLE + TOL
C934-80-5	1.53e-4	1,2-dimethyl-4-ethylbenzene	ARO2	2 PAR + XYL
C124-10-7	1.51e-4	methyl myristate {methyl tetradecanoate}	ALK5	14 PAR + UNR
C3875-51-2	1.51e-4	isopropylcyclopentane	ALK5	8 PAR
C584-94-1	1.44e-4	2,3-dimethylhexane	ALK5	8 PAR
C933-98-2	1.42e-4	1,2-dimethyl-3-ethylbenzene	ARO2	2 PAR + XYL
C4485-13-6	1.40e-4	4-propyl-3-heptene	OLE2	6 PAR + 2 ALD2
C35648-55-6	1.40e-4	3-propyl-1-heptene	OLE1	8 PAR + OLE
C4984-01-4	1.40e-4	3,7-dimethyl-1-octene	OLE2	6 PAR + 2 ALD2

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C19780-61-1	1.40e-4	3-ethyl-2-methyl-2-heptene	OLE2	6 PAR + 2 ALD2
C19398-89-1	1.40e-4	Trans-4-Decene	OLE2	3 PAR + 2 ALD2 + 3 UNR
C1119-40-0	1.39e-4	pentanedioic acid, dimethyl ester (dimethyl glutarate)	ALK4	5 PAR + 2 UNR
S2-91120	1.39e-4	1-methyl-4-n-pentylbenzene	ARO2	4 PAR + XYL
C1595-04-6	1.39e-4	1-methyl-3-butylbenzene	ARO2	3 PAR + XYL
C17302-32-8	1.38e-4	3,7-dimethylnonane	ALK5	11 PAR
C1759-58-6	1.37e-4	trans-1,3-dimethylcyclopentane	ALK5	7 PAR
C62016-37-9	1.35e-4	2,4,6-trimethyloctane	ALK5	11 PAR
C934-74-7	1.33e-4	1,3-dimethyl-5-ethylbenzene	ARO2	2 PAR + XYL
C3982-64-7	1.32e-4	1,3-dimethyl-5-propylbenzene	ARO2	3 PAR + XYL
C29316-05-0	1.32e-4	s-pentylbenzene	ARO1	4 PAR + TOL
C16021-20-8	1.32e-4	1-ethyl-2-propylbenzene	ARO2	3 PAR + XYL
C13732-80-4	1.32e-4	1,2-diethyl-4-methylbenzene	ARO2	3 PAR + XYL
C616-12-6	1.30e-4	3-methyl-trans-2-pentene	OLE2	4 PAR + ALD2
C874-35-1	1.28e-4	5-methylindan	ARO2	2 PAR + XYL
C877-44-1	1.26e-4	1,2,4-triethylbenzene	ARO2	4 PAR + XYL
C1077-16-3	1.26e-4	n-hexylbenzene	ARO1	5 PAR + TOL
C1074-55-1	1.26e-4	1-methyl-4n-propylbenzene	ARO2	2 PAR + XYL
S2-99041	1.23e-4	1-methyl-2-isopropylcyclohexane	ALK5	10 PAR
C29949-27-7	1.22e-4	n-pentylcyclohexane	ALK5	11 PAR
C7154-80-5	1.22e-4	3,3,5-trimethylheptane	ALK5	10 PAR
C493-01-6	1.17e-4	cis-decalin	ALK5	10 PAR
C488-23-3	1.15e-4	1,2,3,4-tetramethylbenzene	ARO2	2 PAR + XYL
C19489-10-2	1.12e-4	cis-1-ethyl-3-methylcyclohexane	ALK5	9 PAR
C760-20-3	1.05e-4	3-methyl-1-pentene	OLE1	4 PAR + OLE
C2532-58-3	1.04e-4	cis-1,3-dimethylcyclopentane	ALK5	7 PAR
C874-41-9	1.03e-4	1,3-dimethyl-4-ethylbenzene	ARO2	2 PAR + XYL
C765-47-9	1.03e-4	1,2-dimethylcyclopentene	OLE2	5 PAR + OLE
C629-92-5	1.03e-4	nonadecane	ALK5	13 PAR + 6 UNR
C1678-97-3	1.01e-4	1,2,3-trimethylcyclohexane	ALK5	9 PAR
C583-48-2	1.01e-4	3,4-dimethylhexane	ALK5	8 PAR
C123-35-3	9.92e-5	myrcene	TERP	4 PAR + 3 OLE
C1636-39-1	9.67e-5	cyclopentylcyclopentane	OLE2	10 PAR
C16747-26-5	9.67e-5	2,2,4-trimethylhexane	ALK5	8 PAR + UNR
C142-96-1	9.63e-5	dibutyl ether	ALK5	8 PAR
C76-15-3	9.60e-5	chloropentafluoroethane (f115)	NROG	2 UNR
C17302-33-9	9.48e-5	6-methylundecane	ALK5	12 PAR
C555-10-2	9.33e-5	b-phellandrene {1(7)-2-p-menthadiene}	TERP	6 PAR + 2 OLE
C26638-19-7	9.19e-5	propylene dichloride	ALK2	1.5 PAR + 1.5 UNR
C2613-66-3	9.14e-5	cis-1-methyl-3-ethylcyclopentane	ALK5	8 PAR
Sx-006	9.08e-5	4,6-dimethyl-2-octyne	OLE2	8 PAR + ALD2
C764-93-2	9.06e-5	1-decyne	OLE1	7 PAR + OLE + UNR
S2-99040	8.87e-5	1-methyl-3-isopropylcyclohexane	ALK5	10 PAR
C24612-75-7	8.73e-5	1,1,3,4-tetramethylcyclohexane	ALK5	10 PAR
C20348-72-5	8.58e-5	cis,trans-1,2,3-trimethylcyclohexane	ALK5	9 PAR
C99-87-6	8.53e-5	1-methyl-4-isopropylbenzene	ARO2	2 PAR + XYL

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
S2-99046	8.48e-5	1,2-dimethyl-3-ethylcyclohexane	ALK5	10 PAR
C74-99-7	8.21e-5	1-propyne	OLE1	PAR + ALD2
C591-49-1	8.12e-5	1-methyl cyclohexene	OLE2	5 PAR + OLE
C208-96-8	8.11e-5	acenaphthylene	ARO2	2 OLE + XYL
C3741-00-2	8.11e-5	pentylcyclopentane	ALK5	10 PAR
C104-87-0	8.06e-5	p-tolualdehyde {4-methylbenzaldehyde}	NROG	8 UNR
C2980-69-0	7.96e-5	4-methylundecane	ALK5	12 PAR
C5794-03-6	7.90e-5	camphene	TERP	8 PAR + OLE
C15869-94-0	7.88e-5	3,6-dimethyloctane	ALK5	10 PAR
C6682-71-9	7.73e-5	4,7-dimethyl-2,3-dihydro-1-h-indenes	ARO2	3 PAR + XYL
C1685-83-2	7.73e-5	4,5-dimethyl-2,3-dihydro-1-h-indenes	ARO2	3 PAR + XYL
C1685-82-1	7.73e-5	4,6-dimethyl-2,3-dihydro-1-h-indenes	ARO2	3 PAR + XYL
C1075-22-5	7.73e-5	5,6-dimethyl-2,3-dihydro-1-h-indenes	ARO2	3 PAR + XYL
S2-99056	7.71e-5	5-isopropylnonane	ALK5	12 PAR
C1678-98-4	7.60e-5	isobutylcyclohexane (2-methylpropyl cyclohexane)	ALK5	10 PAR
C564-02-3	7.57e-5	2,2,3-trimethylpentane	ALK5	8 PAR
C691-37-2	7.43e-5	4-methyl-1-pentene	OLE1	4 PAR + OLE
C107-00-6	7.35e-5	1-butyne (ethylacetylene)	OLE1	2 PAR + ALD2
C107-39-1	7.32e-5	2,4,4-trimethyl-1-pentene	OLE1	6 PAR + FORM + UNR
C13269-52-8	7.09e-5	trans-3-hexene	OLE2	2 PAR + 2 ALD2
C10143-23-4	7.06e-5	dimethylpentanol (2,3-dimethyl-1-pentanol)	ALK5	7 PAR
C4551-51-3	7.02e-5	cis-bicyclo[4.3.0]nonane	ALK5	9 PAR
C7642-09-3	6.78e-5	cis-3-hexene	OLE2	2 PAR + 2 ALD2
S2-99053	6.76e-5	1,2-diethyl-1-methylcyclohexane	ALK5	11 PAR
C54105-77-0	6.70e-5	(2-methylbutyl)cyclohexane	ALK5	11 PAR
C111-66-0	6.66e-5	1-octene	OLE1	6 PAR + OLE
C1072-16-8	6.61e-5	2,7-dimethyloctane	ALK5	10 PAR
C4032-94-4	6.55e-5	2,4-dimethyloctane	ALK5	10 PAR
C20278-84-6	6.36e-5	2,4,5-trimethylheptane	ALK5	10 PAR
C1004-29-1	6.33e-5	2-butyltetrahydrofuran	ALK5	6 PAR + ALD2
C563-16-6	6.31e-5	3,3-dimethylhexane	ALK5	8 PAR
C15870-10-7	6.19e-5	2-methyl-1-heptene	OLE1	6 PAR + OLE
C5364-83-0	5.88e-5	propenylcyclohexane	OLE2	7 PAR + OLE
C4926-76-5	5.83e-5	trans-1-ethyl-3-methylcyclohexane	ALK5	9 PAR
C92-52-4	5.81e-5	biphenyl {phenyl benzene}	ARO1	TOL + 5 UNR
C1071-26-7	5.80e-5	2,2-dimethylheptane	ALK5	9 PAR
C593-45-3	5.79e-5	octadecane	ALK5	12 PAR + 6 UNR
C76-14-2	5.78e-5	1,2-dichloro-1,1,2,2-tetrafluoroethane {cfc-114}	NROG	2 UNR
C1331-14-2	5.71e-5	2,2-dichloronitroaniline	0.295 ARO1	PAR + 5 UNR
C84-65-1	5.61e-5	9,10-anthraquinone	ARO2	2 TOL
C120-82-1	5.56e-5	1,2,4-trichlorobenzene	NROG	PAR + 5 UNR
C135-98-8	5.46e-5	(1-methylpropyl)benzene (sec-butyl benzene)	ARO1	3 PAR + TOL
C56147-63-8	5.34e-5	2-ethylindan	ARO2	3 PAR + XYL
S2-99377	5.30e-5	ethyl-phenyl-phenyl-ethane	ARO1	PAR + TOL + XYL
C584-48-5	5.24e-5	bromodinitrobenzene	0.295 ARO1	PAR + 5 UNR

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C3238-38-8	5.17e-5	2,3,4,6-Tetramethylphenol (Isodurenonol)	CRES	3 PAR + TOL
C926-82-9	5.09e-5	3,5-dimethylheptane	ALK5	9 PAR
C922-28-1	5.04e-5	3,4-dimethylheptane	ALK5	9 PAR
Sx-012	5.02e-5	3,4,6-trimethyl-2-heptene	OLE2	9 PAR + 2 ALD2
Sx-011	5.02e-5	3,4,6-trimethyl-1-heptene	OLE1	11 PAR + OLE
C563-79-1	5.01e-5	2,3-dimethyl-2-butene	OLE2	2 PAR + 2 ALD2
C563-78-0	5.01e-5	2,3-dimethyl-1-butene	OLE2	5 PAR + FORM
C66-25-1	5.01e-5	hexanal (hexanaldehyde)	RCHO	4 PAR + ALD2
C1069-53-0	4.90e-5	2,3,5-trimethylhexane	ALK5	9 PAR
C15869-96-2	4.81e-5	4,5-dimethyloctane	ALK5	10 PAR
C14676-29-0	4.81e-5	3-ethyl-2-methylheptane	ALK5	10 PAR
C1126-18-7	4.79e-5	2-butyl cyclohexanone	ALK5	10 PAR
C115-11-7	4.75e-5	2-methylpropene (isobutene)	OLE2	3 PAR + FORM
C2958-76-1	4.61e-5	2-methyldecalin	ALK5	11 PAR
C4110-44-5	4.59e-5	3,3-dimethyloctane	ALK5	10 PAR
C15869-87-1	4.59e-5	2,2-dimethyloctane	ALK5	10 PAR
C360769-33-1	4.55e-5	2,3,3-trimethyl-1-hexene	OLE1	7 PAR + OLE
Sx-010	4.46e-5	3,4,8-trimethyldecane	ALK5	13 PAR
C1196-58-3	4.43e-5	3-phenylpentane	ARO1	4 PAR + TOL
C99-82-1	4.42e-5	1-methyl-4-isopropylcyclohexane	ALK5	10 PAR
C1074-43-7	4.40e-5	1-methyl-3n-propylbenzene	ARO2	2 PAR + XYL
C15869-80-4	4.39e-5	3-ethylheptane	ALK5	9 PAR
C13151-28-5	4.36e-5	3-methyl-1-decene	OLE1	9 PAR + OLE
C101823-01-2	4.36e-5	trans-4-methyl-2-decene	OLE2	7 PAR + 2 ALD2
C1068-87-7	4.33e-5	3-ethyl-2,4-dimethyl pentane	ALK5	9 PAR
C4049-81-4	4.17e-5	2-methyl-1,5-hexadiene	OLE2	3 PAR + 2 ALD2
C28823-42-9	4.17e-5	3-methyl-2,4-hexadiene	OLE2	3 PAR + 2 ALD2
C7058-01-7	4.17e-5	sec-butylcyclohexane	ALK5	10 PAR
C17302-24-8	4.12e-5	2,4-dimethylnonane	ALK5	11 PAR
C1636-44-8	4.05e-5	4-ethyldecane	ALK5	12 PAR
C206-44-0	3.97e-5	fluoranthene	ARO2	2 XYL
C86-73-7	3.94e-5	fluorene	ARO2	5 PAR + XYL
C129-00-0	3.89e-5	pyrene	ARO2	2 XYL
S2-91058	3.84e-5	trans-2,2-trimethyl-3-heptene	OLE2	5 PAR + 2 ALD2
C6434-77-1	3.84e-5	cis-2-nonene	OLE2	5 PAR + 2 ALD2
C124-11-8	3.84e-5	1-nonene	OLE1	7 PAR + OLE
C10405-85-3	3.84e-5	Trans-4-Nonene	OLE2	5 PAR + 2 ALD2
C1192-14-9	3.84e-5	2,2-dimethyl cyclobutanone	PRD2	6 PAR
C4292-75-5	3.82e-5	hexylcyclohexane	ALK5	8 PAR + 4 UNR
C7094-27-1	3.80e-5	1,1,4-trimethylcyclohexane	ALK5	9 PAR
C4218-48-8	3.69e-5	1-ethyl-4-isopropylbenzene	ARO2	3 PAR + XYL
C218-01-9	3.69e-5	chrysene	ARO2	XYL + 10 UNR
C503-17-3	3.68e-5	2-butyne	OLE2	2 PAR + ALD2
S2-99061	3.60e-5	1-ethyl-1,2-dimethylcyclohexane	ALK5	10 PAR
C75736-67-3	3.57e-5	1-Methyl-4-Pentyl Cyclohexane	ALK5	8 PAR + 4 UNR
C164259-42-1	3.46e-5	1,3-Diethyl-5-Methyl Cyclohexane	ALK5	11 PAR
S2-99068	3.36e-5	3,5-dimethylnonane	ALK5	11 PAR

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
S2-99063	3.35e-5	1-ethyl-2,4-dimethylcyclohexane	ALK5	10 PAR
Sx-002	3.34e-5	2,4-dimethyl-1,3-hexadiene	OLE2	2 PAR + OLE + 2 ALD2
C164259-43-2	3.32e-5	1,3,5-Triethyl Cyclohexane	ALK5	12 PAR
C541-73-1	3.30e-5	1,3-dichlorobenzene {m-dichlorobenzene}	0.295 ARO1	PAR + 5 UNR
S2-99054	3.29e-5	cis,cis-1,2,4-trimethylcyclohexane	ALK5	9 PAR
C4923-78-8	3.29e-5	trans-1-ethyl-2-methylcyclohexane	ALK5	9 PAR
C7642-04-8	3.21e-5	cis-2-octene	OLE2	4 PAR + 2 ALD2
C692-70-6	3.15e-5	Trans 2,5-Dimethyl 3-Hexene	OLE2	3 PAR + 2 ALD2 + UNR
C1632-16-2	3.15e-5	2-ethyl-1-hexene	OLE1	6 PAR + OLE
C14850-23-8	3.15e-5	trans-4-octene	OLE2	3 PAR + 2 ALD2 + UNR
C4457-00-5	3.13e-5	hexylcyclopentane	ALK5	11 PAR
C821-95-4	3.12e-5	1-undecene	OLE1	9 PAR + OLE
C4292-92-6	3.06e-5	pentyl Cyclohexane	ALK5	8 PAR + 3 UNR
C1502-38-1	3.05e-5	methylcyclooctane	ALK5	9 PAR
C3404-56-6	3.04e-5	4-methyl-2-heptene	OLE2	4 PAR + 2 ALD2
C13151-05-8	3.04e-5	4-methyl-1-heptene	OLE1	6 PAR + OLE
C590-35-2	3.01e-5	2,2-dimethylpentane	ALK3	7 PAR
C16580-24-8	2.81e-5	1-Methyl-3-Isopropyl Cyclohexane	ALK5	10 PAR
C6891-45-8	2.80e-5	2-butyl-4-methyl-phenol	CRES	4 PAR + TOL
S2-99055	2.79e-5	2-ethyl-1,3-dimethylcyclohexane	ALK5	10 PAR
C2613-65-2	2.66e-5	trans-1-methyl-3-ethylcyclopentane	ALK5	8 PAR
C56700-77-7	2.66e-5	trans 1,3-nonadiene	OLE2	3 PAR + OLE + 2 ALD2
C52688-89-8	2.64e-5	1,1,2,2-tetramethylcyclopentane	ALK5	9 PAR
C2040-95-1	2.60e-5	n-butylcyclopentane	ALK5	9 PAR
C16747-30-1	2.58e-5	2,4,4-trimethylhexane	ALK5	9 PAR
C16747-25-4	2.58e-5	2,2,3,trimethylhexane	ALK5	9 PAR
C3404-78-2	2.22e-5	2,5-dimethylhex-2-ene	OLE2	6 PAR + ETH
C824-22-6	2.21e-5	4-methylindan	ARO2	2 PAR + XYL
C463-49-0	2.10e-5	1,2-propadiene	OLE1	1.5 OLE
S2-99060	2.03e-5	1-ethyl-2,2,6-trimethylcyclohexane	ALK5	11 PAR
S2-99059	2.03e-5	1,1-dimethyl-2-propylcyclohexane	ALK5	11 PAR
C2040-96-2	2.03e-5	propylcyclopentane	ALK5	8 PAR
C447-53-0	2.00e-5	1,2-Dihydronaphthalene	OLE2	2 PAR + XYL
C2146-38-5	2.00e-5	1-ethyl cyclopentene	OLE2	5 PAR + OLE
C123-66-0	1.89e-5	ethylhexanoate (ethyl n-hexanoate)	ALK5	7 PAR + UNR
S2-99066	1.86e-5	4,5-dimethyldecane	ALK5	12 PAR
C16747-50-5	1.77e-5	1,1-methylethylcyclopentane	ALK5	8 PAR
C85893-67-0	1.66e-5	2,3,4-trimethyl 1,3-pentadiene	OLE2	4 PAR + 2 OLE
C16002-93-0	1.66e-5	trans-1-phenyl-1-pentene	OLE2	PAR + OLE + XYL
S2-99062	1.52e-5	1,1,2,3-tetramethylcyclohexane	ALK5	10 PAR
S2-99064	1.48e-5	1-methyl-4-isobutylbenzene	ARO2	3 PAR + XYL
C3200-65-5	1.45e-5	trans-1,2,3,4-Tetramethyl-1-cyclobutene	OLE2	6 PAR + OLE
C692-24-0	1.39e-5	2-methyl-trans-3-hexene	OLE2	3 PAR + 2 ALD2

Table A-2 (continued)

Database ID [a]	Weight Fraction (MF ^{ROG})	Description	Lumped Model Species Representation (Rep) SAPRC-99 CB4	
C3769-23-1	1.39e-5	4-methyl-1-hexene	OLE1	5 PAR + OLE
C3683-22-5	1.39e-5	4-methyl-trans-2-hexene	OLE2	3 PAR + 2 ALD2
C3404-61-3	1.39e-5	3-methyl-1-hexene	OLE1	5 PAR + OLE
C79004-85-6	1.38e-5	tetramethylhexane	ALK5	10 PAR

[a] Designation of the profile in the Carter (2005) emissions profile and speciation database. The composition is based on the profile provided by the EPA (EPA, 1998) to represent total anthropogenic emissions for a Models-3 scenario. The composition as provided was given in terms of mass emissions of EPA SAROAD categories. These were converted to emissions of actual chemical compounds using the SAROAD and mixture assignments in the Carter (2005) emissions speciation database as of 2/21/2005. Methane, unidentified mixtures, compounds judged to be nonvolatile, and the group of compounds that, as a whole, contribute less than 0.05% of the mass of the total in the profile were removed, and the profile was renormalized to 100% mass.

[b] Categorization codes for the compounds used in the Carter (2005) emissions speciation database. Codes starting with "C" are based on the CAS number of the compound. Codes starting with "S" are used for compounds whose CAS numbers are unknown.