PROPOSED OZONE REACTIVITY METRICS TO BE USED IN PRELIMINARY RRWG REACTIVITY ASSESSMENTS

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Given below is a summary of the relative ozone impact (reactivity) metrics proposed for use in the presentations of the reactivity modeling data for the regional model calculations the preliminary RRWG reactivity modeling projects. A total of 8 scales will be calculated for each episode, using two different methods to quantify ozone impacts in a cell and four different methods to use the multi-cell impacts to derive a single regional reactivity metric. These impact quantification and aggregation methods, and what is meant by an "episode" is described below.

Episodes and Data to be Used

Types of Data

The data to be used will be the hourly average ozone concentrations and hourly average sensitivity coefficients for each of the VOC species of interest. Instantaneous concentration or sensitivity data will not be used. Note that the discussion below assumes that the first hourly average output in the day, referred to as "Hour 1" in the subsequent discussion, is the average of the data between midnight and 1 AM, and the last hourly average ("Hour 24") is the average of the data between 11 PM and midnight.

Units of Data

The units of the O_3 data should be ppm. The documentation should state the temperatures and pressures needed to computer absolute concentrations (e.g., moles/liter) from these data.

The sensitivity coefficients to be used should be in units that are proportional to the ppm O_3 concentration change resulting from adding a mole of VOC model species to the emissions. The proportionality factor between the sensitivity units actually used and ppm O_3 per mole VOC must be the same for all model species and all times and locations in the simulations. However, since we are concerned only with relative reactivity metrics, the value of the proportionality factor is immaterial.

The incremental reactivities for model species should be computed on a molar basis because mass based reactivities are not well defined for lumped model species. The incremental reactivities of the base ROG should be computed on a carbon basis because that is how its composition is normalized, and the number of moles of "inert" species are not well defined. Its composition will be specified in terms of moles of model species per mole carbon of base ROG, so this can be used to directly compute the per carbon reactivity of the base ROG from the molar reactivities of the model species. The relative reactivities of model species should be computed as ratios of molar incremental reactivities of the model species to per-carbon incremental reactivities of the base ROG.

The relative reactivity data for individual compounds should be report using either a mole or mass basis, depending on the context of the discussion. For lumped models, the molar reactivities of the compounds can be computed from the molar reactivities of the model species (or sum of model species molar reactivities for CB4), and the molecular weight of the compound can be used to place the results on a

mass basis. The per-carbon molecular weight of the base ROG, which is also needed to compute mass based relative reactivities, will be included with the specification of the base ROG.

Excluded Cells

Cells where O_3 concentration are below a set minimum concentration, which depends on the ozone impact metric used, will be excluded from consideration when deriving global reactivity metrics. The upper limit O_3 will be 80 ppb for metrics based on 1-hour averages and 60 ppb for metrics based on 8-hour averages. This approach is used to minimize the influences of cells where O_3 levels are sufficiently low that small increases are not considered to be problematic.

Cells with zero anthropogenic NO emissions will also be excluded from consideration when deriving global reactivity metrics. This approach is used to minimize the influence of cells over the ocean.

Definition of an Episode

For the purpose of this study, each 24-hour period of the multi-day simulation is treated as a separate "episode" for the purpose of deriving a regional reactivity metric using the 8 different sets of quantification and aggregation methods. The episode day defined from 1 AM to midnight. Note that the "midnight" (Hour 24) data go with the day that ended and not the day that is beginning because it is the average for the previous hour.

Note that the Environ CAMx East Coast simulations of the July 7-15 East Coast episode end at hour 18 (6 PM) East Coast time on July 15, while the Georgia Tech simulations end at midnight on that day. In order to use equivalent daytime periods for both models, July 15 is not used as an episode day for the purpose of model comparisons. The Georgia Tech group may wish to calculate 1-hour reactivity metrics for July 15, but the results should not be aggregated into the results for the other days when presented for comparison with the Environ CAMx results for that episode. Neither group will be able to compute 8-hour reactivity metrics for the last day because as discussed below the averages are associated with the starting hour so computing the averages for all hours of the day requires data for the first 7 hours of the following day.

Initialization Days

Because of concern about initial and boundary conditions in affecting the results, data from at least the first two days of the simulation will not be used for calculating reactivity metrics. For the July 7-15 East Coast episode, the data from the first three days (July 7-9) should be excluded. This is because the Environ CAMx model does not begin using finer grids until July 10.

Daily Ozone Impact Metrics for a Grid Cell

The two ozone impact metrics to be used will be impacts of the VOC on daily maximum 1-hour averages and impacts of the VOC on daily maximum 8-hour averages in each grid cell. Methods for computing these impacts are as follows

Computation of Maximum 1-Hour Average Impacts

The procedure for calculating the episode day maximum 1-hour impacts for a given cell shall consist of the following steps:

1. Determine the hour between Hour 1 to Hour 24 on the episode day that the O_3 has the maximum concentration. If two different hours have exactly the same ozone concentration, use the first hour.
2. Use the hourly average sensitivities for each of the VOC model species for that hour as the reactivity results for this cell for this episode day.
3. Convert the sensitivity coefficients to molar-based units if appropriate.

8-Hour Averaging Period

For regulatory purposes the 8-hour average is assigned to the starting hour, and this convention will be used in these calculations. Therefore, the set of 24 8-hour averages for an episode day will begin with averaging the data between Hour 1 (1 AM) through Hour 8 (8 AM) of the day, and end averaging the data between Hour 24 (midnight) to Hour 7 (7 AM) of the following day. Note that because data are not available for hour 1 of the day following the last day of the episode, 8-hour average metrics will not be calculated for the last simulated day.

Computation of 8-hour averages

The procedure for calculating the episode day maximum 8-hour impacts for a given cell shall consist of the following steps:

1. For each hour between Hour 1 to Hour 24 on the episode day, calculate the average of the 1-hour average ozone concentrations starting at that hour to the next 7 hours. Note that this will require including hours in the following day for the later hours of the episode day.
2. Determine the hour that had the highest 8-hour average ozone concentration. If two different hours have exactly the same average, use the first hour. Determine the start and end time period used for computing the average associated with that hour.
3. Calculate the average of the 1-hour averages of the sensitivities of each of the model species for the 8-hour period that gave the highest 8-hour average ozone. These are the reactivity results for these species for this cell for this episode day.
4. Convert the sensitivity coefficients to molar-based units if appropriate.

Multi-Cell Aggregation Methods

Four different methods will be used to derive a single relative reactivity metric for type of VOC model species for each of the two ozone quantification methods for each episode day. In all cases the reactivities are computed relative to the reactivity of the base ROG mixture, which is a standard mixture of VOC model species derived as discussed in the following section. Two of these methods involve determining relative reactivity values that minimize sum of squares changes of O_3 concentrations in the non-excluded cells resulting from two types of reactivity-based substitutions, and the other two involve finding the cell in the domain that has either the maximum ozone or maximum base ROG reactivity and using the relative reactivity results for those cells. The specific procedures involved are enumerated below.

Least Squares Substitution Error: Base ROG for VOC

This method involves determining a relative reactivity value that minimizes the sum of squares change in ozone concentrations in non-excluded cells resulting by a reactivity-based substitution of the base ROG for the model species. In particular, it derives the value of RR(species) that minimizes the quantity

$$\text{Substitution Error} = \Sigma_{cells}\,[RR(Species)\cdot IR_{cell}(Base\ ROG) - IR_{cell}(Species)]^2 \qquad (I)$$

where RR(Species) is the reactivity of the species relative to the base ROG mixture, IR_{cell}(Species) is the ozone impact of the species a the cell for the chosen impact quantification method, derived as described in the previous section, and IR_{cell} is the ozone impact of the base ROG mixture in the same cell, derived as discussed in the following section. The sum is over non-excluded cells using the data for the selected episode day, as discussed above. The step-by-step procedure is as follows:

1. For each cell in the model, determine if the total daily anthropogenic NOx and VOC emissions into the cell are greater than zero. Skip this cell if both are zero.
2. Determine if the daily maximum ozone for the quantification method used is greater than or equal to the minimum for this method, which is 80 ppb for 1-hour averages and 60 ppb for 8-hour averages. Skip this cell if they are less than the minimum.
3. Determine the incremental reactivities for each model species for this cell and episode day using the procedures appropriate for the quantification method used as described in the previous section.
4. Increment the number of cells to be used in the computation if both of the above tests are passed. Add the incremental reactivity of the each model species to an IR_{cell}(Species) array for each species.
5. Compute the incremental reactivity of the base ROG mixture from the incremental reactivities of the model species for the cell as described in the previous section, and add the result to the IR_{cell}(Base ROG) array.
6. For each model species, compute RR(Species) as follows, where Σ_{cells} refer to summation over all the non-excluded cells used in the computation

$$RR(Species) = [\Sigma_{cells}\ IR_{cell}(Species)\ IR_{cell}(Base\ ROG)] \,/\, [\Sigma_{cells}\ IR_{cell}(Base\ ROG)^2] \qquad (II)$$

7. A measure of the scatter of the data can be obtained by computing the square root of the substitution error divided by the number of cells used, where the substitution error is derived using Equation (I), above

Least Squares Substitution Error: VOC for Base ROG

This method involves determining a relative reactivity value that minimizes the sum of squares change in ozone concentrations in non-excluded cells resulting by a reactivity-based substitution of the model species for the base ROG. In particular, it derives the value of RR(species) that minimizes the quantity

$$\text{Substitution Error} = \Sigma_{cells}\,[IR_{cell}(Base\ ROG) - IR_{cell}(Species)/RR(Species)]^2 \qquad (III)$$

where RR(Species) are as indicated above, and the sum is over non-excluded cells using the data for the selected episode day, as discussed above. The step-by-step procedure is as follows:

1. Same as steps 1-5 above.
6. For each model species, compute RR(Species) as follows, where Σ_{cells} refer to summation over all the non-excluded cells used in the computation

$$RR(Species) = [\Sigma_{cells}\ IR_{cell}(Species)^2] / [\Sigma_{cells}\ IR_{cell}(Species)\ IR_{cell}(Base\ ROG)] \quad (IV)$$

7. A measure of the scatter of the data can be obtained by computing the square root of the substitution error divided by the number of cells used, where the substitution error is derived using Equation (III), above

3-D MIR

This method involves finding the cell that has the highest incremental reactivity of the base ROG mixture and using the ratios of reactivities for that cell, based on the ozone impact quantification method employed. The step-by-step procedure is as follows.

1. Initialize MIR(Base ROG) to zero.
2. For each cell in the model, determine if the total daily anthropogenic NOx and VOC emissions into the cell are greater than zero. Skip this cell if both are zero.
3. Determine if the daily maximum ozone for the quantification method used is greater than or equal to the minimum for this method, which is 80 ppb for 1-hour averages and 60 ppb for 8-hour averages. Skip this cell if they are less than the minimum.
4. Determine the incremental reactivities for each model species for this cell and episode day using the procedures appropriate for the quantification method used as described in the previous section.
5. Compute the incremental reactivity of the base ROG mixture from the incremental reactivities of the model species for the cell as described in the previous section
6. If this incremental reactivity of the base ROG mixture is greater than the current value of MIR(Base ROG), then replace the MIR(Base ROG) with this incremental reactivity of the base ROG mixture for this cell, and set the MIR(Species) values to the incremental reactivities of the VOC model species in this cell.
7. Once all cells have been checked, the 3-D MIR relative reactivities of the model species are given by

$$RR_{MIR}(Species) = MIR(Species) / MIR(Base\ ROG)$$

3-D MOIR

This method involves finding the cell that has the highest maximum ozone concentration (using the quantification method being employed), and using the ratios of reactivities for that cell. The step-by-step procedure is as follows.

1. Initialize Maximum O_3 to zero.
2. For each cell in the model, determine if the total daily anthropogenic NOx and VOC emissions into the cell are greater than zero. Skip this cell if both are zero.
3. Determine if the daily maximum ozone for the quantification method used is greater than the maximum O_3 value found so far. Skip the cell if not.
4. Set the current maximum O_3 to the maximum O_3 for this cell.
5. Determine the incremental reactivities for each model species for this cell and episode day using the procedures appropriate for the quantification method used as described in the previous section. Assign these values to MOIR(Species).

6. Compute the incremental reactivity of the base ROG mixture from the incremental reactivities of the model species for the cell as described in the previous section. Assign this value to MOIR(Base ROG).
7. Once all cells have been checked, the 3-D MOIR relative reactivities of the model species are given by

$$RR_{MOIR}(Species) = MOIR(Species) / MOIR(Base\ ROG)$$

Base ROG Composition

The relative reactivities will be reported as ratios of incremental reactivities of the model species to the incremental reactivities of the base ROG mixture. The base ROG mixture should approximate the composition of the total mixture of all non-methane anthropogenic VOC emissions into the models. Although the total emissions composition should be generally the same for current regional models using the same generation of emissions inventories, there may be slight differences among the modeling databases used in the RRWG studies. For model intercomparison purposes it is more important that the same mixture be used as the standard than that they necessarily exactly represent the emissions inventory used in each simulation, which may differ in some respects among the models, provided that the standard mixture is reasonably representative.

Because the RRWG modeling studies are national in scope, the base ROG mixture to be used for this study consists of the mixture of VOCs from the total emissions profile that was provided by the EPA to represent total anthropogenic emissions into regional models (EPA, 1998). This composition was used to derive the fixed parameter version of the SAPRC-99 mechanism for Models-3 (Carter, 2000). Although this may not be exactly the same as the composition of the total anthropogenic emissions profiles used in the specific models in this study, and may not necessarily reflect the current state of the EPA's emissions databases (see comments in EPA, 1998 reference), it is considered to be a sufficiently close approximation for the purpose of this study.

The composition of the base ROG is specified in terms of moles of model species per mole carbon of base ROG. The data provided by the EPA (1998) were provided in terms of mass emissions of EPA SAROAD classes. The data provided by the EPA included methane, which was removed from the mixture before further analysis. The non-methane composition was converted into molar emissions of SAPRC-99 and other mechanism model species using emissions assignments made for use with a comprehensive emissions database that is in preparation (Carter, 2002). Methane is removed from the mixture because the base ROG represents non methane organics.

A total of 353 SAPRC-99 detailed model species are required to represent the EPA emissions profile with the current assignments, which are too numerous to list here. Assignments of these species into SAPRC-99 fixed parameter mechanism species and also to the set of species whose reactivities were explicitly calculated by the Georgia Tech group (Hakami et al., 2002) were made by assigning these detailed model species (and some compounds that were not assigned detailed model species) to various lumped emissions categories. These lumped emissions categories are listed in Table 1, along their assignments to SAPRC-99 and fixed parameter species and the species whose reactivities were calculated by Hakami et al. (2002) (referred to as "GIT Explicit" species in the tabulations).

Approximately 5% of the mass of the non-methane emissions could be assigned to SAPRC-99 detailed model species. Since lumped model species assignments were made for all SAPRC-99 detailed species, this means that this could also be assigned to lumped species. In addition, about 4% of the mass consisted of compounds for which SAPRC-99 detailed species assignments have not been made, but for which

lumped emissions group assignments have been made (Carter, 2002). (An additional 0.1% of the mass consist of species for which Carbon Bond assignments are available but which are not assigned a lumped emissions group.) Since lumped model species assignments have been made for most of these emissions groups (as shown on Table 1), this means that about 99% of the emitted mass could be assigned to lumped species. The remaining 1% is not counted when normalizing to 1 ppmC, which means that in effect this 1% is represented as if it had the same composition and reactivity characteristics as the 99% that could be assigned.

Table 2 gives the model species distribution derived for this EPA emissions profile for the SAPRC-99 fixed parameter and the Carbon Bond mechanisms, and also in terms of the GIT explicit species based on the assignments shown in Table 1. The base ROG reactivities are then calculated from the reactivities of the model species by,

$$IR_{cell}\text{ (Base ROG)} = \Sigma_{\text{Model Species}}\text{ (Moles Species / Mole C ROG) } IR_{cell}\text{(Species)} \qquad \text{(V)}$$

where the "(Moles Species / Mole C ROG)" are the values tabulated in Table 2 for the respective mechanisms. Note that IR(Species) should be molar ozone impacts to give IR(Base ROG) which give ozone impacts per mole carbon.

Although ideally the base ROG reactivities for the SAPRC-99 mechanisms should be calculated from the SAPRC-99 lumped model species as shown on the "SAPRC-99 (Fixed Parm.)" columns on Table 2, it is our understanding that at present the Georgia Tech SAPRC-99 calculations to date did include calculation of reactivities of species other than those listed by Hakami et al. (2002). In this case, the "GIT Explicit" assignments shown on Table 2 can be used to obtain an estimate of the base ROG reactivity until more reactivity data are available for all the SAPRC-99 lumped model species.

Table 2 also gives the molecular weights per carbon of the assigned portions of the base ROG for the various mechanisms. These should be used for converting mole based reactivities to mass basis, as follows:

$$\text{RR(Compound, Mass basis)} = \text{RR(Compound, Mole basis) } 18.21 / \text{Mwt(Compound)}$$

where 18.21 is the molecular weight per carbon of the base ROG in grams per mole carbon, and Mwt(compound) is the molecular weight of the compound in grams per mole.

References and Notes

Carter, W. P. L. (2000): "Implementation of the SAPRC-99 Chemical Mechanism into the Models-3 Framework," Report to the United States Environmental Protection Agency, January 29. Available at http://www.cert.ucr.edu/~carter/absts.htm#s99mod3.

Carter, W. P. L. (2002): Emissions database work in progress under contract for the University of Houston.

EPA (1998). Emissions received by email from Deborah Luecken of EPA on Thu, 31 Dec 1998. The email message indicated that the data were forwarded from nmm@hpcc.epa.gov on 12/30/98 06:58:57 PM. The message also included the following text: "These ASCII files contain SAROAD emission totals for Benjyey's 36km evaluation grid. These attached files …are based on the 1995-NET EPA US inventory. These files contain the emission summaries for the US part of the grid." The comments also note that the emissions have not been completely reviewed and should be regarded as preliminary. Separate totals were given for area and point source totals. These were summed up to get the total emissions.

Hakami, A., R. A. Harley, J. B. Milford, M. T. Odman and A. G. Russell (2002): "Regional, Three-Dimensional Reactivity Assessment of Organic Compounds," Manuscript in preparation. (Personal communication to W. P. L. Carter, April, 2002).

Table 1. Composition of the Base ROG mixture in terms of SAPRC-99 lumped emissions categories, and assignments of these species to SAPRC-99 fixed parameter and GIT Explicit species.

Grp. Code	Lumped Emissions Group Description	Saprc-99 Fixed Prm.	GIT Explicit		Moles / Mole C
			Code	Desc.	
ETHA	Ethane	ALK1	C2H6	Ethane	6.95e-3
PROP	Propane	ALK2	*ALK2	0.5 (C2H6 + N_C4)	7.15e-3
ALK2	Alkanes (kOH = 0.05-0.25 ppm-1 min-1)	ALK2	*ALK2	0.5 (C2H6 + N_C4)	1.39e-5
ALK3	Alkanes (kOH =0.25-0.50 ppm-1 min-1)	ALK3	N_C4	n-Butane	1.50e-2
ALK4	Alkanes (kOH =0.50-1.00 ppm-1 min-1)	ALK4	*ALK4	0.25 (MCPT + IPNT + N_C5 + 224P)	1.78e-2
ALK5	Alkanes (kOH =1.00-2.00 ppm-1 min-1)	ALK5	*ALK4	0.25 (MCPT + IPNT + N_C5 + 224P)	1.55e-2
ALK6	Alkanes (kOH>2.00 ppm-1 min-1)	ALK5	*ALK4	0.25 (MCPT + IPNT + N_C5 + 224P)	1.83e-3
ETHE	Ethene	ETHENE	ETHE	Ethylene	2.02e-2
OLE1	Alkenes (Primary)	OLE1	OLE1	Higher lumped olefines	1.16e-2
OLE2	Alkenes (Internal)	OLE2	2MBT	2-Methyl 2-butene	4.56e-3
13BDE	1,3-Butadiene	OLE2	BUTD	1,3-Butadiene	1.36e-3
ISOP	Isoprene	ISOPRENE	ISOP	Isoprene	3.77e-4
TERP	Terpenes	TRP1	APIN	a-Pinene	7.23e-4
BENZ	Benzene	0.295 ARO1	C6H6	Benzene	4.81e-3
HBEN	Halo and nitrobenzenes	0.295 ARO1	C6H6	Benzene	2.44e-3
ARO1	Aromatics (kOH <2 ppm-1 min-1)	ARO1	TOLU	Toluene	9.94e-3
ARO2	Aromatics (kOH >2 ppm-1 min-1)	ARO2	XYLM	m-Xylene	7.04e-3
NAPT	Naphthalenes	ARO2	TOLU	Toluene	4.60e-4
PHEN	Phenols	PHEN	*CRES	0.5 (TOLU + BALD)	5.27e-4
CRES	Cresols	CRES	*CRES	0.5 (TOLU + BALD)	3.65e-4
STYR	Styrenes	OLE2	TOLU	Toluene	1.67e-3
HCHO	Formaldehyde	HCHO	HCHO	Formaldehyde	9.75e-3
CCHO	Acetaldehyde	CCHO	CCHO	Acetaldehyde	2.16e-3
RCHO	Higher Aldehydes	RCHO	RCHO	Higher aldehydes	1.60e-3
AALD	Aromatic Aldehydes	BALD	BALD	Benzaldehyde	7.68e-5
ACET	Acetone	ACET	ACET	Acetone	4.66e-3
KET1	Ketones (kOH <0.73 ppm-1 min-1)	MEK	MEK	Methyl ethyl ketone	2.84e-3
KET2	Ketones (kOH >0.73 ppm-1 min-1)	PROD2	MEK	Methyl ethyl ketone	1.72e-3
HCOOH	Formic Acid	ALK2	INERT	Not represented	5.89e-4
CCOOH	Acetic Acid	ALK2	C2H6	Ethane	1.01e-3
RCOOH	Higher organic acids	ALK2	C2H6	Ethane	3.41e-4
ACTYL	Acetylene	ALK2	C2H2	Acetylene	5.30e-3
HALKE	Other Haloalkenes	ALK3	ETHE	Ethylene	2.11e-3
OTH1	Others (kOH =0.02-0.05 ppm-1 min-1)	ALK1	INERT	Not represented	2.03e-3
OTH2	Others (kOH =0.05-0.25 ppm-1 min-1)	ALK2	MEOH	Methanol	3.92e-3
OTH3	Others (kOH =0.25-0.5 ppm-1 min-1)	ALK3	MTBE	Methyl t-butyl ether	5.07e-3
OTH4	Others (kOH =0.5-1.0 ppm-1 min-1)	ALK4	BACT	n-Butyl acetate	1.88e-2
OTH5	Others (kOH =1-2 ppm-1 min-1)	ALK5	BACT	n-Butyl acetate	6.32e-3
OTH6	Others (kOH >2 ppm-1 min-1)	ALK5	BACT	n-Butyl acetate	8.35e-3
MEOH	Methanol	MEOH	MEOH	Methanol	5.17e-3
ETOH	Ethanol	ALK3	ETOH	Ethanol	2.12e-2
INHIB	Inhibitors	INERT	BALD	Benzaldehyde	9.71e-4
GLY	Glyoxal	GLY	HCHO	Formaldehyde	1.06e-4
MGLY	Methyl Glyoxal	MGLY	RCHO	Higher aldehydes	7.28e-5
MACR	Methacrolein	METHACRO	ACRO	Acrolein	1.13e-3

Table 1 (continued)

Grp. Code	Lumped Emissions Group Description	Saprc-99 Fixed Prm.	GIT Explicit Code	GIT Explicit Desc.	Moles / Mole C
UALD	Other Unsaturated Aldehydes	ISO-PROD	ACRO	Acrolein	7.83e-5
UKET	Unsaturated Ketones	MVK	ACRO	Acrolein	6.76e-7
PHOT	Other photoreactive	BACL	ACRO	Acrolein	2.79e-6
PAH	Polycyclic aromatic hydrocarbons	ARO2	TOLU	Toluene	5.04e-5
BOAT	Pthallates and benzoates	ARO1	TOLU	Toluene	8.21e-4
MARO	Miscellaneous other heteroatom-containing aromatics	ARO1	TOLU	Toluene	9.62e-7
MRCT	Miscellaneous heteroatom-containing non-aromatic reactive compounds	ALK5	BACT	n-Butyl acetate	2.71e-3
AMIN	Amines and amides	ALK5	BACT	n-Butyl acetate	9.35e-4
TCE	Trichloroethylene	ALK1	C2H6	Ethane	3.74e-4
INERT	Unreactive	INERT	INERT	Not represented	4.99e-3
NVOC	Non-volatile	INERT	INERT	Not represented	3.48e-3
	GIT Explicit Species not assigned to any particular emissions group		MCPT	Methylcyclopentane	
			IPNT	iso-Pentane	
			N_C5	n-Pentane	
			224P	2,2,4 Trimethyl pentane	
			124B	1,2,4 Trimethyl benzene	
			XYLP	p-Xylene	
			PRPE	Propene	

Table 2. Composition of Base ROG mixture in terms of GIT Explicit species and model species in the Carbon Bond IV and the fixed parameter version of the SAPRC-99 mechanism.

	GIT Explicit		CB4		SAPRC-99 (Fixed Parm.)	
	Species or Group	Moles / MoleC	Species	Moles / MoleC	Species	Moles / MoleC
Weight Fraction Assigned		98.9%		98.9%		98.9%
Molecular Weight / Carbon		17.13		17.14		17.13
Average Carbons / Mole		4.01		4.01		4.01
	C2H6	8.68e-3	PAR	5.47e-1	ALK1	9.36e-3
	*ALK2	7.16e-3	OLE	2.01e-2	ALK2	1.83e-2
	N_C4	1.50e-2	TOL	1.25e-2	ALK3	4.34e-2
	*ALK4	3.51e-2	XYL	7.55e-3	ALK4	3.67e-2
	ETHE	2.23e-2	HCHO	1.04e-2	ALK5	3.56e-2
	OLE1	1.16e-2	ALD2	1.91e-2	ETHENE	2.02e-2
	2MBT	4.56e-3	ETH	2.09e-2	OLE1	1.16e-2
	BUTD	1.36e-3	ISOP	3.77e-4	OLE2	7.59e-3
	ISOP	3.77e-4	MEOH	5.17e-3	ISOPRENE	3.77e-4
	APIN	7.23e-4	ETOH	2.12e-2	TRP1	7.23e-4
	C6H6	7.25e-3	MTBE	2.39e-4	ARO1	1.29e-2
	TOLU	1.29e-2	UNR	1.24e-1	ARO2	7.55e-3
	XYLM	7.04e-3			PHEN	5.27e-4
	*CRES	8.92e-4			CRES	3.65e-4
	HCHO	9.86e-3			HCHO	9.75e-3
	CCHO	2.16e-3			CCHO	2.16e-3
	RCHO	1.68e-3			RCHO	1.60e-3
	BALD	1.05e-3			BALD	7.68e-5
	ACET	4.66e-3			ACET	4.66e-3
	MEK	4.56e-3			MEK	2.84e-3
	INERT	7.77e-3			PROD2	1.72e-3
	C2H2	5.30e-3			MEOH	5.17e-3
	MEOH	9.09e-3			INERT	6.11e-3
	MTBE	5.07e-3			GLY	1.06e-4
	BACT	3.71e-2			MGLY	7.28e-5
	ETOH	2.12e-2			BACL	2.79e-6
	ACRO	1.21e-3			METHACRO	1.13e-3
					ISO-PROD	7.83e-5
					MVK	6.76e-7

[a] *ALK2 is 0.5 (C2H6 + N_C4)
[b] *ALK4 is 0.25 (MCPT + IPNT + N_C5 + 224P)
[c] *CRES is 0.5 (TOLU + BALD)