DEVELOPMENT OF A CONDENSED SAPRC-07 CHEMICAL MECHANISM

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By

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ABSTRACT

Condensed versions of the SAPRC-07 mechanism, designated CS07A and CS07B, have been developed and are documented. They are derived directly from detailed SAPRC-07, which serves as the basis for their chemical validity and evaluation against chamber data. Both incorporate condensations involving removing or lumping less reactive compounds, lumping some product species in isoprene or aromatic mechanisms with other species with similar mechanisms using reactivity weighting, removing some compounds and reactions that are rapidly reversed, and using fewer model species to represent emitted alkanes and similar species. Mechanism CS07A is comparable in size to CB05 and incorporates the more condensed and approximate peroxy radical lumped operator method employed in SAPRC99, CB4, and CB05. It gives predictions of O_3, total PANs and OH radicals that are very close to the uncondensed mechanism, but overpredicts H_2O_2 by about 15%. Mechanism CS07B retains the more detailed peroxy radical representation of uncondensed SAPRC-07, giving it ~40% more species than CS07A, and giving it better agreements in predictions of H_2O_2. Use of CS07A is suitable for models where the priority is O_3 formation, while CS07B should be used if more accurate hydroperoxide predictions are a priority. Files for implementing these mechanisms are available at http://www .cert.ucr.edu/~carter/SAPRC.

Since the completion of first version of this report in July, 2008, several corrections to the base SAPRC-07 were made as a result of ongoing reviews. These required corresponding corrections to be made to the condensed versions of the mechanism documented in this report, and to this report. The changes to the mechanism and the report since its initial distribution in July, 2008, are summarized in Appendix B to this report.

ACKNOWLEDGEMENTS AND DISCLAIMERS

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INTRODUCTION

Airshed models are essential for the development of effective control strategies for reducing photochemical air pollution because they provide the only available scientific basis for making quantitative estimates of changes in air quality resulting from changes in emissions. The chemical mechanism is the portion of the model that represents the processes by which emitted primary pollutants, such as volatile organic compounds (VOCs) and oxides of nitrogen (NO_x), interact in the gas phase to form secondary pollutants such as ozone (O_3) and other oxidants. This is an important component of airshed models because if the mechanism is incorrect or incomplete in significant respects, then the model's predictions of secondary pollutant formation may also be incorrect, and its use might result in implementation of inappropriate or even counter-productive air pollution control strategies.

For many years the SAPRC-99 chemical mechanisms (Carter, 2000a,b), which were developed primarily under funding from the California Air Resources Board (CARB), has been used in airshed models for research and control strategy purposes. This consisted of a "detailed" mechanism that contained explicit representation of the atmospheric reactions of many hundreds of types of VOCs for the purpose of calculating VOC reactivity scales and other applications requiring this level of chemical detail, which was comprehensively evaluated against environmental chamber data (Carter, 2000a). Under U.S. EPA funding this was used to develop a "fixed parameter" mechanism using a smaller number of lumped species to represent VOCs in ambient simulations where this level of detail is not practical or appropriate (Carter, 2000b). The mechanisms for these lumped species were derived based on the detailed mechanisms for the components of the ambient VOC mixture that was taken as representative of VOC emissions from all anthropogenic sources in the reactivity scale calculations (Carter, 1994, 2000b). This fixed parameter version of SAPRC-99 is implemented in the current versions of the CMAQ (2008) and CAMx (Environ, 2006) urban and regional airshed models and used in a number of airshed modeling studies (e.g., Tonnesen et al, 1998, and references therein).

Since the SAPRC-99 mechanism was becoming out-of-date, the CARB funded the development of the SAPRC-07 mechanism to reflect new kinetic and mechanistic data as of mid-2007, and to incorporate new data on many types of stationary source VOCs (Carter, 2010a). As with SAPRC-99 this consists of a detailed mechanism that separately represents the many types of VOCs for reactivity scale calculations, and a fixed parameter mechanism for ambient airshed calculations. The fixed parameter SAPRC-07 mechanism has a similar level of chemical detail as fixed parameter SAPRC-99 in terms of lumped species used to represent emitted VOCs, though it has a larger number of reactions and intermediate species because it incorporates a less approximate method to represent low NO_x peroxy radical reactions and products. Unlike SAPRC-99, this mechanism incorporates a representation of chlorine chemistry as an option. It has a total of 124 model species and 347 reactions, making it larger than most mechanisms used in 3-D airshed models in the United States.

Representation of the chemistry makes significant demands of computer time and resources and memory in 3-D airshed model applications, and use of more condensed and computationally efficient would permit the available computer resources to be used for other priorities such as improved grid resolution or modeling more cases. For that reason, the highly compact Carbon Bond 4 (CB4) (Gery et al, 1998) has been widely used in research and regulatory applications where chemical detail is seen as less of a priority. This mechanism is now being replaced by the more up-to-date Carbon Bond 05 (CB05) mechanism (Yarwood et al, 2005; Sarwar et al, 2008), which is somewhat larger and more chemically detailed than CB4 but still much smaller than fixed parameter SAPRC-99 and especially SAPRC-07.

In this report we document the development of condensed versions of SAPRC-07 that are based on detailed SAPRC-07 as documented by Carter (2010a), and compare their predictions with uncondensed SAPRC-07. Two versions are presented, designated CS07A and CS07B. Version CS07A is the more condensed version and is comparable in size to CB05 and is suitable for predictions of ozone formation and for use with the current generation of PM modules used in airshed models. To minimize the number of reactions and species, this version incorporates the more approximate "chemical operator" representation of peroxy + peroxy reactions used in SAPRC-99 (and also CB4 and CB05) that is satisfactory for modeling ozone formation but is less accurate in representing chemical species such as hydroperoxides formed in the absence of NO_x (Carter, 2000a). Version CS07B incorporates the more chemically accurate representation of the peroxy radical reactions as used in the uncondensed version of SAPRC-07. This version gives a potentially more accurate representation of the formation and reactions of the hydroperoxide species that may be needed when more chemically detailed PM modules are developed (Carter, 2010a). In addition to being larger, implementation of version CS07B into current airshed models will require some modification to the model software, as is the case for the uncondensed SAPRC-07. Therefore, CS07A may be more useful for immediate implementation in the current generation of models.

MECHANISM DESCRIPTION AND TESTS

General Approach

The general approach used in this work is to take the uncondensed fixed-parameter SAPRC-07 mechanism as the starting point, and derive a series of mechanisms by making stepwise condensations to the previous mechanism in the series. This way the effects of the various condensations can be assessed, to determine what condensations can be employed without yielding unacceptable changes to model predictions. The condensed mechanisms so developed are summarized in Table 1 and discussed in more detail below, and Figure 1 shows a comparison of the number of non-constant model species and reactions in the mechanisms. The predictions of these mechanisms on selected species are compared using a series of test calculations and based on the results of these comparisons a set of condensed mechanisms recommended for use was chosen. This is discussed in the remainder of this report.

Mechanism Descriptions

Uncondensed Mechanism (SAPRC-07 or S07B)

The starting point for this work was the fixed parameter version of SAPRC-07 mechanism as documented by Carter (2010a). This in turn was derived from the detailed SAPRC-07 mechanism, with parameters for the lumped model species being derived based from the mechanisms of the components of the base ROG mixture used to represent anthropogenic emissions from all sources in the atmospheric reactivity calculations (Carter 1994a, 2000a, 2010a). This is the version of the mechanism that was recommended for use in airshed model calculations where use of a standard composition of emitted VOCs is considered appropriate. This version of the mechanism is referred to as "SAPRC-07" in the subsequent discussion, though it should be noted that there are other versions of SAPRC-07 that are available (e.g., detailed or with parameters adjusted based on other mixtures or different lumping approaches).

Note that the some changes were made to the uncondensed mechanism as a result of minor problems, errors or omissions that were discovered subsequent to its initial release. These are incorporated in the version documented by Carter (2010a) and the changes made to the uncondensed mechanism are summarized in Appendix E of Carter (2010a). The mechanism used as the starting point for the condensed mechanisms documented in this report is consistent with that given by Carter (2010a) as of the date of the report given in the reference list below.

The model species used in this mechanism are listed in Table A-1 in Appendix A (with the species in this version of the mechanism being those indicated with the "B" or "x" in the "Unc" column), and the reactions and rate constants are given in Table A-2. The absorption cross-sections and quantum yields are given in supplementary material associated with the SAPRC07 mechanism (Carter, 2010) and are not reproduced here. The absorption cross-sections and quantum yields were not changed in any versions of the condensed mechanisms developed in this work.

Uncondensed Mechanism with SAPRC-99 Peroxy Lumping (SAPRC-07A or S07A)

One of the major changes made when developing SAPRC-07 from SAPRC-99 was to revise the procedure used to represent effects of peroxy + peroxy radical reactions in the mechanism. Because of the large number of peroxy radicals that are involved even in condensed atmospheric chemistry mechanisms,

Table 1. Summary of versions of the SAPRC-07 mechanism used or developed for this project. Number of species and reactions in the CB05 mechanism are shown for comparison.

Label	Description	Number [a] Spec	Rxns	Description or Modifications [b]
SAPRC-07 (S07B)	Fixed parameter SAPRC-07 mechanism (Carter, 2010a)	118 104	339 275	See text and Carter (2010a) for a list of the minor corrections made relative to the version that was initially distributed and documented. Designated "B" to indicate the type of peroxy radical representation used. Mechanism listed in Table A-2 in Appendix A.
SAPRC-07A (S07A)	Same as SAPRC-07 except uses the peroxy radical representation "A" of SAPRC-99.	85 72	286 218	The SAPRC-99 peroxy radical representation "A", documented by Carter (2000) was employed instead of the representation "B" in the standard uncondensed SAPRC-07 (Carter, 2007). See text. Mechanism listed in Table A-3 in Appendix A.
C1	Low reactivity compounds lumped using reactivity weighting and other changes expected to have relatively small impacts are made.	75 63	257 205	The following substitutions made, using reactivity weighting where applicable: TBUO = ACET + HCHO + RO2R; RO2CL = CL + R2O2; HCOOH = 0.048 ALK3; CCOOH = 0.243 ALK3 + 0.086 CCHO; RCOOH = 0.526 ALK3 + 0.190 CCHO; MEOH = 0.288 ALK3; MEK = 0.369 PROD2; ACET = 0.071 PROD2; BENZENE = 0.045 ARO1 + 0.154 CRES; ACETYLEN = 0.308 ALK3 (Methane is retained to permit the mechanisms to be used in remote simulations)
C2	Methyl peroxy lumped with RO2R + HCHO	73 61	242 190	MEO2 removed from the mechanism and replaced by HCHO + RO2R
C3	Higher PANs lumped with PAN2	69 57	215 165	BZCO3 and MACO3 represented by RCO3; PBZN and MAPAN represented by PAN2
C4	Number of model species used for aromatics and isoprene reduced. One-product isoprene mechanism used and Aromatics mechanisms simplified	62 50	191 143	MVK and MACR represented by IPRD, and IPRD mechanism revised to incorporate MVK and MACR mechanisms. BALD (benzaldehyde) removed. NPHE formation in NO3 + CRES represented by 0.5 CRES. Following aromatic product model species substituted using reactivity weighting: GLY = 0.582 MGLY + 0.016 AFG1; BACL = 1.455 MGLY; AFG3 = 0.724 MGLY + 0.918 AFG2;

Table 1 (continued)

Label	Description	Number [a] Spec	Number [a] Rxns	Description or Modifications [b]
C5	Chlorine mechanism simplified	55 50	179 143	Formation and reactions of CLNO, CLNO2, CLONO, and HOCL removed (only small net effects), and following substitutions made using reactivity weighting: CLCCHO = 0.261 RCHO + 0.713 MGLY CLACET = 0.400 RCHO + 0.583 MGLY
C6 (CS07A)	Lumped alkane species reduced from 5 to 2 using reactivity weighting. This is the version recommended for general use	52 47	173 140	ALK1, ALK2, and ALK5 removed and following substitutions made to emissions assignments: SAPRC-07 ALK1 = 0.132 CS07 ALK3; SAPRC-07 ALK2 = 0.334 CS07 ALK3; SAPRC-07 ALK3 = CS07 ALK3; SAPRC-07 ALK4 = CS07 ALK4; SAPRC-07 ALK5 = CS07 ALK4 Mechanism for ALK4 modified based on parameters of species in base ROG mixture represented by ALK4 and ALK5 in SAPRC-07. Mechanism listed in Table A-4 in Appendix A.
C7	PAN lumped with PAN2	50 45	161 129	PAN2 lumped with PAN and MECO3 lumped with RCO3. Rate constants for PAN2 used because that caused the smallest changes in the simulations.
C8	Acetaldehyde lumped with RCHO	49 44	158 126	RCHO represented by CCHO, whose rate constants were not changed.
CS07B	C6 (CS07) except with SAPRC-07 peroxy representation "B" This is the version recommended for more accurate hydro-peroxide predictions	70 64	207 171	SAPRC-07 with substitutions and modifications as indicated above for C1 through C6. Mechanism listed in Table A-5 in Appendix A.
CB05	Carbon Bond 05 mechanism (Yarwood et al, 2005) for CMAQ	57 51	177 156	Version of CB05 mechanism as implemented into CMAQ (Sarwar et al, 2008), with reactions added for SOA calculation excluded.

[a] Number of model species (excluding constant) or reactions in the full version of the mechanisms and in the mechanisms without chlorine chemistry, respectively.

[b] Except for SAPRC-07, CS07B and CB05, all modifications are made relative to the version listed immediately above it in the table.

[c] The HCHO + HO_2 reaction was removed from the uncondensed mechanism when it was revised in March 2009. See Appendix E of Carter (2010a).

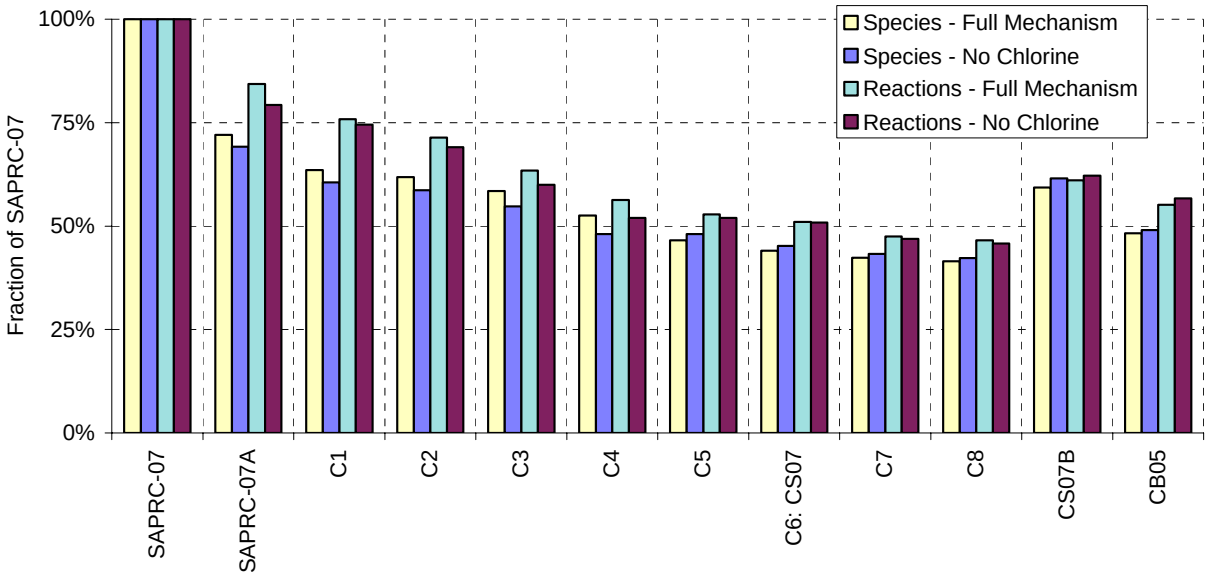

Figure 1. Comparison of number of model species and reactions in various mechanisms and condensation levels.

it is generally not practical to represent the many possible peroxy + peroxy reactions explicitly, especially considering that these reactions are relatively unimportant under conditions favorable for O_3 formation. SAPRC-99 represents methyl peroxy radicals explicitly, but uses a limited number of "chemical operators" to represent effects of peroxy radical reactions on NO_x and radicals, and represents the organic products formed when higher peroxy radicals react with other peroxy radicals by those formed when they react with NO_x (Carter, 2000a). This is referred to as the peroxy radical lumping method "A" in the subsequent discussion. The CB4/05 mechanisms use a similar approach (Gery et al, 1988; Yarwood et al, 2005). Although this representation has been shown to have relatively little effects on predictions of O_3 formation, it does not represent the changes in organic oxidation products that occur when these peroxy + peroxy reactions become non-negligible, which may be important in models for secondary organic aerosol (SOA) formation. For that reason, SAPRC-07 employed a modified chemical operator method that permits representation of changes in organic product formation in oxidations of VOCs under low NO_x conditions (Carter, 2010a). This is referred to as peroxy radical lumping method "B" in the subsequent discussion.

The SAPRC-07 peroxy radical lumping method "B" requires a larger number of model species and reactions than the SAPRC-99 method "A", and since it has relatively little effect on O_3 formation compared to method "B" and makes implementation into many airshed model software systems more difficult (Carter, 2010a), reverting to the method "A" was the first condensation approach that was considered. The otherwise uncondensed SAPRC-07 mechanism modified to use peroxy lumping method "A" is referred to as the "SAPRC-07A" mechanism in the subsequent discussion. The modification consisted of the following steps (see Carter 2000a, 2010a for a discussion of the chemical operators and methods used in the two approaches):

- RO2C + xHO2 is replaced by RO2R, using the SAPRC-99 reactions for this operator and the SAPRC-07 rate constants of RO2C

- RO2C formation not associated with xHO2 is represented by R2O2, using the SAPRC-99 reactions for this operator and the SAPRC-07 rate constants of RO2C
- RO2XC + zRNO3 is replaced by RO2N using the SAPRC-99 reactions for this operator and the SAPRC-07 rate constants of RO2C. Since all zRNO3 formation is associated with RO2XC, this means that zRNO3 and its reactions are deleted.
- RO2C + xCL is replaced by the operator RO2CL, whose reactions are like those for RO2R except that Cl rather than HO2 is formed in the NO reaction.
- Formations of all xPROD and xRAD species are replaced by the corresponding product or radical species (e.g., xHCHO is replaced by HCHO and xHO2 is replaced by HO2) and their reactions are deleted.
- The yROOH, yR6OOH, yRAOOH operators and their reactions are deleted. The hydroperoxide species they form in the HO2 reactions are represented by an XOOH operator formed in the reactions of RO2R+HO2 and RO2N+HO2 reactions.
- The hydroperoxide species ROOH, R6OOH, and RAOOH are deleted and replaced by the XOOH lumped hydroperoxide group. The effects of their reactions are represented by the reactions of the organic products formed in the peroxy + NO reactions. The radicals formed in their photolysis are represented by the photolysis of the XOOH operator, similar to the ROOH species in SAPRC-99.

Note that the elimination of the xPROD, xRAD, yROOH, and zRNO3 species eliminates the need to calculate the parameter values used to derive the rate constants of these reactions, which requires modifications to mechanism implementation software in most airshed models. Thus this mechanism, and the more condensed mechanisms derived from it, can be implemented into the current airshed model systems without the software modifications that may be required for uncondensed SAPRC-07.

The model species used in this mechanism are listed in Table A-1 in Appendix A (with the species in this version of the mechanism being those indicated with the "A" or "x" in the "Unc" column), and the reactions and rate constants are given in Table A-3. The absorption cross-sections and quantum yields are unchanged.

Condensed Mechanisms C1-C8

The condensed mechanisms designated C1-C8 were derived by applying incremental condensations starting with mechanism SAPRC-07A, with C1 being derived from SAPRC-07A, C2 being derived from C1, etc. Table 1 summarizes the condensations employed and the resulting number of reactions and non-constant model species. These condensations are discussed further below.

Condensed mechanism C1 was derived by applying various condensations that are expected not to have significant effects on model predictions. These consisted the following. (1) Various chemical operators that are of relatively small importance for most VOCs are removed and replaced by chemical operators that have the same effects under most conditions. (2) Various relatively low reactivity or low yield organic product and emitted VOC species that are represented explicitly in the uncondensed mechanism are represented using other model species using reactivity weighting. The derivation of the reactivity weighting factors shown in Table 1 is discussed later in this section.

Condensed mechanism C2 is derived from mechanism C1 by replacing the methyl peroxy radical model species, MEO2, by chemical operators and species that represent the same net effect under conditions where O_3 formation occurs. An additional effect of this substitution is the representation of the relatively unreactive methyl hydroperoxide model species by the lumped hydroperoxide group (XOOH) and formaldehyde.

Condensed mechanism C3 is derived from mechanism C2 by lumping the higher PAN analogues PBZN (formed from benzaldehyde) and MAPAN (formed from methacrolein and related compounds) with the generic higher PAN species PAN2. PAN itself is still represented separately since lumping PAN with PAN2 was found to have a larger effect on mode simulations, as discussed below.

Mechanism C4 was derived from C3 by making condensations to the isoprene and aromatics mechanisms. The isoprene product species methacrolein (MACR) and MVK are lumped with the model species used in the uncondensed mechanism to represent the C_5 isoprene products (IPRD), and the mechanistic parameters for that species are re-derived based on those for MACR, MVK, and IPRD in the condensed mechanism, weighted by their relative yields in the OH + isoprene reaction. This is analogous to the "one product" isoprene mechanism of Carter (1996), except that the parameters are updated to be consistent with the current uncondensed isoprene mechanism in SAPRC-07 (Carter, 2010a).

Mechanism C4 also employed various simplifications to the aromatics mechanisms, as follows: (1) The aromatic aldehyde (BALD) model species was removed because it is formed in relatively low yields in the lumped aromatic model species reactions, and the effect of its removal was found to be relatively small. It is not represented by other model species because it is negatively reactive and the other remaining model species in the mechanism have positive reactivity under most conditions. (2) The "nitrophenol" model species (NPHE) that is formed in the NO_3 + cresol (CRES) reaction was removed and was represented by replacing its formation in that reaction by 0.5 CRES. Using the factor of 0.5 in this reaction was found to have the least impact on the model simulations. (3) The aromatic ring fragmentation products GLY (glyoxal) and AFG3 (non-photoreactive unsaturated dicarbonyls) were represented by other aromatic ring fragmentation products whose reactivities are most similar to them using reactivity weighting, as shown on Table 1. Various combinations were examined but those shown on Table 1 were found to give the best correspondence to the reactivities of these model species.

Mechanism C5 was derived from C4 by applying various simplifications to the chlorine mechanism. The formation and rapid photolysis of CLNO, CLNO2, CLONO, and HOCL were removed because these reactions are calculated to have little or no net effect. The chloroacetone and chloroacetaldehyde model species, which are formed in the reactions of Cl with lumped olefin species, were represented by other photoreactive species by reactivity weighting. The chemical operator RO2CL, representing the formation of chlorine atoms after an NO to NO_2 conversion, is replaced by the prompt formation of chlorine atoms plus the operator R2O2 to represent the NO to NO_2 conversion. The chlorine nitrate (CLONO2) model species retained because the effect of removing it was found to be non-negligible.

Mechanism C6 was derived from C5 by lumping the alkane model species as shown on Table 1. Alkane species ALK1 and ALK2 are represented by ALK3 using reactivity weighting, and ALK4 and ALK5 are lumped together as a modified ALK4 model species whose parameters are derived from the mechanisms of the compounds in the ambient base ROG mixture that were used to derive the parameters for ALK4 and ALK5 in the uncondensed mechanism. Thus, this mechanism uses two model species to represent all alkane and alkane-like compounds instead of the five used in the uncondensed mechanism.

Mechanism C7 was derived from C6 by lumping PAN and the higher PAN analogue model species with a single PAN species, as is done in the CB4 (but not CB05) mechanism. The corresponding acyl peroxy model species MECO3 and RCO3 were also lumped. Test calculations indicated that the change in model predictions was less if the lumped PAN and MECO3 model species used the rate constants of PAN2 and RCO3 rather than PAN and MECO3, so this was employed in this mechanism.

Finally, Mechanism C8 was derived from C7 by lumping the aldehyde species CCHO (acetaldehyde) and RCHO (lumped higher aldehydes) into a single acetaldehyde species, as is also done

in CB4 but not CB05. The rate constants and mechanism used for the lumped species is the same as the acetaldehyde model species.

As indicated above, a number of the condensations involved representing certain model species by others using reactivity weighting. The model species used to represent the removed model species or compounds were chosen based on considerations of similar types of mechanisms, with the weighting factors derived minimizing sum of square differences in incremental reactivities for ozone formation in the EKMA box-model airshed scenarios used for deriving the reactivity scales of Carter (1994a, 2000a, 2010a). These incremental reactivities were calculated using the uncondensed SAPRC-07 mechanism using the procedures and mechanisms as documented by Carter (2010a), except that the reactivities used were on a molar rather than a mass basis because this is how the substitutions were made. Figure 2 and Figure 3 show plots of incremental reactivities of the model species calculated using the substitutions indicated in Table 1 against the incremental reactivities calculated explicitly for all the MIR, MOIR, EBIR and base case reactivity scenarios. These indicate how well these substitutions perform in these scenarios in predictions of ozone formation in the various scenarios. In general, the substitutions perform reasonably well, as would be expected considering the similar chemical nature and reactivity characteristics of the substituted and substituting species. The slight biases shown for ALK5 and ALK5 are due to the fact that reactivity weighting was not used for these species.

As discussed below, the test calculations given in the "Results" section indicated that making further condensations from mechanism C6 resulted in larger changes in model predictions than the other condensations, suggesting that level of condensation in C6 represents probably the best balance between mechanism reduction and chemical accuracy. For that reason, mechanism C6 is one of the recommended condensed SAPRC-07 mechanisms derived in this work. It is also designated "CS07A" mechanism, for condensed SAPRC-07 mechanism employing the peroxy radical "A" representation.

Condensed Mechanism CS07B

As indicated on Table 1 and Figure 1 above, the largest reduction in number of species came from incorporating the more approximate SAPRC-99 peroxy radical representation method "A" in place of the uncondensed SAPRC-07 peroxy representation "B". However, a condensed mechanism using peroxy representation method "A" may not be suitable for model applications, such as those using more explicit SOA mechanisms, that require better representation of reactions of hydroperoxides and other compounds formed under low NO_x conditions. Therefore, for such model applications we also derived a version of the SAPRC-07 condensed mechanism that retained the peroxy representation method "B" used in the condensed mechanism, but incorporated the other condensations used for mechanism C6 or CS07A. This is designated mechanism "CS07B", or condensed SAPRC-07 mechanism employing the peroxy radical "B" representation. Its reactions are listed in Table A-5 in Appendix A.

Emissions Assignments

In order to use the mechanism ambient simulations, including many of the test calculations discussed in the following section, it is necessary to make assignments of model species to the many types of individual compounds that are emitted. For the fixed-parameter SAPRC-99 and SAPRC-07 mechanisms the approach used was to assign the hundreds of emitted compounds to smaller numbers of "emissions groups" on a mole-for-mole basis, and then assign those emissions groups to the model species in the mechanisms. This is based on the approach initially developed for the RADM2 mechanism (Middleton et al, 1990), and is incorporated in the current emissions speciation database (Carter, 2009). Table 2 lists the emissions categories used in the current emissions speciation database, and the assignments of these categories to model species in the fixed-parameter uncondensed SAPRC-07 mechanism and the C6 condensed mechanisms (CS07A and CS07B) developed in this work. The

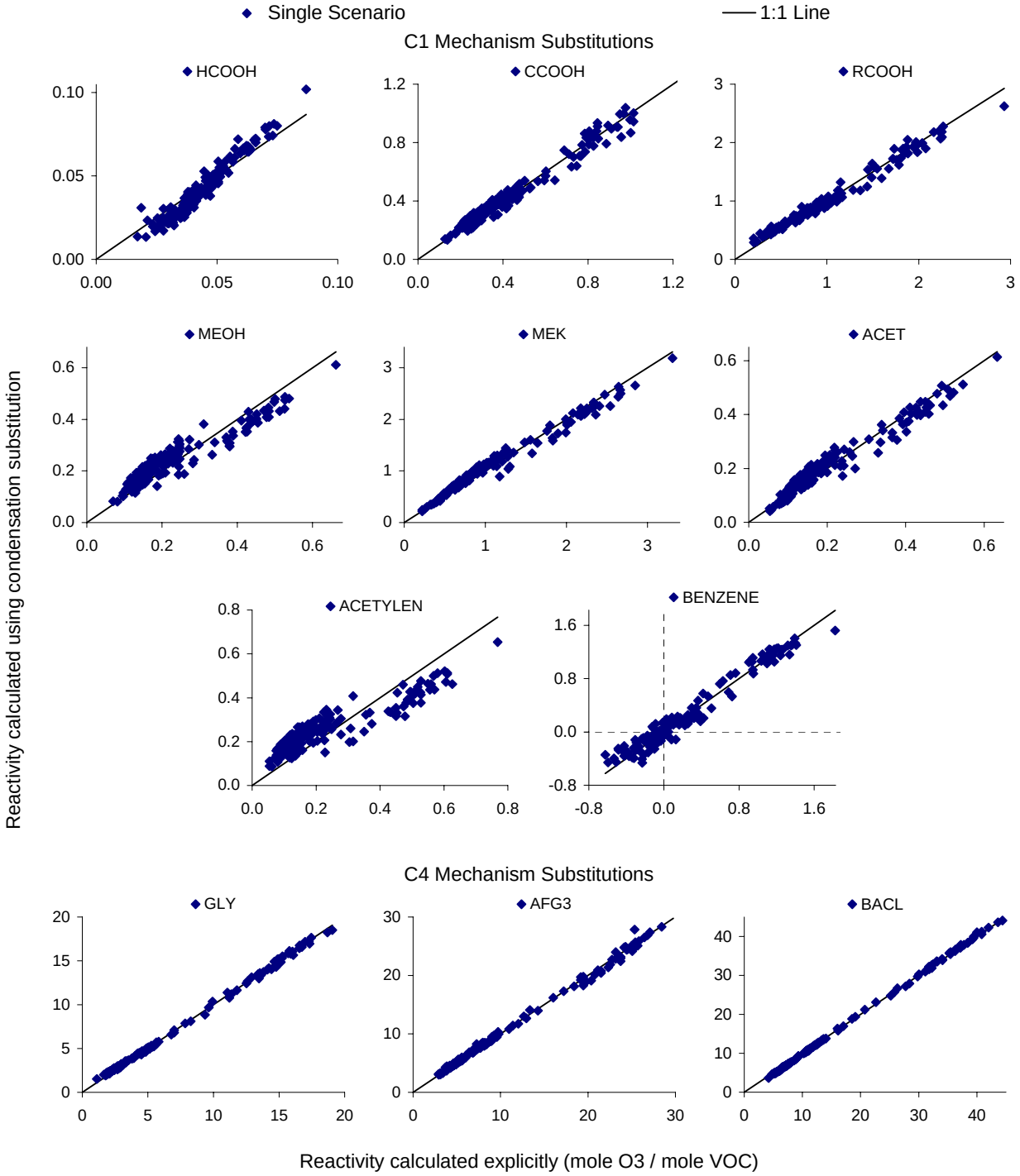

Figure 2. Plots of incremental reactivities of model species derived using the substitutions incorporated in the C1 and C4 condensed mechanisms as indicated on Table 1 against incremental reactivities for all the EKMA box model scenarios used to derive MIR, MOIR, EBIR, and base case reactivity scales.

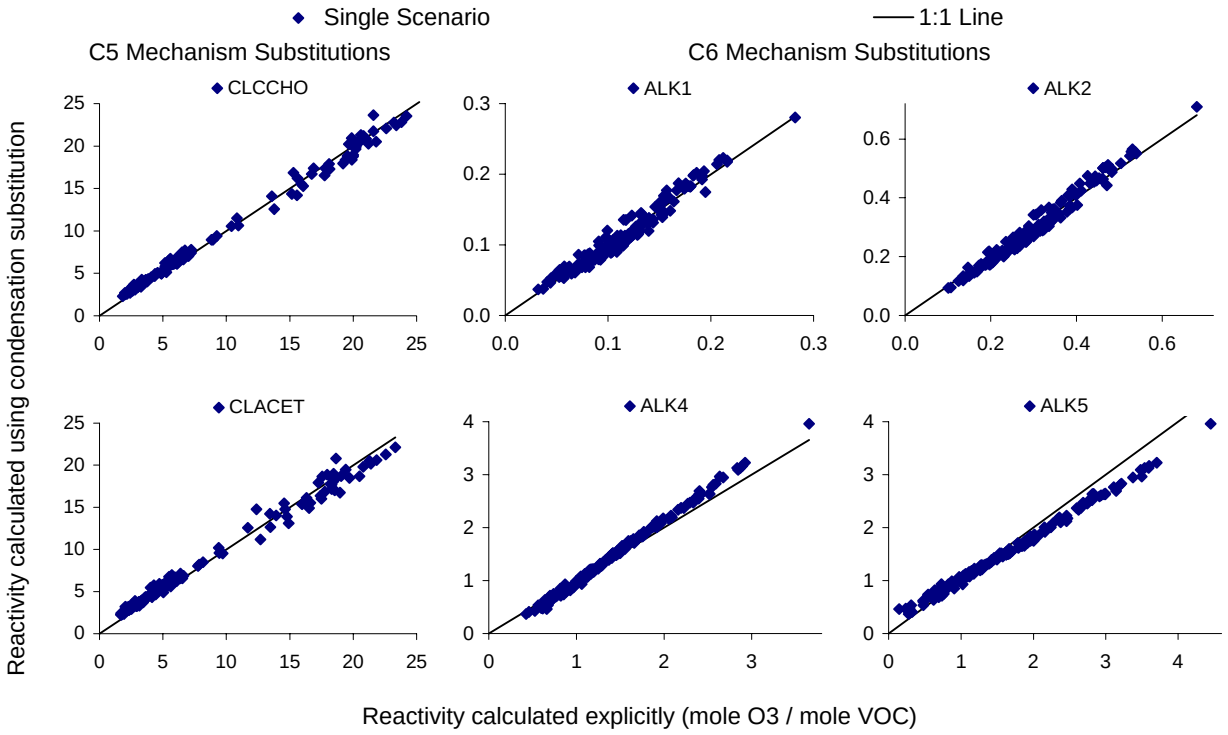

Figure 3. Plots of incremental reactivities of model species derived using the substitutions incorporated in the C5 and C6 condensed mechanisms as indicated on Table 1 against incremental reactivities for all the EKMA box model scenarios used to derive MIR, MOIR, EBIR, and base case reactivity scales.

assignments for the condensed mechanisms are based on those for uncondensed SAPRC-07, applying the substitutions given through C6 on Table 1 where applicable.

Note that the same emissions assignments are used for CS07A as CS07B and likewise the assignments are the same for SAPRC-07A as uncondensed SAPRC-07. This is because the peroxy radical lumping approach does not affect the model species used to represent primary VOC emissions.

Test Scenarios

The effects of the condensation methods were assessed using a series of box model test calculations designed to compare various aspects of the mechanisms under various conditions. The inputs for these calculations are summarized on Table 3 and Table 4. The scenarios included static simulations with constant light intensity, no dilution, and all reactants present initially for the purpose of comparing the general mechanisms or specific aspects of the mechanisms such as the isoprene, aromatics or chlorine chemistry, multi-day continuous dilution scenarios to compare mechanisms under multi-day conditions, and the one-day EKMA model city-specific scenarios used to calculate the Carter (1994a, 2000a, 2010a) reactivity scales. For some of the static scenarios NO_x was added after 6-hour of the irradiation in order to compare model predictions of aged mixtures where NO_x was restored so O_3 formation could continue.

Table 2. Listing of emissions categories used in the current SAPRC emissions speciation database (Carter, 2008) and the assignments of these categories to model species in the SAPRC-07 and CS07 mechanisms.

Description	SAPRC-07		CS07			
	Species	Moles	Species1	Moles	Species2	Moles
Methane	CH4	1	CH4	1		
Ethane	ALK1	1	ALK3	0.132		
Propane	ALK2	1	ALK3	0.334		
Alkanes (kOH = 0.05-0.25 x 10^4 ppm^{-1} min^{-1})	ALK2	1	ALK3	0.334		
Alkanes (kOH =0.25-0.50 x 10^4 ppm^{-1} min^{-1})	ALK3	1	ALK3	1		
Alkanes (kOH =0.50-1.00 x 10^4 ppm^{-1} min^{-1})	ALK4	1	ALK4	1		
Alkanes (kOH =1.00-2.00 x 10^4 ppm^{-1} min^{-1})	ALK5	1	ALK4	1		
Alkanes (kOH>2.00 x 10^4 ppm^{-1} min^{-1})	ALK5	1	ALK4	1		
Ethene	ETHE	1	ETHE	1		
Propene	OLE1	1	OLE1	1		
Alkenes (Primary) (also primary allenes)	OLE1	1	OLE1	1		
Alkenes (Internal) (also internal allenes)	OLE2	1	OLE2	1		
Alkenes with multiple double bonds (excluding allenes)	OLE2	1	OLE2	1		
1,3-Butadiene	OLE2	1	OLE2	1		
Isoprene	ISOP	1	ISOP	1		
Terpenes with 1 double bond	TERP	1	TERP	1		
Terpenes with 2 double bonds	TERP	1	TERP	1		
Alpha pinene	TERP	1	TERP	1		
Beta pinene	TERP	1	TERP	1		
Sesquiterpenes	TERP	1	TERP	1		
Benzene	BENZ	1	ARO1	0.045	CRES	0.154
Halo and nitrobenzenes	ARO1	0.15	ARO1	0.045	CRES	0.154
Halo and nitrotoluenes	ARO1	0.3	ARO1	0.3		
Monosubstituted alkylbenzenes	ARO1	1	ARO1	1		
Di- and polysubstituted alkylbenzenes	ARO2	1	ARO2	1		
Naphthalenes and tetralins	ARO2	1	ARO2	1		
Toluene	ARO1	1	ARO1	1		
o-Xylene	ARO2	1	ARO2	1		
m-Xylene	ARO2	1	ARO2	1		
p-Xylene	ARO2	1	ARO2	1		
1,2,4-Trimethylbenzene	ARO2	1	ARO2	1		
Phenols	CRES	1	CRES	1		
Cresols	CRES	1	CRES	1		
Styrenes	OLE2	1	OLE2	1		
Formaldehyde	HCHO	1	HCHO	1		
Acetaldehyde	CCHO	1	CCHO	1		
Higher Aldehydes	RCHO	1	RCHO	1		
Aromatic Aldehydes	BALD	1	NROG	1		
Acetone	ACET	1	PRD2	0.071		
Ketones (kOH <0.73 x 10^4 ppm^{-1} min^{-1})	MEK	1	PRD2	0.369		
Ketones (kOH >0.73 x 10^4 ppm^{-1} min^{-1})	PRD2	1	PRD2	1		
Formic Acid	FACD	1	ALK3	0.048		
Acetic Acid	AACD	1	ALK3	0.243		

Table 2 (continued)

Description	SAPRC-07		CS07			
	Species	Moles	Species1	Moles	Species2	Moles
Higher organic acids	PACD	1	ALK3	0.526		
Acetylene	ACYE	1	ALK3	0.308		
Terminal Alkynes	OLE1	1	OLE1	1		
Internal Alkynes	OLE2	1	OLE2	1		
Allene and Terminal Allenes	OLE1	1	OLE1	1		
Internal Allenes	OLE2	1	OLE2	1		
Perchloroethylene	ALK1	1	ALK3	0.132		
Trichloroethylene	ALK3	1	ALK3	1		
Others (kOH =0.02-0.05 x 10^4 ppm^{-1} min^{-1})	ALK1	1	ALK3	0.132		
Others (kOH =0.05-0.25 x 10^4 ppm^{-1} min^{-1})	ALK2	1	ALK3	0.334		
Others (kOH =0.25-0.5 x 10^4 ppm^{-1} min^{-1})	ALK3	1	ALK3	1		
Others (kOH =0.5-1.0 x 10^4 ppm^{-1} min^{-1})	ALK4	1	ALK4	1		
Others (kOH =1-2 x 10^4 ppm^{-1} min^{-1})	ALK5	1	ALK4	1		
Others (kOH >2 x 10^4 ppm^{-1} min^{-1})	ALK5	1	ALK4	1		
Methanol	MEOH	1	ALK3	0.288		
Ethanol	ALK3	1	ALK3	1		
Inhibitors	NROG	1	NROG	1		
Glyoxal	GLY	1	MGLY	0.582	AFG1	0.016
Methyl Glyoxal	MGLY	1	MGLY	1		
Biacetyl	BACL	1	MGLY	1.455		
Glycolaldehyde (and other aldehydes usually lumped with acetaldehyde)	CCHO	1	CCHO	1		
Acrolein	MACR	1	IPRD	1		
Methacrolein	MACR	1	IPRD	1		
Other Unsaturated Aldehydes	IPRD	1	IPRD	1		
Unsaturated Ketones	MVK	1	IPRD	1		
Other photoreactive	BACL	1	MGLY	1.455		
Polycyclic aromatic hydrocarbons	ARO2	1	ARO2	1		
Pthallates and benzoates	ARO1	1	ARO1	1		
Miscellaneous other heteroatom-containing aromatics (Lumped with ARO1)	ARO1	1	ARO1	1		
Miscellaneous other heteroatom-containing aromatics (Lumped with ARO2)	ARO2	1	ARO2	1		
Miscellaneous heteroatom-containing non-aromatic reactive compounds	ALK5	1	ALK4	1		
Amines and amides	ALK5	1	ALK4	1		
Organic nitrates	RNO3	1	RNO3	1		
Miscellaneous unreactive unsaturated compounds lumped as alkenes	OLE2	1	OLE2	1		
Unreactive	NROG	1	NROG	1		

The NO_x and total ROG inputs for the EKMA model reactivity scale scenarios are summarized on Table 4, and the daily maximum O_3 concentrations are also summarized. The other inputs for these scenarios are given by Carter (1994a,b). As discussed by Carter (1994a, 2000a, 2010a) the NO_x inputs for the base case scenarios were derived by Baugues (1990) to represent various urban areas around the United States in the 70's or 80's, and the NO_x inputs in the MIR, MOIR, and EBIR scenarios are adjusted to yield either maximum incremental reactivities of the base ROG mixture, maximum ozone concentrations, or equal sensitivities of O_3 to relative changes in ROG or NO_x inputs, respectively. Since the NO_x inputs for these later 3 types of scenarios are adjusted to yield specified conditions, in general they are mechanism dependent. In this case, the NO_x inputs derived using the uncondensed SAPRC-07 mechanism were used for all the mechanisms that are compared. This is necessary in order that the various mechanisms be compared using the same inputs.

The incremental reactivities that were used to used to derive the reactivity weighting factors employed for the condensed mechanisms as indicated on Table 1 and to calculate the data on Figure 2 and Figure 3 were calculated using the uncondensed SAPRC-07 mechanism for the reactivity scale scenarios summarized on Table 4. The incremental reactivities are comparable to those given by Carter (2010a) except that molar units are used.

Table 3 includes several types of scenarios added in order to provide more sensitive tests to condensations of the mechanism concerning isoprene, aromatics, and chlorine chemistry. The isoprene test scenarios contained only isoprene as the VOC reactant, and the scenarios to test the aromatic mechanisms contained only toluene (ARO1) or m-xylene (ARO2). To test chlorine chemistry, which is not tested in the other scenarios because chlorine species are not reactants, scenarios are included where either Cl_2 or chloroform ($CHCl_3$) is added. Since Cl_2 is removed rapidly by photolysis, in some scenarios it was added in the middle of the simulation to simulate its reactions in a more aged mixture. Simulations with added chloroform are also included to simulate cases with more gradual chlorine atom input, since chloroform reacts relatively slowly. Since chloroform is not part of the fixed parameter SAPRC-07 mechanisms, its reactions were added for the purpose of these test calculations only, and its reactions included with the mechanism listings in Appendix A.

Table 3. Summary of box model scenarios used for mechanism comparison tests

Description	ID	Reactants [a]		Additional reactants (ppb)		
		NOx	VOC	Compound	Initial	Injected [b]
General Mechanism Tests - Static scenarios						
Static scenarios [c]; VOCs = ambient	A	10	0.6	NO_2		10
mixture [d]; NO_x injected at 6 hours	B	50	0.6	NO_2		50
for cases A, B, and D. See Figure 6	C	50	0.3			
for concentration-time plots calculated	D	5	0.6	NO_2		5
for selected species.	E	10	0.3			
General Mechanism Tests - Multi-day continuous emissions scenarios						
5-Day continuous emissions airshed	A	2	7.69			
scenarios. [e] VOCs = ambient	B	1.56	7.69			
mixture. [d]. See Figure 7 for	C	1.09	7.69			
concentration-time plots calculated for	D	0.70	7.69			
selected species.	E	0.11	7.69			
Isoprene Mechanism Tests						
Static scenarios [c] VOC = isoprene	A	10	0.5	NO_2		10
only. NOx injected at 6 hours for	B	50	0.5	NO_2		50
cases A, B, and D	C	50	0.125			
	D	5	0.5	NO_2		5
	E	10	0.125			
Aromatic Mechanism Tests - ARO1						
Static scenarios [c]; VOC = toluene	A	10	0.7	NO_2		10
only; NOx injected at 6 hours for	B	50	0.7	NO_2		50
cases A, B, and D	C	50	0.28			
	D	5	0.7	NO_2		5
	E	10	0.28			
Aromatic Mechanism Tests - ARO2						
Static scenarios [c]; VOC =m-xylene	A	10	0.24	NO_2		10
only; NOx injected at 6 hours for	B	50	0.24	NO_2		50
cases A, B, and D	C	50	0.12			
	D	5	0.24	NO_2		5
	E	10	0.12			
Chlorine mechanism Tests						
Static scenarios [c]; VOCs = ambient	A	30	0.3	Cl_2	10	300
mixture [d]; Cl_2 or $CHCl_3$ present	B	10	0.6	Cl_2	10	300
initially and added at 6 hours for cases	C	30	0.3	$CHCl_3$	10,000	
A, B, and E	D	5	0.3	$CHCL_3$	10,000	
	E	50	0.6	CL_2	50	300
Reactivity Scale Scenarios						
Same scenarios as used to calculate the MIR, MOIR, EBIR and base case scales (Carter, 1994a, 2000a, 2010a). Also includes "averaged conditions" scenarios with NOx inputs varied. The total ROG and NO_x inputs employed and the maximum O_3 concentrations calculated using the uncondensed mechanism are given in Table 4 and the other inputs are given by Carter (1994b).						

Table 3 (continued)

[a] NO_x given in units of ppb except for the multi-day scenarios, where the units are millimoles/m^2. VOC given in units of ppmC, except for multi-day scenarios, where the units are millimoles C/m^2.

[b] Injected after 6 hours of irradiation.

[c] Static conditions; all reactants present initially except for injections at 6 hours if indicated. 12-hour simulations with constant light with NO2 photolysis rate of 0.5 min-1 and solar Z=0 relative spectral distribution. In some cases NO_2 is injected at 6 hours. NO_x consisted of 25% NO2 75% NO. Temperature constant at 300K.

[d] Ambient mixture used is the base ROG mixture used in the reactivity scale calculations (Carter, 1994, 2000a, 2010a).

[e] 5-Day EKMA-type box model simulations with meteorology and emissions the same on each day. Diurnal solar light input derived for conditions of Los Angeles on June 21 (latitude=34.1 degrees, declination=23.5 degrees, daylight savings time). Temperature constant at 300K and 50% RH. No initial or aloft pollutants. Emissions of both NO_x and VOCs start at 0800 local time, level off to a constant value at 0800, begin to decrease at 1830, end at 1930, and start again with the same schedule the next day. The inversion height is 100 meters when emissions start each day until 0900 local time, raises at a constant rate at 540 meters at 2100 local time, and returns to 100 meters when emissions start the following day. Only clean air is entrained when the inversion height raises. NOx consisted of 25% NO_2 and 75% NO.

Table 4. Summary of ROG and NO_x inputs and maximum ozone concentrations calculated using the SAPRC-07 mechanism for the reactivity scale scenarios.

ScenID		ROG ($mmol/m^3$)	NOx Input ($mmol/m^3$)				Daily Maximum O_3 (ppb)			
			Base	MIR	MOIR	EBIR	Base	MIR	MOIR	EBIR
Avg Cond		15.4		4.16	2.73	1.74		179	229	213
ATL	GA	11.8	1.62	3.32	2.19	1.54	173	146	179	171
AUS	TX	11.2	1.21	3.34	2.21	1.40	171	156	189	178
BAL	MD	16.8	3.26	4.31	2.84	1.67	318	246	322	295
BAT	LA	11.1	1.63	2.58	1.75	1.32	237	188	238	228
BIR	AL	12.8	1.85	4.73	3.13	2.05	239	205	261	245
BOS	MA	14.3	2.20	5.30	3.45	2.19	191	163	202	191
CHA	NC	7.5	0.96	4.15	2.69	1.93	139	138	165	160
CHI	IL	25.0	2.15	5.82	3.91	2.56	286	243	325	302
CIN	OH	17.3	2.71	5.25	3.43	1.92	196	159	200	183
CLE	OH	15.7	2.37	3.70	2.36	1.55	245	195	245	230
DAL	TX	17.5	3.70	4.39	2.87	1.98	194	163	206	196
DEN	CO	29.3	4.64	6.02	3.98	2.58	197	163	201	189
DET	MI	17.3	2.54	4.76	3.12	1.76	237	184	241	220
ELP	TX	12.3	1.86	2.73	1.76	1.27	178	146	178	170
HAR	CT	10.7	1.28	3.91	2.52	1.51	167	149	187	174
HOU	TX	25.5	4.19	6.46	4.27	2.72	303	227	303	281
IND	IN	12.1	1.82	3.12	1.94	1.26	205	160	205	193
JAC	FL	7.7	1.01	2.25	1.49	1.07	150	126	159	152
KAN	MO	9.1	1.28	3.07	1.98	1.09	152	127	160	147
LAK	LA	7.0	0.94	2.01	1.39	1.01	289	232	310	295
LOS	CA	23.1	3.04	4.51	2.97	2.08	566	405	566	534
LOU	KY	13.7	2.48	4.44	2.88	1.92	204	162	206	195
MEM	TN	14.9	2.20	4.64	3.11	1.96	224	180	234	218
MIA	FL	9.5	0.98	3.50	2.26	1.56	129	122	151	145
NAS	TN	7.4	0.92	3.00	1.97	1.27	162	147	190	178
NEW	NY	39.2	4.85	8.54	6.12	4.11	371	300	380	358
PHI	PA	19.0	3.07	4.77	3.17	2.01	237	182	237	221
PHO	AZ	39.9	5.26	8.19	5.24	3.07	271	210	271	246
POR	OR	6.2	0.96	2.15	1.34	0.93	160	131	166	159
RIC	VA	16.4	2.65	4.76	3.12	1.76	233	181	236	215
SAC	CA	7.4	1.12	1.99	1.29	0.83	198	153	200	187
SAI	MO	25.6	4.22	5.64	3.70	2.23	311	239	315	290
SAL	UT	10.7	1.26	3.18	2.02	1.19	181	157	192	179
SAN	TX	6.0	1.53	2.11	1.36	0.98	124	104	125	120
SDO	CA	7.7	1.08	1.69	1.12	0.80	188	150	188	179
SFO	CA	25.0	5.24	4.18	2.82	2.11	231	350	461	439
TAM	FL	7.9	1.81	2.38	1.60	1.18	219	174	222	213
TUL	OK	14.9	2.80	4.82	2.94	1.73	221	151	221	204
WAS	DC	13.5	2.54	4.41	2.94	1.87	274	214	277	259

MECHANISM COMPARISON RESULTS

General Mechanism Tests

Figure 4 shows the changes in maximum O_3, H_2O_2, total PANs, and average OH in the static and multi-day general mechanism test calculations resulting from the various condensations, relative to the uncondensed SAPRC-07 mechanism, and the changes in these quantities caused by the individual condensation steps are shown on Figure 5. Concentration-time plots for these species in these scenarios are shown for selected mechanisms in Figure 6 and Figure 7.

These calculations show that the condensations through C6 have relatively little effect on O_3 in these general test scenarios, with the average change for a given type of scenario being less than 2% in all cases. However, the differences in O_3 predictions become considerably greater for condensation C7 (lumping PAN with PAN2) and C8 (lumping acetaldehyde and RCHO), suggesting that these condensations introduce a greater degree of inaccuracy in model predictions. The changes in total PANs and average OH are somewhat greater than changes in O_3, but the averages changes for the two types of scenarios are less than 5% except for C7 and C8. The changes for H_2O_2 are greater yet, with the average change in maximum H_2O_2 concentrations in most cases being on the order of 7-15% for the condensed mechanisms through C6 employing peroxy representation "A". For CS07B, the condensed mechanism employing the uncondensed peroxy representation "B", the differences in the PAN and H_2O_2 simulations are less, though the difference in O_3 is only slightly better, and the difference in average OH somewhat worse, then the corresponding condensed mechanism using peroxy representation "A".

Figure 5 shows the effects of the stepwise condensations that were made, starting with changing from peroxy "B" to peroxy "A", then making the other condensations one after the other. (The effects of the chlorine mechanism condensations are not shown because they do not affect these general mechanism test calculations.) Consistent with the results shown on Figure 4, the changes in O_3 concentrations are insignificant until the PANs and aldehydes are lumped, and the differences in H_2O_2 and total PAN predictions are primarily due to the effects of going from peroxy representation "B" to "A". On the other hand, the main condensation steps through C6 that caused changes in average OH concentrations were those incorporated in C1. This is probably due to the lumping of the MEK model species used to represent the lower reactivity oxygenated products, since similar differences in OH are seen in test calculations with benzene and acetylene removed from the base ROG mixture, and the other condensations associated with C1 are expected to be less important.

Special Mechanism Tests

The general mechanism test calculations are not particularly sensitive to changes in the isoprene mechanism because of the relatively low level of isoprene in the base ROG mixture used in those calculations, so as indicated in Table 3 separate sets of test calculations are used to test changes in this mechanism. The effects of the condensations of the isoprene mechanism on these isoprene test calculations is shown on Figure 8, which shows concentration-time plots of selected compounds calculated using uncondensed SAPRC-99, the condensed mechanism version (C3) with the condensations prior to the isoprene condensations, and the condensed mechanism incorporating the isoprene condensations (C4, which is the same as C07A for these isoprene-only simulations). It can be seen that the condensation has essentially no effect on O_3 except for the lowest ROG/NO_x simulation, and that the effect on H_2O_2 is small compared to the larger effect of changing the peroxy radical representation. The

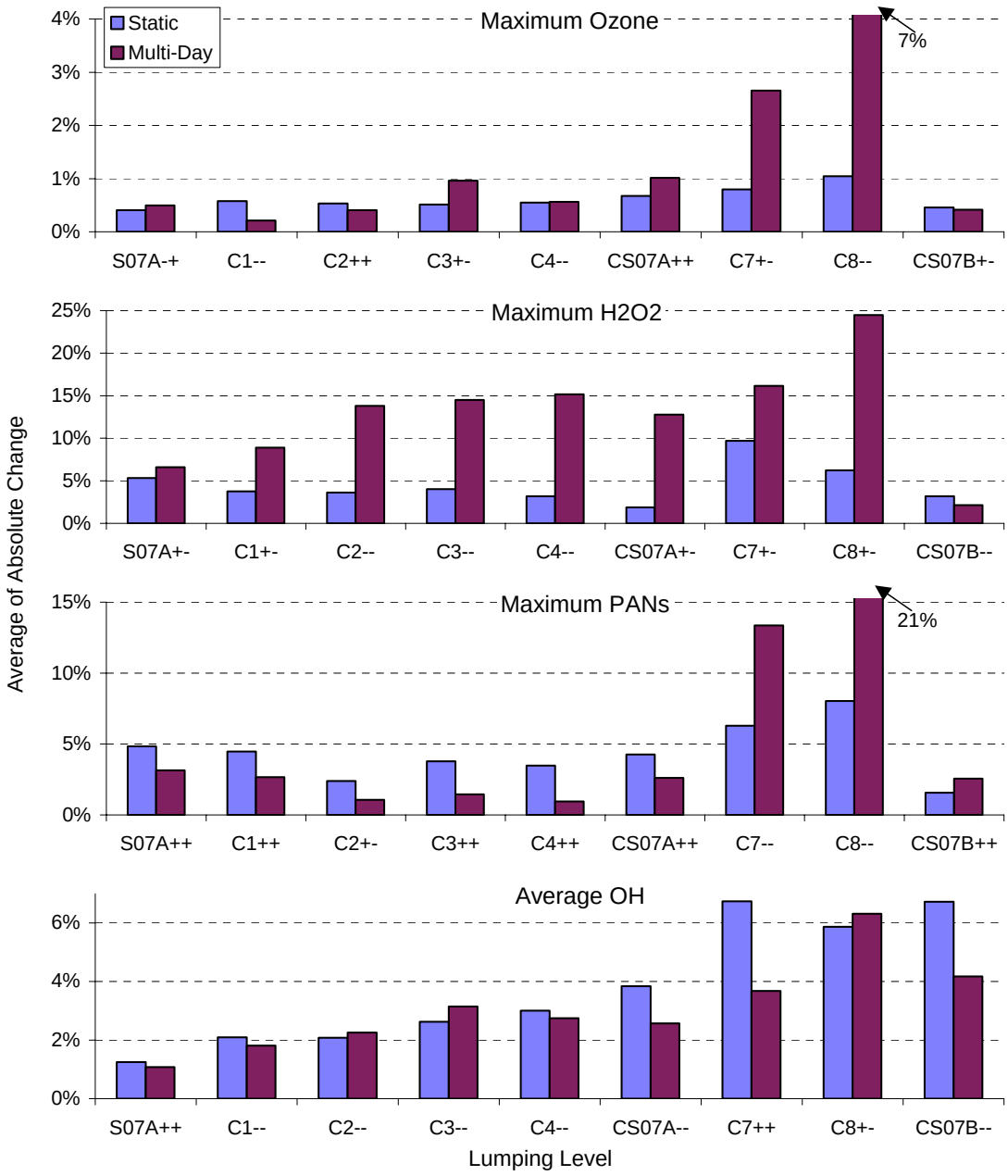

Figure 4. Average changes for maximum O3, H_2O_2, PANs and average OH for the static and multi-day ROG - NO_x test calculations, relative to the uncondensed SAPRC-07 mechanism. "A" = uncondensed mechanism using the SAPRC-99 peroxy radical operators, C1 … C8 = condensed mechanisms. C6B = C6 mechanism using SAPRC-07 peroxy radical operators (see Table 1). The signs after lumping level indicate the sign for the average differences for the static and multi-day scenarios, respectively.

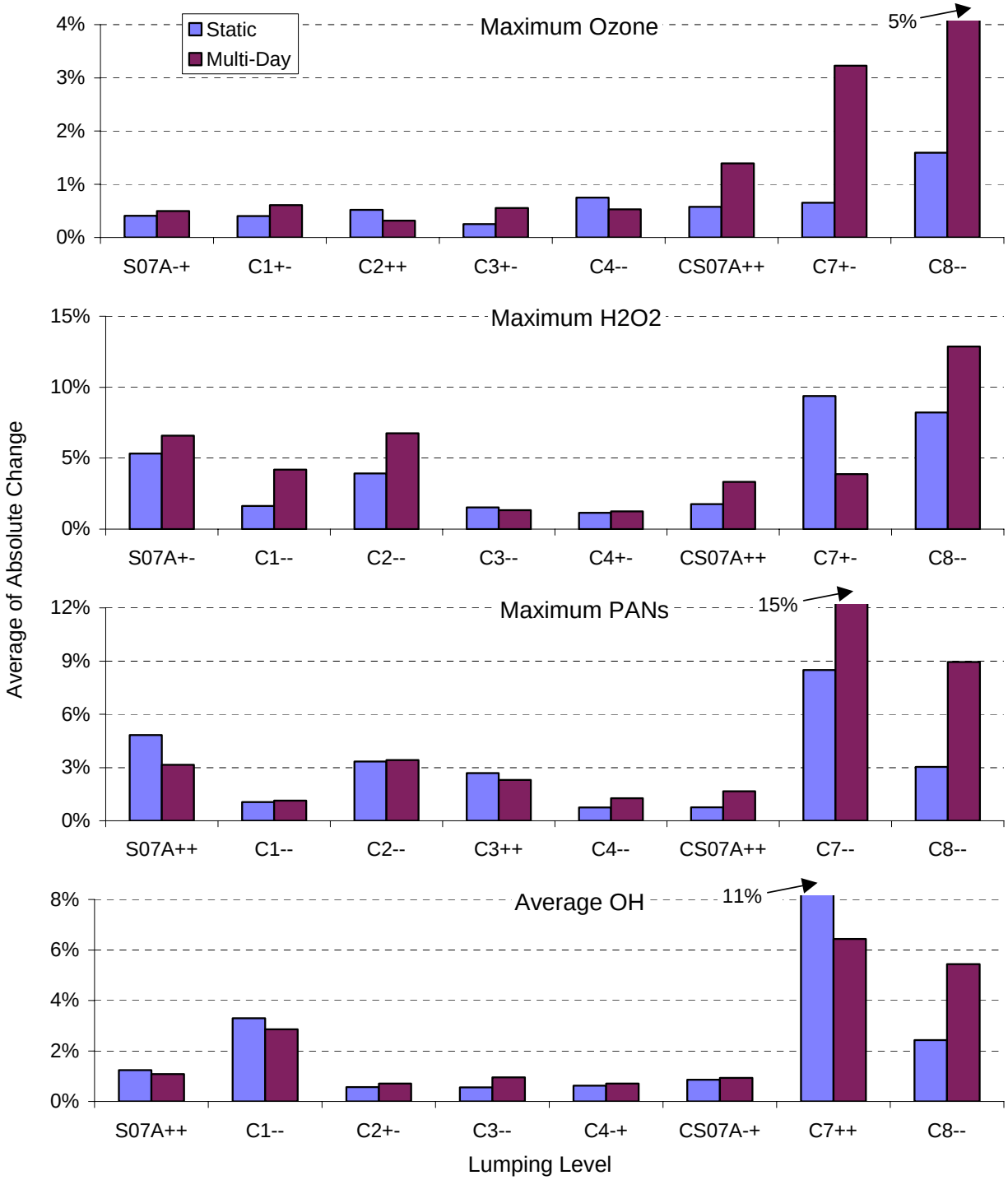

Figure 5. Average changes for maximum O3, H_2O_2, PANs and average OH for the static and multi-day ROG - NO_x test calculations, relative to previous condensation level. "A" = uncondensed mechanism using the SAPRC-99 peroxy radical operators relative to standard SAPRC-07, C1 … C8 = condensed mechanisms (see Table 1) relative to previous condensation level. The signs after lumping level indicate the sign for the average differences for the static and multi-day scenarios, respectively.

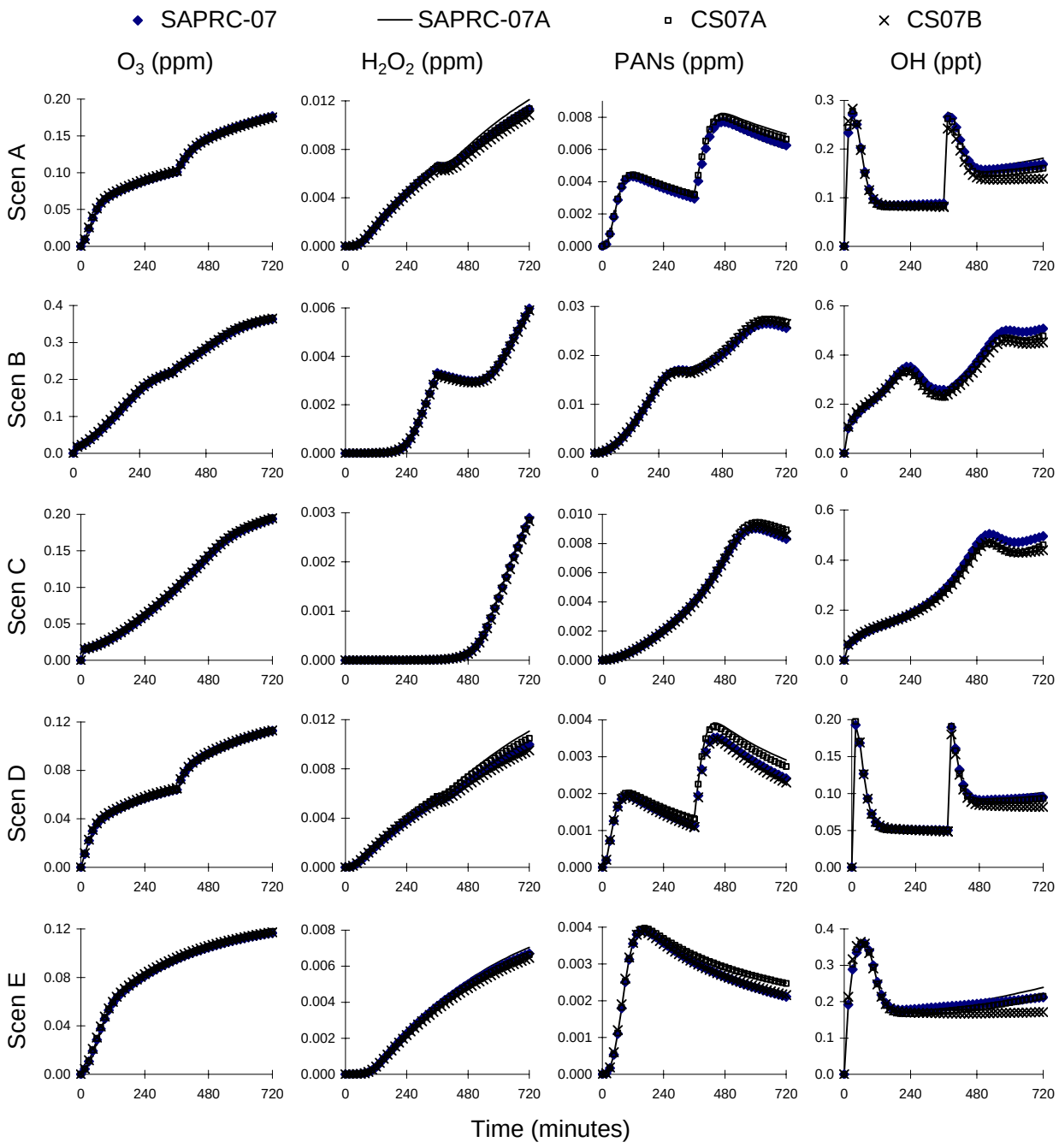

Figure 6. Concentration-time plots for selected species in the static general mechanism test simulations using the standard uncondensed mechanism (SAPRC-07), the uncondensed mechanism with the SAPRC-99 peroxy radical operators (SAPRC-07A) and the "C6" condensed mechanisms derived in this work (CS07A and CS07B) .

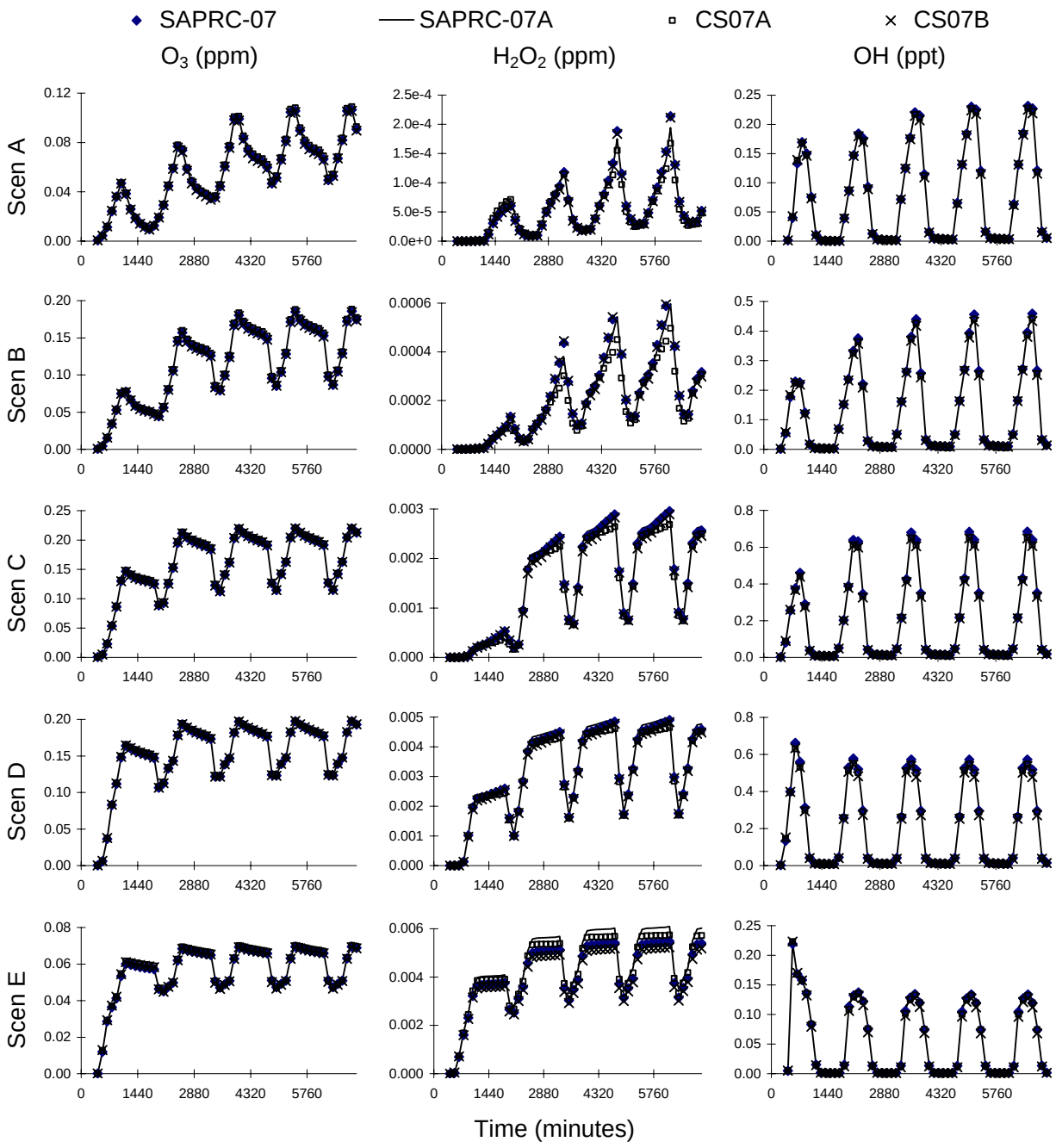

Figure 7. Concentration-time plots for selected species in the multi-day general mechanism test simulations using the standard uncondensed mechanism (SAPRC-07), the uncondensed mechanism with the SAPRC-99 peroxy radical operators (SAPRC-07A) and the "C6" condensed mechanisms derived in this work (CS07A and CS07B).

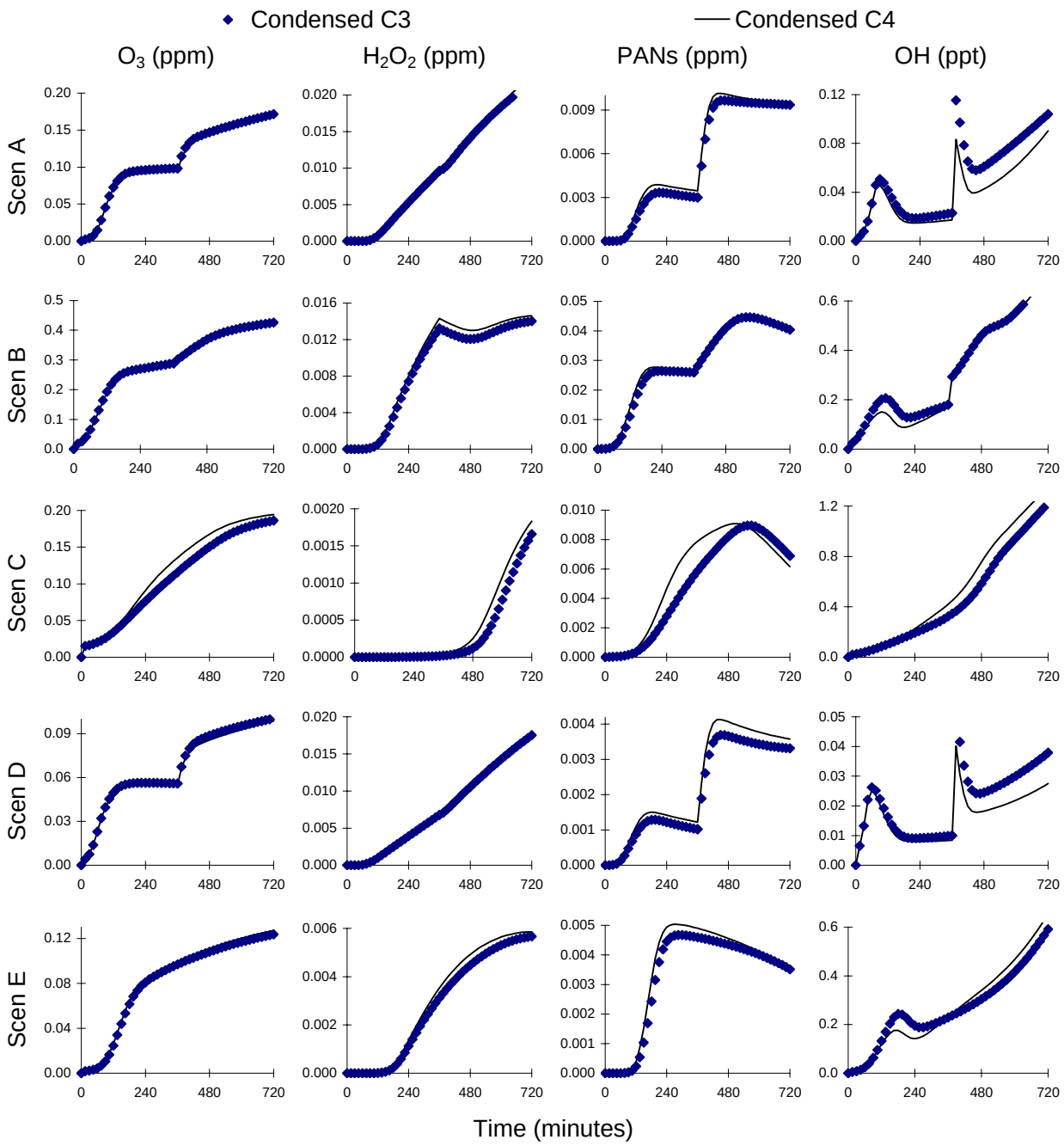

Figure 8. Concentration time plots for selected species in the calculations used to test the condensations to the isoprene products mechanism (C3 to C4).

effects of the isoprene condensation on PANs and OH are somewhat larger, especially after the 2nd NO_x injection in Scenarios "A" and "D". This is due to the fact that the initial isoprene is essentially reacted at the later stages of these simulations, and the reactivity of the simulation is dominated by isoprene's products, which are represented differently in the condensed mechanism.

Although the condensations to the aromatics mechanism should affect the general mechanism test calculations, because of the importance of aromatics their effects were also examined in special test scenarios where aromatics were the only added VOC reactants. The simulations of these scenarios with the condensed mechanism at the level prior to the aromatic simulations (C3), and the condensed mechanism incorporating the aromatics condensations (C4, which is the same as S07A for these simulations) are shown on Figure 9 and Figure 10. In general the effects of the aromatic mechanism condensations are small compared to the effects of the other condensations implemented through C3, except for some relatively small changes in OH and PANs in some scenarios.

The general mechanism test calculations do not test the chlorine mechanism condensations because chlorine species are not present in those scenarios. Therefore, special scenarios were used to test effects of changes to this aspect of the mechanism. Scenarios with added Cl_2 test effects of rapid injections of chlorine atoms because of the rapid photolysis of Cl_2, while those with added $CHCl_3$ test effects of continuous inputs of chlorine atoms. The results of simulations of these scenarios with the uncondensed mechanism, the condensed mechanism version without the chlorine condensations (C4) and the version after chlorine condensation (C5) are shown on Figure 11. In all cases the difference between the version of the mechanism with (C5) and without (C4) were relatively small, indicating that these chlorine mechanism condensations, by themselves, should have relatively small effects on the model simulations.

Test Calculations with Reactivity Scenarios

Simulations were carried out on the EKMA city-specific and "averaged conditions" scenarios used to derive the reactivity scales were conducted using the uncondensed and selected condensed mechanisms. The condensed mechanisms used were SAPRC-07A, the uncondensed mechanism with the condensed peroxy radical representation "A" and CS07A, the most condensed mechanism version that gave satisfactory simulations of O_3 in the general mechanism test scenarios. The simulations using the three mechanisms are shown on Figure 12 through Figure 14, where Figure 12 compares the most and least condensed mechanisms, Figure 13 shows the effects of changing the peroxy radical representation from "B" to "A", and Figure 14 shows the effects of implementing condensations C1 through C6 with the same peroxy radical model. The quantities compared are maximum O_3, PANs and H_2O_2 and incremental reactivities relative to the base ROG and NO_x. The latter two provide a comparison of how the mechanisms differ predictions of effects of VOC and NO_x controls on ozone.

Figure 12 shows that the maximum O_3 predictions of the condensed mechanism were generally within 2-3% of those of the uncondensed mechanism, though the condensed mechanism usually predicted about 1% more ozone. The total PAN predictions were generally within 7%, but also tended to be somewhat higher, while the H_2O_2 predictions were within ~5% for the MIR to MOIR scenarios but the discrepancy tended to increase with lower NO_x conditions. Figure 13 and Figure 14 indicate that the peroxy radical condensations tend to have an opposite effect on H_2O_2 predictions than condensations C1 through C6, and thus tend to cancel out, but are still within ±5% except for the MIR scenarios. For the other species the two types of condensations tend to have similar effects.

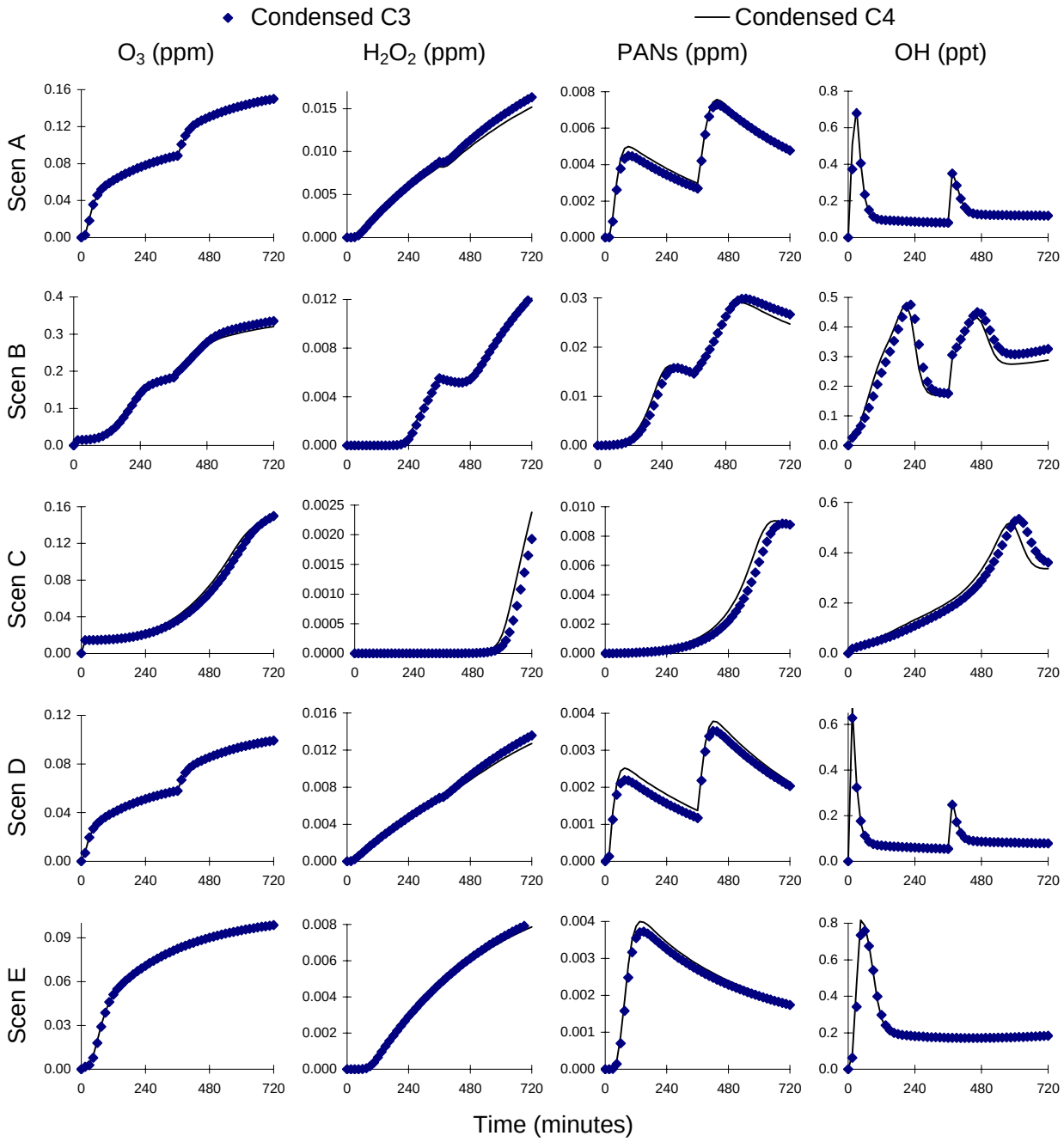

Figure 9. Concentration time plots for selected species in the ARO1 (toluene) calculations used to test the condensations to the aromatic mechanisms (C3 to C4).

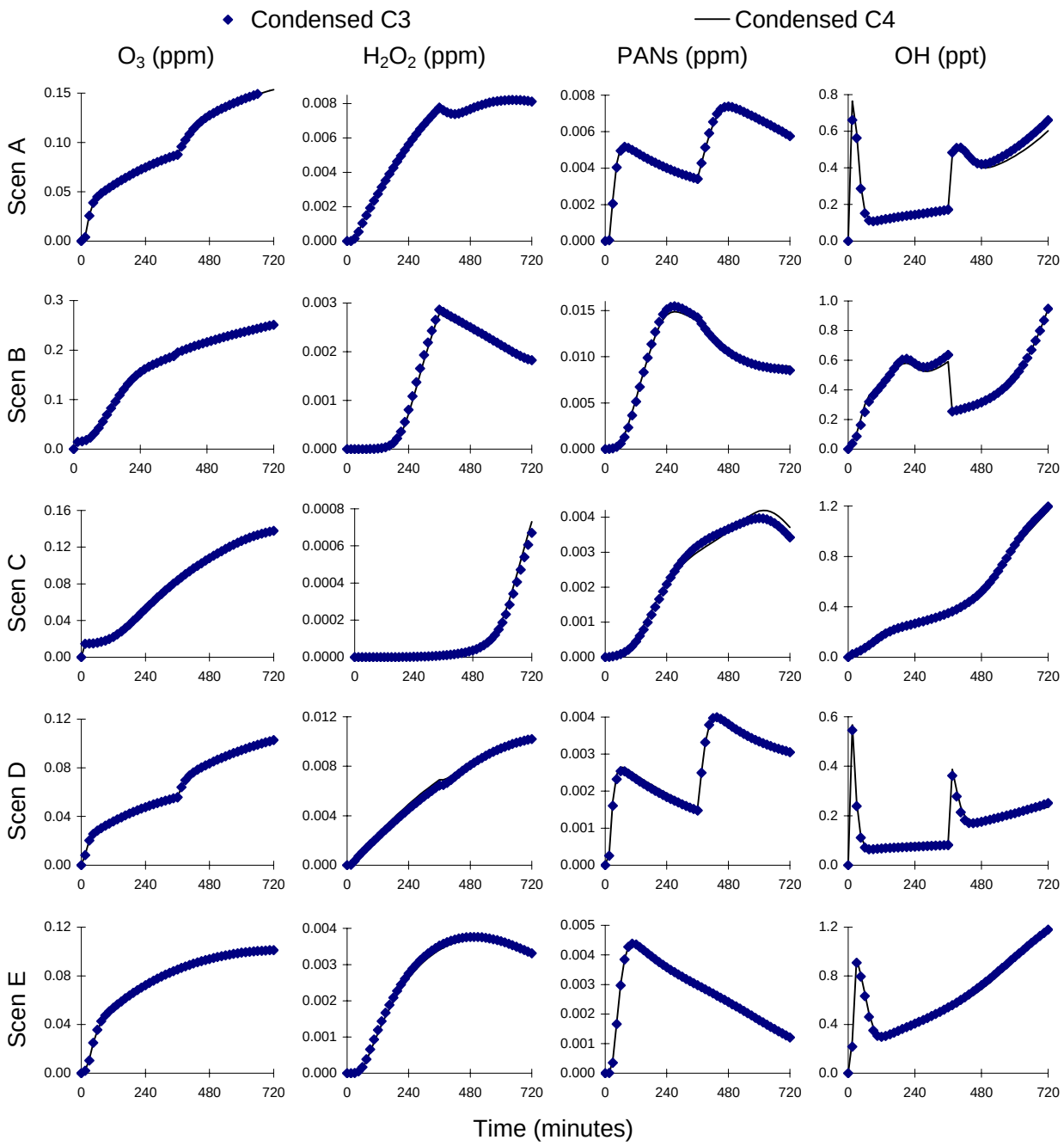

Figure 10. Concentration time plots for selected species in the ARO2 (m-xylene) calculations used to test the condensations to the aromatic mechanisms (C3 to C4).

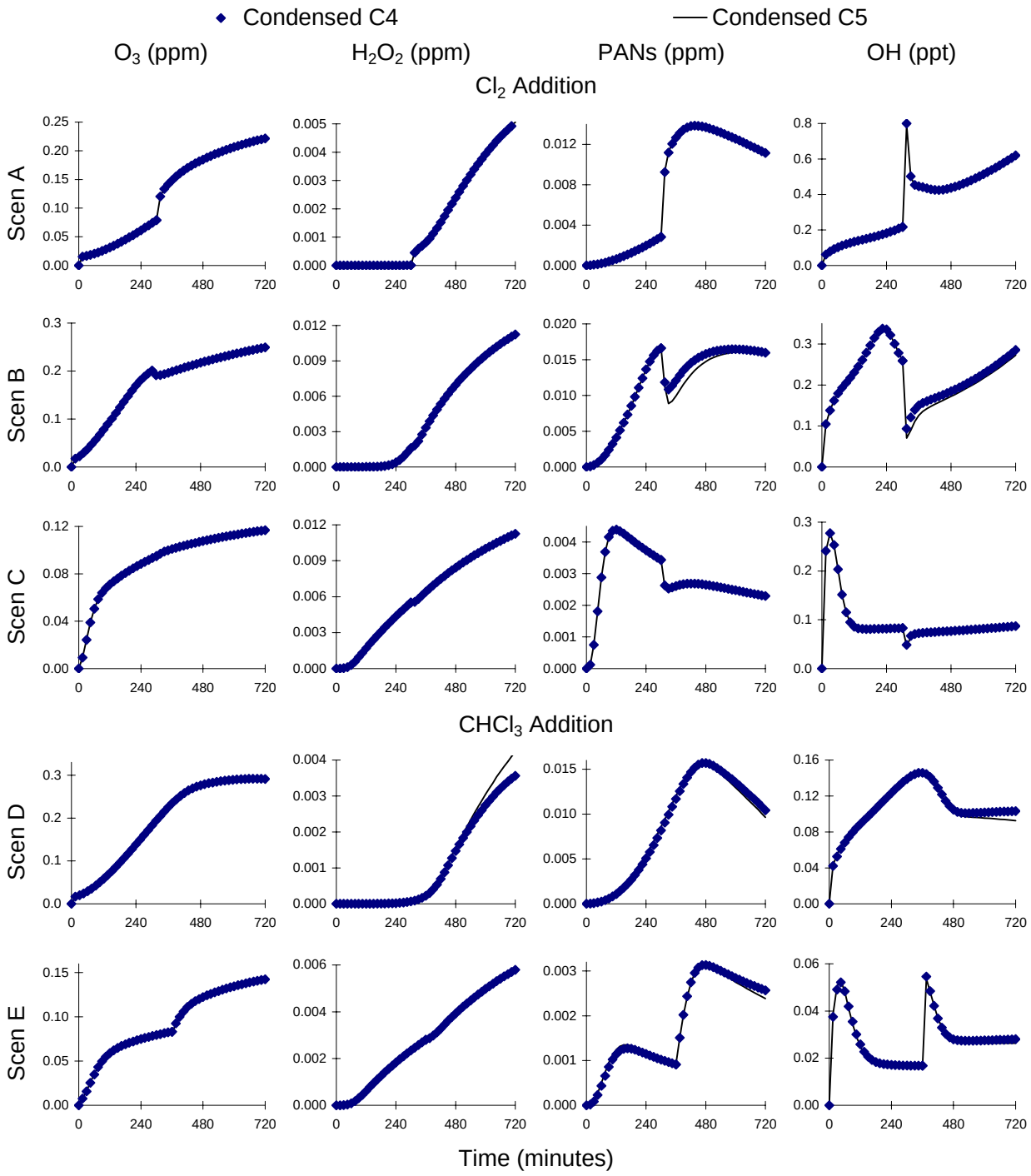

Figure 11. Concentration time plots for selected species in the calculations used to test the condensations to chlorine mechanism (C4 to C5).

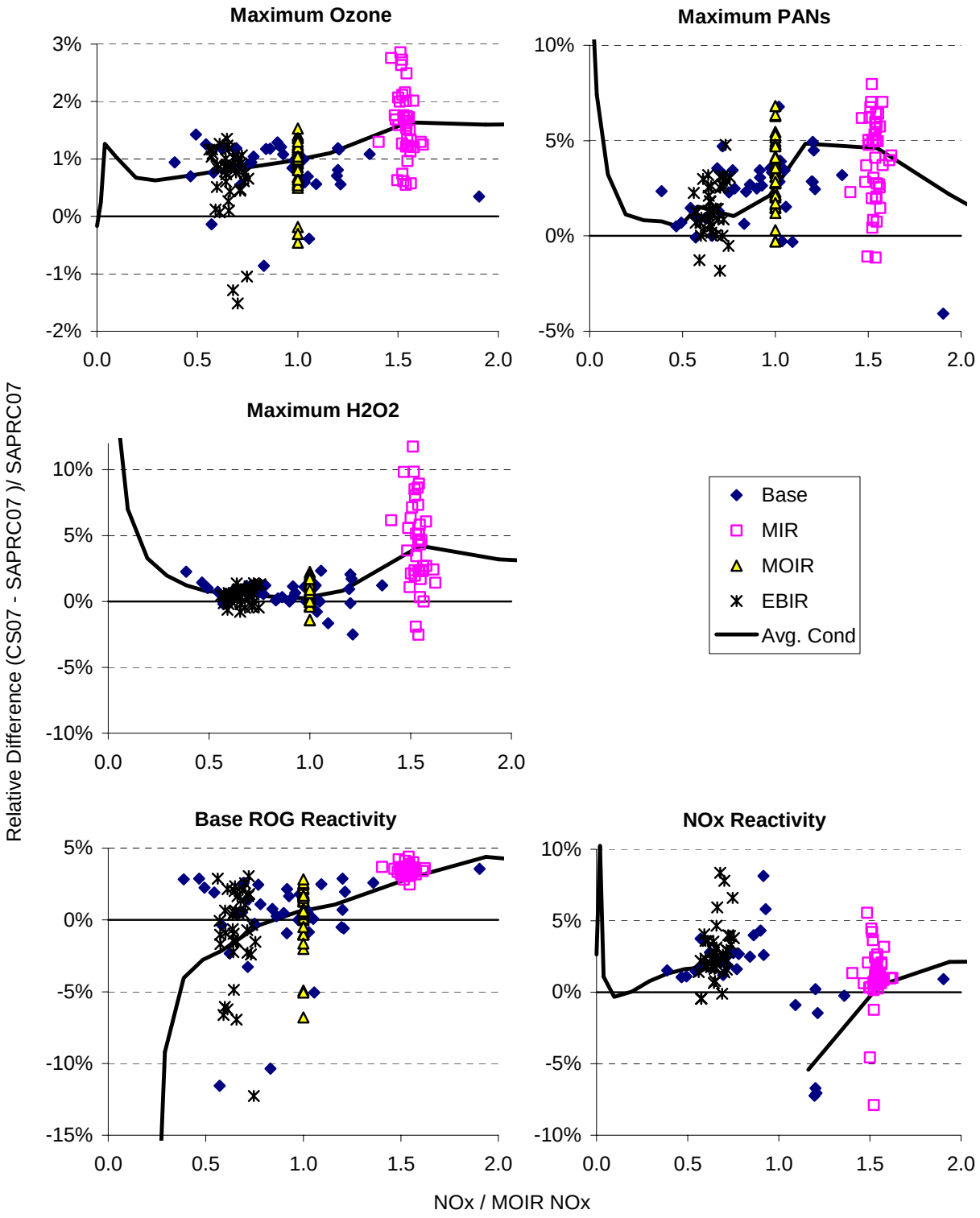

Figure 12. Differences in selected calculated quantities in the reactivity scenario simulations between the condensed (CS07A) and the uncondensed SAPRC-07 mechanisms.

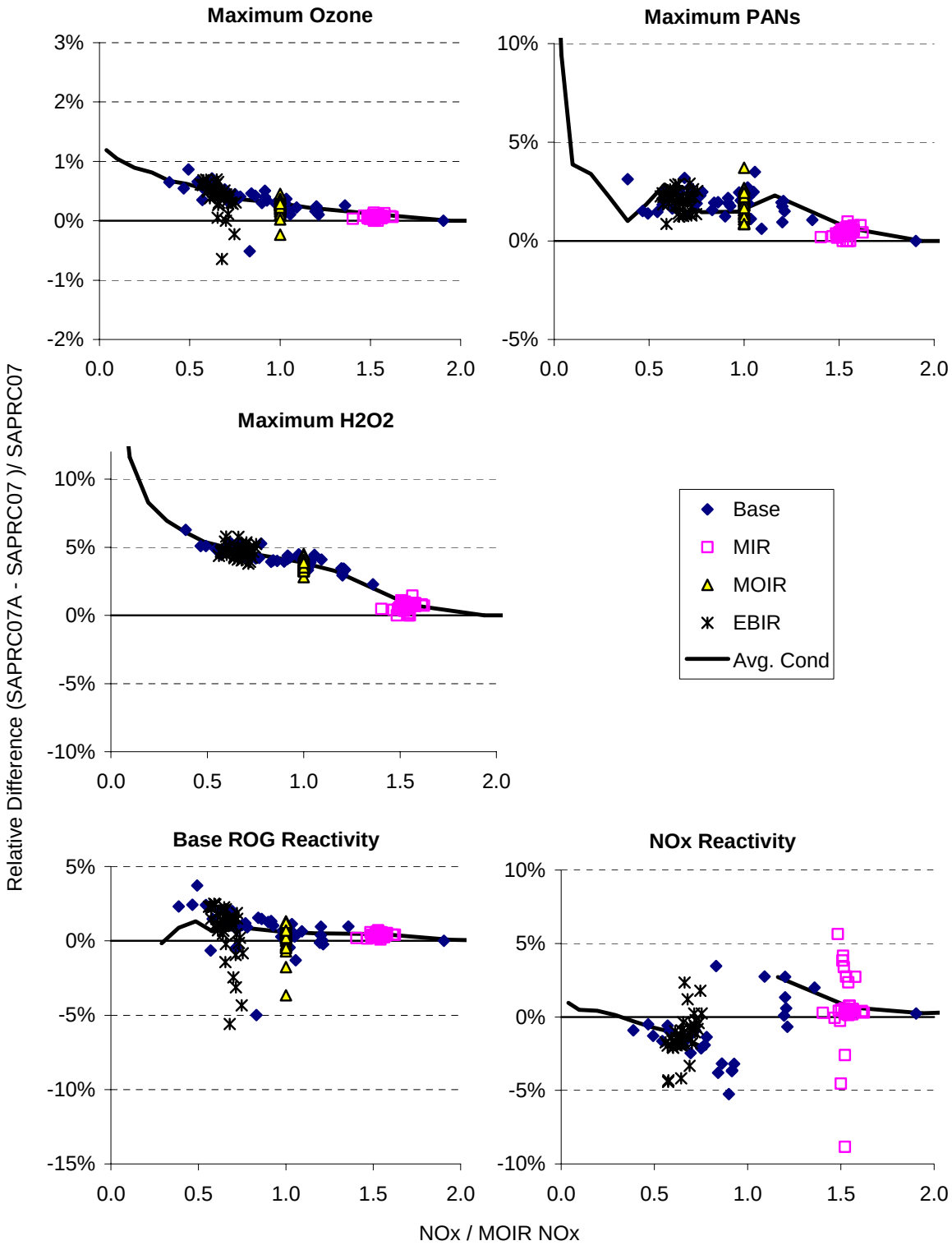

Figure 13. Differences in selected calculated quantities in the reactivity scenario simulations between the uncondensed SAPRC-07 mechanism and the version of the otherwise uncondensed mechanism using peroxy radical representation "A" (SAPRC-07A).

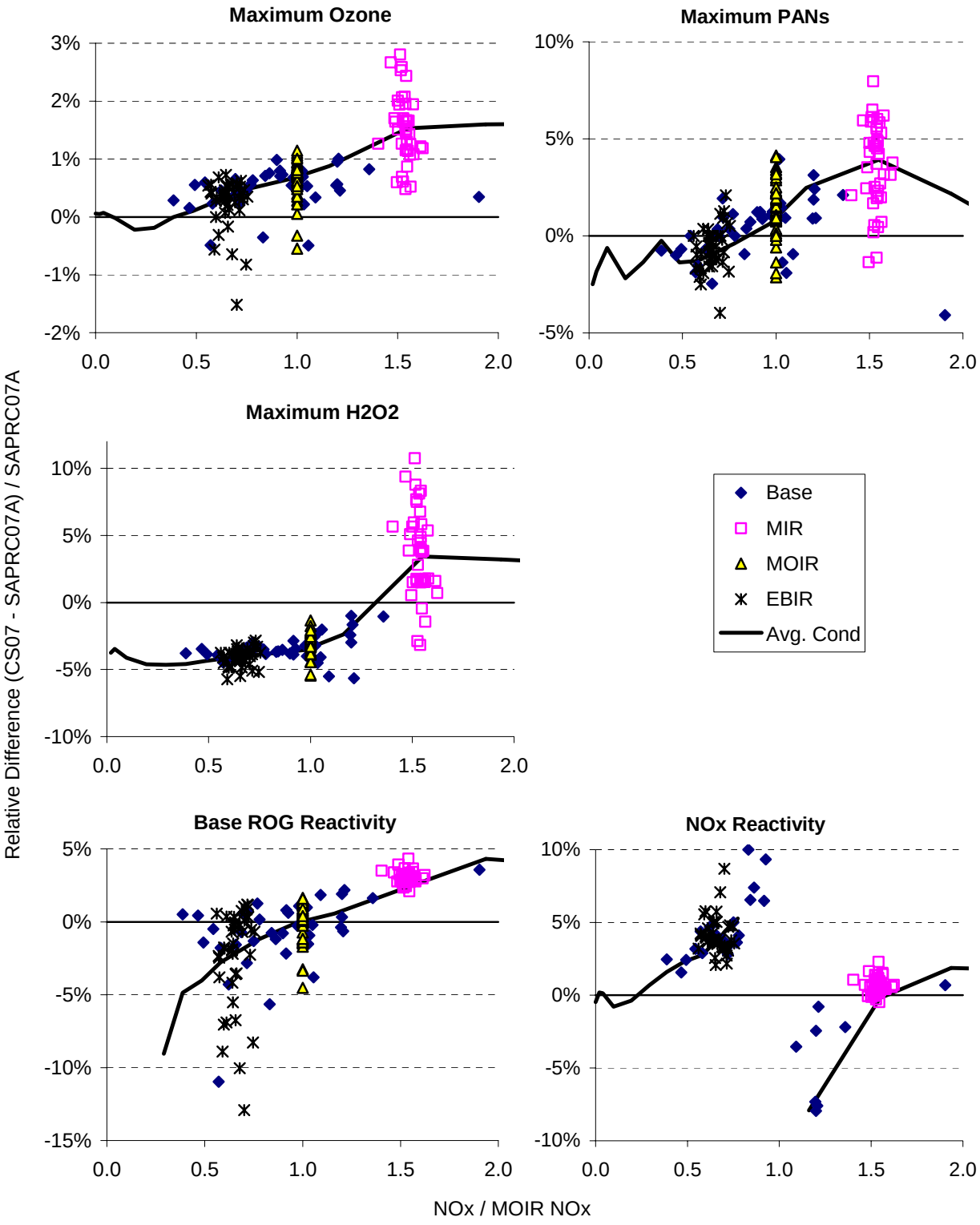

Figure 14. Differences in selected calculated quantities in the reactivity scenario simulations between the condensed (CS07A) and the uncondensed mechanisms using the condensed peroxy radical condensation approach (SAPRC-07A).

Figure 12 shows that the effects of the condensations on the base ROG and NO_x reactivities tend to vary from scenario to scenario, but are generally within ±10%. The condensed mechanism predicts somewhat less effectiveness of ROG controls under low NO_x conditions and somewhat more effectiveness of ROG controls in MOIR and higher NO_x scenarios, while there appears to be relatively little consistent difference in the case of predictions of effectiveness of NO_x controls. The differences in base ROG reactivity are primarily due to effects of the C1 through C6 condensations, not the change in peroxy radical model, as can be seen by comparing Figure 13 and Figure 14.

The differences in reactivities of individual VOCs calculated using the condensed mechanisms were not examined because condensed mechanisms are generally not appropriate for calculation of VOC reactivity scales. However, differences in calculations of total VOCs (base ROG) or total NO_x is relevant because condensed mechanisms may well be used for determining effects of changes in total VOC or NO_x emissions.

DISCUSSION AND CONCLUSIONS

The objective of this project is to develop a condensed version of the SAPRC-07 mechanisms whose chemical basis and validity is derived from the fully detailed mechanism, and which gives essentially the same predictions of species of interest in model applications where the condensed mechanism will be used. If the primary objective is the prediction of ozone formation, then this objective has been achieved. The mechanism described above designated "C6", employing the SAPRC-99 peroxy radical representation and other condensations that reduce the number of reactions and species by more than a factor of two, give predictions of ozone that are within a few percent of the uncondensed mechanism even in multi-day simulations, gives reasonably close predictions of PANs, OH radicals, and gives predictions of H_2O_2 within about 15%. For that reason, we conclude that mechanism C6, or CS07A, can serve as the condensed version of SAPRC-07 where the priority is ozone predictions, and highly accurate predictions of H_2O_2 and other hydroperoxides are not as critical. If more accurate predictions of H_2O_2 and organic hydroperoxides are important, then mechanism CS07B, the version of mechanism C6 that retains the less approximate SAPRC-07 peroxy radical representation, should be employed. This has about 60% of the species and reactions as uncondensed SAPRC-07, or 40% more species and 20% more reactions, than the more condensed CS07A.

The condensations found to have small and generally acceptable effects on predictions of O_3, PANs, H_2O_2 and OH radicals involved removing or lumping less reactive compounds, lumping some product species in isoprene or aromatic mechanisms with other species with similar mechanisms using reactivity weighting, removing some compounds and reactions that are rapidly reversed, and using fewer model species to represent emitted alkanes and similar species. On the other hand, it was found that lumping PAN with the higher PAN species PPN and other PANs represented by PAN2, and lumping acetaldehyde with the higher acetaldehyde species RCHO, causes larger changes in O_3 predictions, and are not considered worthwhile approximations given the relatively small decrease in model species and reactions that result. Therefore these approximations are not employed in the versions of condensed SAPRC-07 recommended for use.

Note that all mechanisms used in regulatory modeling applications must ultimately be based on current scientific data and theories, have their predictive capabilities evaluated by comparing their predictions with environmental chamber data (Jeffries et al, 1992). The scientific validity and predictive capabilities of separately-developed condensed mechanisms are difficult to assess because there is no way to assess effects of condensation approximations they employ, and they can only be evaluated against a small subset of the available environmental chamber data base because many chamber experiments do not contain compounds or mixtures of compounds they are designed to represent. The scientific basis and evaluation of the condensed mechanisms developed in this work are based on those of the detailed SAPRC-07 mechanism as documented by Carter (2010a). That detailed mechanism reflects the state of the science as of mid-2007, and was extensively evaluated against results of ~2400 environmental chamber experiments carried out in 11 different environmental chambers, including experiments to test mechanisms for over 120 types of VOCs. Although the performance in simulating the chamber data was not perfect in all cases, it was generally satisfactory for most important types of VOCs and mixtures, and is probably the best can be obtained given the current state of the science. The effects of the condensations employed in these mechanisms can be directly assessed by comparing its predictions with those of the detailed or uncondensed mechanism, as done in the test calculations employed in this work.

The most condensed mechanism developed in this work that is recommended for use, CS07A, is comparable in size to the recently developed Carbon Bond 05 mechanism (Yarwood et al, 2005) that is being implemented in the CMAQ model (Sarwar et al, 2008). CB05 employs a peroxy radical

representation that is comparable to the SAPRC-99 method "A" that is used in CS07A, and generally employs similar numbers of lumped species to represent reactive organic products. It has 5 more species and 16 more reactions than CS07A, but also contains explicit representations of methanol, ethanol, acetic and formic acids, methyl hydroperoxide and ethane, which are lumped in CS07A. If these compounds were represented explicitly in CS07A, or if they were removed from CB05, then the mechanisms would be almost equal in size. Therefore, CS07A would be appropriate for any application where use of CB05 is contemplated, and if properly implemented the computer resource requirements should be comparable. Note that use of implementation of CS07A would not require the changes to chemical mechanism implementation software that may be required for uncondensed SAPRC-07 or CS07B.

The development of mechanisms for predictions of SOA formation was beyond the scope of this project, so the mechanisms developed in this work represent only gas-phase species. Existing SOA modules developed for SAPRC-99 or CB05 could be added to CS07A or CS07B in a relatively straightforward manner. More detailed SOA modules would probably have to use uncondensed SAPRC-07 or at least CS07B as the starting point in order to appropriately represent differences on condensable product formation under low NO_x conditions where peroxy + peroxy radical reactions are important.

The condensed and fixed-parameter SAPRC-07 mechanisms depend in part on the composition used for the base ROG mixture that was used to derive the parameters of some of the lumped species. As discussed by Carter (2010a) the mixture used for this purpose when deriving the current fixed-parameter and condensed SAPRC-07 mechanisms is the same as that used for that purpose in SAPRC-99, and in calculation of the VOC reactivity scales, and is based on measurements of ambient air in urban areas in the 1980's (Lonneman, 1986; Jeffries et al, 1989, Carter, 1994a). If that mixture were updated then the fixed-parameter and condensed SAPRC-07 mechanisms would need to be updated accordingly. This is beyond the scope of the present project.

Since the validity of the CS07A and CS07B mechanisms depend on the detailed SAPRC07 mechanisms, these mechanisms would need to be updated whenever the detailed mechanism is updated. The procedures employed to derive the fixed-parameter SAPRC-07 from the detailed mechanisms as discussed by Carter (2010a), and to derive the condensed mechanisms from the fixed-parameter mechanism as discussed in this report, can be then used to derive the updated condensed mechanisms. This would preserve the relationship between the detailed and condensed mechanism that is important for maintaining its validity and traceability to basic laboratory and environmental chamber data.

The files necessary to implement the CS07A and CS07B mechanisms in airshed models are available at the SAPRC mechanism web page at http://www.cert.ucr.edu/~carter/SAPRC. These include listings of the reactions and rate constant in the format used by the SAPRC and CMAQ mechanism implementation systems, and files containing the absorption cross sections and quantum yields, and assignments of model species to VOC categories used in emissions inventories.

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APPENDIX A. GENERAL MECHANISM LISTING TABLES

This appendix contains the tables giving a complete listing of the condensed SAPRC-07 mechanisms developed in this work and the uncondensed mechanism used as the starting point. Note that the absorption cross sections and quantum yields for the photolysis reactions are the same for all the mechanisms, and as documented by Carter (2010a), and available at http://www.cert.ucr.edu/~carter /SAPRC (Carter, 2010b)

Table A-1. List of model species used in the fixed parameter uncondensed SAPRC-07 mechanism that was used as the starting point for the mechanism developed in this work.

Name	Version [a] Unc	Cnd	Description
Constant Species.			
O2	x	x	Oxygen
M	x	x	Air
H2O	x	x	Water
H2	x	x	Hydrogen Molecules
HV	x	x	Light
Active Inorganic Species.			
O3	x	x	Ozone
NO	x	x	Nitric Oxide
NO2	x	x	Nitrogen Dioxide
NO3	x	x	Nitrate Radical
N2O5	x	x	Nitrogen Pentoxide
HONO	x	x	Nitrous Acid
HNO3	x	x	Nitric Acid
HNO4	x	x	Peroxynitric Acid
HO2H	x	x	Hydrogen Peroxide
CO	x	x	Carbon Monoxide
SO2	x	x	Sulfur Dioxide
Active Radical Species			
OH	x	x	Hydroxyl Radicals
HO2	x	x	Hydroperoxide Radicals
MEO2	x		Methyl Peroxy Radicals
MECO3	x	x	Acetyl Peroxy Radicals
RCO3	x	x	Peroxy Propionyl and higher peroxy acyl Radicals
BZCO3	x		Peroxyacyl radical formed from Aromatic Aldehydes
MACO3	x		Peroxyacyl radicals formed from methacrolein and other acroleins.
Active Peroxy Radical Operators - SAPRC-07 peroxy representation "B"			
RO2C	B	B	Peroxy Radical Operator representing NO to NO_2 and NO_3 to NO_2 conversions, and the effects of peroxy radical reactions on acyl peroxy and other peroxy radicals.

Table A-1 (continued)

Name	Version [a] Unc	Cnd	Description
RO2XC	B	B	Peroxy Radical Operator representing NO consumption (used in conjunction with organic nitrate formation), and the effects of peroxy radical reactions on NO_3, acyl peroxy radicals, and other peroxy radicals.
Active Peroxy Radical Operators - SAPRC-99 peroxy representation "A"			
RO2R	A	A	Peroxy Radical Operator representing NO to NO_2 conversion with HO_2 formation.
R2O2	A	A	Peroxy Radical Operator representing NO to NO_2 conversion without HO_2 formation.
RO2N	A	A	Peroxy Radical Operator representing NO consumption with organic nitrate formation.
Steady State Radical Species			
O3P	x	x	Ground State Oxygen Atoms
O1D	x	x	Excited Oxygen Atoms
TBUO	x		t-Butoxy Radicals
BZO	x	x	Phenoxy Radicals
PAN and PAN Analogues			
PAN	x	x	Peroxy Acetyl Nitrate
PAN2	x	x	PPN and other higher alkyl PAN analogues
PBZN	x		PAN analogues formed from Aromatic Aldehydes
MAPAN	x		PAN analogue formed from Methacrolein
Explicit and Lumped Molecule Reactive Organic Product Species			
HCHO	x	x	Formaldehyde
CCHO	x	x	Acetaldehyde
RCHO	x	x	Lumped C3+ Aldehydes
ACET	x		Acetone
MEK	x		Ketones and other non-aldehyde oxygenated products that react with OH radicals faster than 5×10^{-13} but slower than 5×10^{-12} cm^3 $molec^{-2}$ sec^{-1}
MEOH	x		Methanol
HCOOH	x		Formic Acid
CCOOH	x		Acetic Acid. Also used for peroxyacetic acid.
RCOOH	x		Higher organic acids and peroxy acids.
COOH	B		Methyl Hydroperoxide
ROOH	B	B	Lumped organic hydroperoxides with 2-4 carbons.
R6OOH	B		Lumped organic hydroperoxides with 5 or more carbons (other than those formed following OH addition to aromatic rings, which are represented separately).
RAOOH	B	B	Organic hydroperoxides formed following OH addition to aromatic rings, which is represented separately because of their probable role in SOA formation.
XOOH	A	A	Lumped organic hydroperoxide structure, used to represent the effect of photolysis of the hydroperoxide group in the SAPRC-99 peroxy radical representation (Carter, 2000).
GLY	x		Glyoxal
MGLY	x	x	Methyl Glyoxal
BACL	x		Biacetyl

Table A-1 (continued)

Name	Version [a] Unc	Cnd	Description
CRES	x	x	Phenols and Cresols.
NPHE	x		Nitrophenols
BALD	x		Aromatic aldehydes
MACR	x		Methacrolein
MVK	x		Methyl Vinyl Ketone
IPRD	x	x	Lumped isoprene product species
Aromatic unsaturated ring fragmentation products			
AFG1	x	x	Lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form radicals.
AFG2	x	x	Lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form non-radical products
AFG3	x		Lumped diunsaturatred dicarbonyl aromatic fragmentation product.
Lumped Parameter Products			
PROD2	x	x	Ketones and other non-aldehyde oxygenated products that react with OH radicals faster than 5×10^{-12} cm^3 $molec^{-2}$ sec^{-1}.
RNO3	x	x	Lumped Organic Nitrates
Steady state operators used to represent radical or product formation in peroxy radical reactions			
xHO2	B	B	Formation of HO_2 from alkoxy radicals formed in peroxy radical reactions with NO and NO_3 (100% yields) and RO_2 (50% yields)
xOH	B	B	As above, but for OH
xNO2	B	B	As above, but for NO_2
xMEO2	B		As above, but for MEO2
xMECO3	B	B	As above, but for MECO3
xRCO3	B	B	As above, but for RCO3
xMACO3	B		As above, but for MACO3
xTBUO	B		As above, but for TBUO
xCO	B		As above, but for CO
xHCHO	B	B	As above, but for HCHO
xCCHO	B	B	As above, but for CCHO
xRCHO	B	B	As above, but for RCHO
xACET	B		As above, but for ACET
xMEK	B		As above, but for MEK
xPROD2	B	B	As above, but for PROD2
xGLY	B		As above, but for GLY
xMGLY	B	B	As above, but for MGLY
xBACL	B		As above, but for BACL
xBALD	B		As above, but for BALD
xAFG1	B	B	As above, but for AFG1
xAFG2	B	B	As above, but for AFG2
xAFG3	B		As above, but for AFG3
xMACR	B		As above, but for MACR
xMVK	B		As above, but for MVK
xIPRD	B	B	As above, but for IPRD
xRNO3	B	B	As above, but for RNO3

Table A-1 (continued)

Name	Version [a] Unc	Cnd	Description
zRNO3	B	B	Formation of RNO3 in the RO_2 + NO, reaction, or formation of corresponding non-nitrate products (represented by PROD2) formed from alkoxy radicals formed in RO_2 + NO_3 and (in 50% yields) RO_2 + RO_2 reactions.
yROOH	B	B	Formation of ROOH following RO_2 + HO_2 reactions, or formation of H-shift disproportionation products (represented by MEK) in the RO_2 + RCO_3 and (in 50% yields) RO_2 + RO_2 reactions.
yR6OOH	B		As above, but with the RO_2 + HO_2 product represented by R6OOH and the H-shift products are represented by PROD2.
yRAOOH	B	B	As above, but with the RO_2 + HO_2 product represented by R6OOH
Non-Reacting Species			
CO2	x	x	Carbon Dioxide
SULF	x	x	Sulfates (SO_3 or H_2SO_4)
XC	x	x	Lost Carbon or carbon in unreactive products
XN	x	x	Lost Nitrogen or nitrogen in unreactive products
Primary Organics Represented explicitly			
CH4	x	x	Methane
ETHENE	x	x	Ethene
ISOPRENE	x	x	Isoprene
ACETYLEN	x		Acetylene
BENZENE	x		Benzene
Lumped model species used to represent emitted VOC species			
ALK1	x		Alkanes and other non-aromatic compounds that react only with OH, and have kOH (OH radical rate constant) between 2 and 5 x 10^2 ppm^{-1} min^{-1}. (Primarily ethane)
ALK2	x		Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 10^2 and 2.5 x 10^3 ppm^{-1} min^{-1}. (Primarily propane)
ALK3	x	x	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 2.5 x 10^3 and 5 x 10^3 ppm^{-1} min^{-1}. For CS07 this is used for all alkanes with kOH less than 5 x 10^3 ppm^{-1} min^{-1}.
ALK4	x	x	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 10^3 and 1 x 10^4 ppm^{-1} min^{-1}. For CS07 this is used for all alkanes with kOH greater than 5 x 10^3 ppm^{-1} min^{-1}.
ALK5	x		Alkanes and other non-aromatic compounds that react only with OH, and have kOH greater than 1 x 10^4 ppm-1 min-1.
ARO1	x	x	Aromatics with kOH < 2x10^4 ppm^{-1} min^{-1}.
ARO2	x	x	Aromatics with kOH > 2x10^4 ppm^{-1} min^{-1}.
OLE1	x	x	Alkenes (other than ethene) with kOH < 7x10^4 ppm^{-1} min^{-1}.
OLE2	x	x	Alkenes with kOH > 7x10^4 ppm^{-1} min^{-1}.
TERP	x	x	Terpenes
			Chlorine Species
Active Inorganic Species.			
CL2	x	x	Chlorine molecules
CLNO	x		ClNO

Table A-1 (continued)

Name	Version [a] Unc	Cnd	Description
CLONO	x		ClONO
CLNO2	x		ClNO2
CLONO2	x	x	ClONO2
HOCL	x		HOCl
HCL	x	x	Hydrochloric acid
Active Chlorine Radical Species			
CL	x	x	Chlorine atoms
CLO	x	x	ClO. Radicals
Steady state operators used to represent radical or product formation in peroxy radical reactions.			
xCL	B	B	Formation of Cl radicals from alkoxy radicals formed in peroxy radical reactions with NO and NO_3 (100% yields) and RO_2 (50% yields)
RO2CL	A		Peroxy Radical Operator representing NO to NO_2 conversion with Cl formation.
xCLCCHO	B		As above, but for CLCCHO
xCLACET	B		As above, but for CLACET
Active Organic Product Species			
CLCCHO	x		Chloroacetaldehyde (and other alpha-chloro aldehydes that are assumed to be similarly photoreactive)
CLACET	x		Chloroacetone (and other alpha-chloro ketones that are assumed to be similarly photoreactive)
Included for testing purposes only – not part of the standard mechanisms			
CHCL3			Chloroform (added for the chlorine mechanism test calculations because its reactions provides a continuous source of chlorine atoms).

[a] Mechanism versions: "Unc" = uncondensed and "Cnd" = condensed mechanisms. "x" = species in mechanism regardless of peroxy radical representation method. "A" = species in mechanism version using SAPRC-99 peroxy radical representation method A and "B" = species in mechanism version using standard SAPRC-07 peroxy radical representation method B.

Table A-2. Listing of reactions and rate parameters in the uncondensed SAPRC-07 mechanism used as the starting point for the condensed mechanisms developed for this work. From Carter (2010a).

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
Inorganic Reactions					
1	NO2 + HV = NO + O3P	Phot Set= NO2-06			
2	O3P + O2 + M = O3 + M	5.68E-34	5.68E-34	0.00	-2.60
3	O3P + O3 = #2 O2	8.34E-15	8.00E-12	4.09	
4	O3P + NO = NO2	1.64E-12	Falloff, F=0.60, N=1.00		
		0:	9.00E-32	0.00	-1.50
		inf:	3.00E-11	0.00	0.00
5	O3P + NO2 = NO + O2	1.03E-11	5.50E-12	-0.37	
6	O3P + NO2 = NO3	3.24E-12	Falloff, F=0.60, N=1.00		
		0:	2.50E-31	0.00	-1.80
		inf:	2.20E-11	0.00	-0.70
7	O3 + NO = NO2 + O2	2.02E-14	3.00E-12	2.98	
8	O3 + NO2 = O2 + NO3	3.72E-17	1.40E-13	4.91	
9	NO + NO3 = #2 NO2	2.60E-11	1.80E-11	-0.22	
10	NO + NO + O2 = #2 NO2	1.93E-38	3.30E-39	-1.05	
11	NO2 + NO3 = N2O5	1.24E-12	Falloff, F=0.35, N=1.33		
		0:	3.60E-30	0.00	-4.10
		inf:	1.90E-12	0.00	0.20
12	N2O5 = NO2 + NO3	5.69E-02	Falloff, F=0.35, N=1.33		
		0:	1.30E-03	21.86	-3.50
		inf:	9.70E+14	22.02	0.10
13	N2O5 + H2O = #2 HNO3	2.50E-22			
14	N2O5 + H2O + H2O = #2 HNO3 + H2O	1.80E-39			
	N2O5 + HV = NO3 + NO + O3P	(Slow)			
	N2O5 + HV = NO3 + NO2	(Slow)			
15	NO2 + NO3 = NO + NO2 + O2	6.75E-16	4.50E-14	2.50	
16	NO3 + HV = NO + O2	Phot Set= NO3NO-06			
17	NO3 + HV = NO2 + O3P	Phot Set= NO3NO2-6			
18	O3 + HV = O1D + O2	Phot Set= O3O1D-06			
19	O3 + HV = O3P + O2	Phot Set= O3O3P-06			
20	O1D + H2O = #2 OH	1.99E-10	1.63E-10	-0.12	
21	O1D + M = O3P + M	3.28E-11	2.38E-11	-0.19	
22	OH + NO = HONO	7.31E-12	Falloff, F=0.60, N=1.00		
		0:	7.00E-31	0.00	-2.60
		inf:	3.60E-11	0.00	-0.10
23	HONO + HV = OH + NO	Phot Set= HONO-06			
24	OH + HONO = H2O + NO2	5.95E-12	2.50E-12	-0.52	
25	OH + NO2 = HNO3	1.05E-11	Falloff, F=0.60, N=1.00		
		0:	1.80E-30	0.00	-3.00
		inf:	2.80E-11	0.00	0.00
26	OH + NO3 = HO2 + NO2	2.00E-11			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
27	OH + HNO3 = H2O + NO3	1.51E-13	k =k0+k3M/(1+k3M/k2)		
		k0:	2.40E-14	-0.91	0.00
		k2:	2.70E-17	-4.37	0.00
		k3:	6.50E-34	-2.65	0.00
28	HNO3 + HV = OH + NO2	Phot Set= HNO3			
29	OH + CO = HO2 + CO2	2.28E-13	k = k1 + k2 [M]		
		k1:	1.44E-13	0.00	0.00
		k2:	3.43E-33	0.00	0.00
30	OH + O3 = HO2 + O2	7.41E-14	1.70E-12	1.87	
31	HO2 + NO = OH + NO2	8.85E-12	3.60E-12	-0.54	
32	HO2 + NO2 = HNO4	1.12E-12	Falloff, F=0.60, N=1.00		
		0:	2.00E-31	0.00	-3.40
		inf:	2.90E-12	0.00	-1.10
33	HNO4 = HO2 + NO2	1.07E-01	Falloff, F=0.60, N=1.00		
		0:	3.72E-05	21.16	-2.40
		inf:	5.42E+15	22.20	-2.30
34	HNO4 + HV = #.61 {HO2 + NO2} + #.39 {OH + NO3}	Phot Set= HNO4-06			
35	HNO4 + OH = H2O + NO2 + O2	4.61E-12	1.30E-12	-0.76	
36	HO2 + O3 = OH + #2 O2	2.05E-15	2.03E-16	-1.38	4.57
37	HO2 + HO2 = HO2H + O2	2.84E-12	k = k1 + k2 [M]		
		k1:	2.20E-13	-1.19	0.00
		k2:	1.90E-33	-1.95	0.00
38	HO2 + HO2 + H2O = HO2H + O2 + H2O	6.09E-30	k = k1 + k2 [M]		
		k1:	3.08E-34	-5.56	0.00
		k2:	2.66E-54	-6.32	0.00
39	NO3 + HO2 = #.8 {OH + NO2 + O2} + #.2 {HNO3 + O2}	4.00E-12			
40	NO3 + NO3 = #2 NO2 + O2	2.41E-16	8.50E-13	4.87	
41	HO2H + HV = #2 OH	Phot Set= H2O2			
42	HO2H + OH = HO2 + H2O	1.80E-12	1.80E-12	0.00	
43	OH + HO2 = H2O + O2	1.10E-10	4.80E-11	-0.50	
44	OH + SO2 = HO2 + SULF	9.49E-13	Falloff, F=0.60, N=1.00		
		0:	3.30E-31	0.00	-4.30
		inf:	1.60E-12	0.00	0.00
45	OH + H2 = HO2 + H2O	7.02E-15	7.70E-12	4.17	
<u>Methyl peroxy and methoxy reactions</u>					
BR01	MEO2 + NO = NO2 + HCHO + HO2	7.64E-12	2.30E-12	-0.72	
BR02	MEO2 + HO2 = COOH + O2	4.65E-12	3.46E-13	-1.55	0.36
BR03	MEO2 + HO2 = HCHO + O2 + H2O	4.50E-13	3.34E-14	-1.55	-3.53
BR04	MEO2 + NO3 = HCHO + HO2 + NO2	1.30E-12			
BR05	MEO2 + MEO2 = MEOH + HCHO + O2	2.16E-13	6.39E-14	-0.73	-1.80
BR06	MEO2 + MEO2 = #2 {HCHO + HO2}	1.31E-13	7.40E-13	1.03	
<u>Active Peroxy Racical Operators</u>					
BR07	RO2C + NO = NO2	9.23E-12	2.60E-12	-0.76	
BR08	RO2C + HO2 =	7.63E-12	3.80E-13	-1.79	
BR09	RO2C + NO3 = NO2	2.30E-12			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BR10	RO2C + MEO2 = #.5 HO2 + #.75 HCHO + #.25 MEOH	2.00E-13			
BR11	RO2C + RO2C =	3.50E-14			
BR12	RO2XC + NO = XN	Same k as rxn BR07			
BR13	RO2XC + HO2 =	Same k as rxn BR08			
BR14	RO2XC + NO3 = NO2	Same k as rxn BR09			
BR15	RO2XC + MEO2 = #.5 HO2 + #.75 HCHO + #.25 MEOH	Same k as rxn BR10			
BR16	RO2XC + RO2C =	Same k as rxn BR11			
BR17	RO2XC + RO2XC =	Same k as rxn BR11			
Reactions of Acyl Peroxy Radicals, PAN, and PAN analogues					
BR18	MECO3 + NO2 = PAN	9.37E-12	Falloff, F=0.30, N=1.41		
		0:	2.70E-28	0.00	-7.10
		inf:	1.21E-11	0.00	-0.90
BR19	PAN = MECO3 + NO2	6.27E-04	Falloff, F=0.30, N=1.41		
		0:	4.90E-03	24.05	0.00
		inf:	4.00E+16	27.03	0.00
BR20	PAN + HV = #.6 {MECO3 + NO2} + #.4 {MEO2 + CO2 + NO3}	Phot Set= PAN			
BR21	MECO3 + NO = MEO2 + CO2 + NO2	1.97E-11	7.50E-12	-0.58	
BR22	MECO3 + HO2 = CCOOH + #.7 O2 + #.3 O3	1.36E-11	5.20E-13	-1.95	
BR23	MECO3 + NO3 = MEO2 + CO2 + NO2 + O2	Same k as rxn BR09			
BR24	MECO3 + MEO2 = #.1 {CCOOH + HCHO + O2} + #.9 {HCHO + HO2 + MEO2 + CO2}	1.06E-11	2.00E-12	-0.99	
BR25	MECO3 + RO2C = MEO2 + CO2	1.56E-11	4.40E-13	-2.13	
BR26	MECO3 + RO2XC = MEO2 + CO2	Same k as rxn BR25			
BR27	MECO3 + MECO3 = #2 {MEO2 + CO2} + O2	1.54E-11	2.90E-12	-0.99	
BR28	RCO3 + NO2 = PAN2	1.21E-11	1.21E-11	0.00	-1.07
BR29	PAN2 = RCO3 + NO2	5.48E-04	8.30E+16	27.70	
BR30	PAN2 + HV = #.6 {RCO3 + NO2} + #.4 {RO2C + xHO2 + yROOH + xCCHO + CO2 + NO3}	Phot Set= PAN			
BR31	RCO3 + NO = NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2	2.08E-11	6.70E-12	-0.68	
BR32	RCO3 + HO2 = RCOOH + #.75 O2 + #.25 O3	Same k as rxn BR22			
BR33	RCO3 + NO3 = NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2 + O2	Same k as rxn BR09			
BR34	RCO3 + MEO2 = HCHO + HO2 + RO2C + xHO2 + xCCHO + yROOH + CO2	Same k as rxn BR24			
BR35	RCO3 + RO2C = RO2C + xHO2 + xCCHO + yROOH + CO2	Same k as rxn BR25			
BR36	RCO3 + RO2XC = RO2C + xHO2 + xCCHO + yROOH + CO2	Same k as rxn BR25			
BR37	RCO3 + MECO3 = #2 CO2 + MEO2 + RO2C + xHO2 + yROOH + xCCHO + O2	Same k as rxn BR27			
BR38	RCO3 + RCO3 = #2 {RO2C + xHO2 + xCCHO + yROOH + CO2}	Same k as rxn BR27			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BR39	BZCO3 + NO2 = PBZN	1.37E-11			
BR40	PBZN = BZCO3 + NO2	4.27E-04	7.90E+16	27.82	
BR41	PBZN + HV = #.6 {BZCO3 + NO2} + #.4 {CO2 + BZO + RO2C + NO3}	Phot Set= PAN			
BR42	BZCO3 + NO = NO2 + CO2 + BZO + RO2C	Same k as rxn BR31			
BR43	BZCO3 + HO2 = RCOOH + #.75 O2 + #.25 O3 + #4 XC	Same k as rxn BR22			
BR44	BZCO3 + NO3 = NO2 + CO2 + BZO + RO2C + O2	Same k as rxn BR09			
BR45	BZCO3 + MEO2 = HCHO + HO2 + RO2C + BZO + CO2	Same k as rxn BR24			
BR46	BZCO3 + RO2C = RO2C + BZO + CO2	Same k as rxn BR25			
BR47	BZCO3 + RO2XC = RO2C + BZO + CO2	Same k as rxn BR25			
BR48	BZCO3 + MECO3 = #2 CO2 + MEO2 + BZO + RO2C	Same k as rxn BR27			
BR49	BZCO3 + RCO3 = #2 CO2 + RO2C + xHO2 + yROOH + xCCHO + BZO + RO2C	Same k as rxn BR27			
BR50	BZCO3 + BZCO3 = #2 {BZO + RO2C + CO2}	Same k as rxn BR27			
BR51	MACO3 + NO2 = MAPAN	Same k as rxn BR28			
BR52	MAPAN = MACO3 + NO2	4.79E-04	1.60E+16	26.80	
BR53	MAPAN + HV = #.6 {MACO3 + NO2} + #.4 {CO2 + HCHO + MECO3 + NO3}	Phot Set= PAN			
BR54	MACO3 + NO = NO2 + CO2 + HCHO + MECO3	Same k as rxn BR31			
BR55	MACO3 + HO2 = RCOOH + #.75 O2 + #.25 O3 + XC	Same k as rxn BR22			
BR56	MACO3 + NO3 = NO2 + CO2 + HCHO + MECO3 + O2	Same k as rxn BR09			
BR57	MACO3 + MEO2 = #2 HCHO + HO2 + CO2 + MECO3	Same k as rxn BR24			
BR58	MACO3 + RO2C = CO2 + HCHO + MECO3	Same k as rxn BR25			
BR59	MACO3 + RO2XC = CO2 + HCHO + MECO3	Same k as rxn BR25			
BR60	MACO3 + MECO3 = #2 CO2 + MEO2 + HCHO + MECO3 + O2	Same k as rxn BR27			
BR61	MACO3 + RCO3 = HCHO + MECO3 + RO2C + xHO2 + yROOH + xCCHO + #2 CO2	Same k as rxn BR27			
BR62	MACO3 + BZCO3 = HCHO + MECO3 + BZO + RO2C + #2 CO2	Same k as rxn BR27			
BR63	MACO3 + MACO3 = #2 {HCHO + MECO3 + CO2}	Same k as rxn BR27			
Other Organic Radical Species					
BR64	TBUO + NO2 = RNO3 + #-2 XC	2.40E-11			
BR65	TBUO = ACET + MEO2	1.18E+03	7.50E+14	16.20	
BR66	BZO + NO2 = NPHE	3.79E-11	2.30E-11	-0.30	
BR67	BZO + HO2 = CRES + #-1 XC	Same k as rxn BR08			
BR68	BZO = CRES + RO2C + xHO2 + #-1 XC	1.00E-03			
Steady-State Peroxy Radical operators (for formation of inorganic and radical products) [c]					
RO01	xHO2 = HO2	k is variable parameter: RO2RO			
RO02	xHO2 =	k is variable parameter: RO2XRO			
RO03	xOH = OH	k is variable parameter: RO2RO			
RO04	xOH =	k is variable parameter: RO2XRO			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
RO05	xNO2 = NO2	k is variable parameter: RO2RO			
RO06	xNO2 = XN	k is variable parameter: RO2XRO			
RO07	xMEO2 = MEO2	k is variable parameter: RO2RO			
RO08	xMEO2 = XC	k is variable parameter: RO2XRO			
RO09	xMECO3 = MECO3	k is variable parameter: RO2RO			
RO10	xMECO3 = #2 XC	k is variable parameter: RO2XRO			
RO11	xRCO3 = RCO3	k is variable parameter: RO2RO			
RO12	xRCO3 = #3 XC	k is variable parameter: RO2XRO			
RO13	xMACO3 = MACO3	k is variable parameter: RO2RO			
RO14	xMACO3 = #4 XC	k is variable parameter: RO2XRO			
RO15	xTBUO = TBUO	k is variable parameter: RO2RO			
RO16	xTBUO = #4 XC	k is variable parameter: RO2XRO			
RO17	xCO = CO	k is variable parameter: RO2RO			
RO18	xCO = XC	k is variable parameter: RO2XRO			
Explicit and Lumped Molecule Organic Products					
BP01	HCHO + HV = #2 HO2 + CO	Phot Set= HCHOR-06			
BP02	HCHO + HV = H2 + CO	Phot Set= HCHOM-06			
BP03	HCHO + OH = HO2 + CO + H2O	8.47E-12	5.40E-12	-0.27	
BP04	HCHO + HO2 = HOCOO	Assumed to be negligible			
BP07	HCHO + NO3 = HNO3 + HO2 + CO	6.06E-16	2.00E-12	4.83	
BP08	CCHO + OH = MECO3 + H2O	1.49E-11	4.40E-12	-0.73	
BP09	CCHO + HV = CO + HO2 + MEO2	Phot Set= CCHO_R			
BP10	CCHO + NO3 = HNO3 + MECO3	2.84E-15	1.40E-12	3.70	
BP11	RCHO + OH = #.965 RCO3 + #.035 {RO2C + xHO2 + xCO + xCCHO + yROOH}	1.97E-11	5.10E-12	-0.80	
BP12	RCHO + HV = RO2C + xHO2 + yROOH + xCCHO + CO + HO2	Phot Set= C2CHO			
BP13	RCHO + NO3 = HNO3 + RCO3	6.74E-15	1.40E-12	3.18	
BP14	ACET + OH = RO2C + xMECO3 + xHCHO + yROOH	1.91E-13	4.56E-14	-0.85	3.65
BP15	ACET + HV = #.62 MECO3 + #1.38 MEO2 + #.38 CO	Phot Set= ACET-06, qy= 0.5			
BP16	MEK + OH = #.967 RO2C + #.039 {RO2XC + zRNO3} + #.376 xHO2 + #.51 xMECO3 + #.074 xRCO3 + #.088 xHCHO + #.504 xCCHO + #.376 xRCHO + yROOH + #.3 XC	1.20E-12	1.30E-12	0.05	2.00
BP17	MEK + HV = MECO3 + RO2C + xHO2 + xCCHO + yROOH	Phot Set= MEK-06, qy= 0.175			
BP18	MEOH + OH = HCHO + HO2	9.02E-13	2.85E-12	0.69	
BP19	HCOOH + OH = HO2 + CO2	4.50E-13			
BP20	CCOOH + OH = #.509 MEO2 + #.491 RO2C + #.509 CO2 + #.491 xHO2 + #.491 xMGLY + #.491 yROOH + #-0.491 XC	7.26E-13	4.20E-14	-1.70	
BP21	RCOOH + OH = RO2C + xHO2 + #.143 CO2 + #.142 xCCHO + #.4 xRCHO + #.457 xBACL + yROOH + #-0.455 XC	1.20E-12			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BP22	COOH + OH = H2O + #.3 {HCHO + OH} + #.7 MEO2	7.40E-12	3.80E-12	-0.40	
BP23	COOH + HV = HCHO + HO2 + OH	Phot Set= COOH			
BP24	ROOH + OH = #.744 OH + #.251 RO2C + #.004 RO2XC + #.004 zRNO3 + #.744 RCHO + #.239 xHO2 + #.012 xOH + #.012 xHCHO + #.012 xCCHO + #.205 xRCHO + #.034 xPROD2 + #.256 yROOH + #-0.115 XC	2.50E-11			
BP25	ROOH + HV = RCHO + HO2 + OH	Phot Set= COOH			
BP26	R6OOH + OH = #.84 OH + #.222 RO2C + #.029 RO2XC + #.029 zRNO3 + #.84 PROD2 + #.09 xHO2 + #.041 xOH + #.02 xCCHO + #.075 xRCHO + #.084 xPROD2 + #.16 yROOH + #.02 XC	5.60E-11			
BP27	R6OOH + HV = OH + #.142 HO2 + #.782 RO2C + #.077 RO2XC + #.077 zRNO3 + #.085 RCHO + #.142 PROD2 + #.782 xHO2 + #.026 xCCHO + #.058 xRCHO + #.698 xPROD2 + #.858 yR6OOH + #.017 XC	Phot Set= COOH			
BP28	RAOOH + OH = #.139 OH + #.148 HO2 + #.589 RO2C + #.124 RO2XC + #.124 zRNO3 + #.074 PROD2 + #.147 MGLY + #.139 IPRD + #.565 xHO2 + #.024 xOH + #.448 xRCHO + #.026 xGLY + #.030 xMEK + #.252 xMGLY + #.073 xAFG1 + #.073 xAFG2 + #.713 yR6OOH + #2.674 XC	1.41E-10			
BP29	RAOOH + HV = OH + HO2 + #.5 {GLY + MGLY + AFG1 + AFG2} + #.5 XC	Phot Set= COOH			
BP30	GLY + HV = #2 {CO + HO2}	Phot Set= GLY-07R			
BP31	GLY + HV = HCHO + CO	Phot Set= GLY-07M			
BP32	GLY + OH = #.63 HO2 + #1.26 CO + #.37 RCO3 + #-.37 XC	1.10E-11			
BP33	GLY + NO3 = HNO3 + #.63 HO2 + #1.26 CO + #.37 RCO3 + #-.37 XC	1.02E-15	2.80E-12	4.72	
BP34	MGLY + HV = HO2 + CO + MECO3	Phot Set= MGLY-06			
BP35	MGLY + OH = CO + MECO3	1.50E-11			
BP36	MGLY + NO3 = HNO3 + CO + MECO3	2.53E-15	1.40E-12	3.77	
BP37	BACL + HV = #2 MECO3	Phot Set= BACL-07			
BP38	CRES + OH = #.2 BZO + #.8 {RO2C + xHO2 + yR6OOH} + #.25 xMGLY + #5.05 XC	4.03E-11	1.70E-12	-1.89	
BP39	CRES + NO3 = HNO3 + BZO + XC	1.40E-11			
BP40	NPHE + OH = BZO + XN	3.50E-12			
BP41	NPHE + HV = HONO + #6 XC	Phot Set= NO2-06, qy= 1.5e-3			
BP42	NPHE + HV = #6 XC + XN	Phot Set= NO2-06, qy= 1.5e-2			
BP43	BALD + OH = BZCO3	1.20E-11			
BP44	BALD + HV = #7 XC	Phot Set= BALD-06, qy= 0.06			
BP45	BALD + NO3 = HNO3 + BZCO3	2.73E-15	1.34E-12	3.70	

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
Lumped Unsaturated Aromatic Ring-Opening Products					
BP46	AFG1 + OH = #.217 MACO3 + #.723 RO2C + #.060 {RO2XC + zRNO3} + #.521 xHO2 + #.201 xMECO3 + #.334 xCO + #.407 xRCHO + #.129 xMEK + #.107 xGLY + #.267 xMGLY + #.783 yR6OOH + #.284 XC	7.40E-11			
BP47	AFG1 + O3 = #.826 OH + #.522 HO2 + #.652 RO2C + #.522 CO + #.174 CO2 + #.432 GLY + #.568 MGLY + #.652 xRCO3 + #.652 xHCHO + #.652 yR6OOH + #-.872 XC	9.66E-18			
BP48	AFG1 + HV = #1.023 HO2 + #.173 MEO2 + #.305 MECO3 + #.500 MACO3 + #.695 CO + #.195 GLY + #.305 MGLY + #.217 XC	Phot Set= AFG1			
BP49	AFG2 + OH = #.217 MACO3 + #.723 RO2C + #.060 {RO2XC + zRNO3} + #.521 xHO2 + #.201 xMECO3 + #.334 xCO + #.407 xRCHO + #.129 xMEK + #.107 xGLY + #.267 xMGLY + #.783 yR6OOH + #.284 XC	7.40E-11			
BP50	AFG2 + O3 = #.826 OH + #.522 HO2 + #.652 RO2C + #.522 CO + #.174 CO2 + #.432 GLY + #.568 MGLY + #.652 xRCO3 + #.652 xHCHO + #.652 yR6OOH + #-.872 XC	9.66E-18			
BP51	AFG2 + HV = PROD2 + #-1 XC	Phot Set= AFG1			
BP52	AFG3 + OH = #.206 MACO3 + #.733 RO2C + #.117 {RO2XC + zRNO3} + #.561 xHO2 + #.117 xMECO3 + #.114 xCO + #.274 xGLY + #.153 xMGLY + #.019 xBACL + #.195 xAFG1 + #.195 xAFG2 + #.231 xIPRD + #.794 yR6OOH + #.938 XC	9.35E-11			
BP53	AFG3 + O3 = #.471 OH + #.554 HO2 + #.013 MECO3 + #.258 RO2C + #.007 {RO2XC + zRNO3} + #.580 CO + #.190 CO2 + #.366 GLY + #.184 MGLY + #.350 AFG1 + #.350 AFG2 + #.139 AFG3 + #.003 MACR + #.004 MVK + #.003 IPRD + #.095 xHO2 + #.163 xRCO3 + #.163 xHCHO + #.095 xMGLY + #.264 yR6OOH + #-.575 XC	1.43E-17			
Isoprene Products					
BP54	MACR + OH = #.5 MACO3 + #.5 {RO2C + xHO2} + #.416 xCO + #.084 xHCHO + #.416 xMEK + #.084 xMGLY + #.5 yROOH + #-0.416 XC	2.84E-11	8.00E-12	-0.76	
BP55	MACR + O3 = #.208 OH + #.108 HO2 + #.1 RO2C + #.45 CO + #.117 CO2 + #.1 HCHO + #.9 MGLY + #.333 HCOOH + #.1 xRCO3 + #.1 xHCHO + #.1 yROOH + #-0.1 XC	1.28E-18	1.40E-15	4.17	
BP56	MACR + NO3 = #.5 {MACO3 + RO2C + HNO3 + xHO2 + xCO} + #.5 yROOH + #1.5 XC + #.5 XN	3.54E-15	1.50E-12	3.61	
BP57	MACR + O3P = RCHO + XC	6.34E-12			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BP58	MACR + HV = #.33 OH + #.67 HO2 + #.34 MECO3 + #.33 MACO3 + #.33 RO2C + #.67 CO + #.34 HCHO + #.33 xMECO3 + #.33 xHCHO + #.33 yROOH	Phot Set= MACR-06			
BP59	MVK + OH = #.975 RO2C + #.025 {RO2XC + zRNO3} + #.3 xHO2 + #.675 xMECO3 + #.3 xHCHO + #.675 xRCHO + #.3 xMGLY + yROOH + #-0.725 XC	1.99E-11	2.60E-12	-1.21	
BP60	MVK + O3 = #.164 OH + #.064 HO2 + #.05 {RO2C + xHO2} + #.475 CO + #.124 CO2 + #.05 HCHO + #.95 MGLY + #.351 HCOOH + #.05 xRCO3 + #.05 xHCHO + #.05 yROOH + #-0.05 XC	5.36E-18	8.50E-16	3.02	
BP61	MVK + NO3 = #4 XC + XN		(Slow)		
BP62	MVK + O3P = #.45 RCHO + #.55 MEK + #.45 XC	4.32E-12			
BP63	MVK + HV = #.4 MEO2 + #.6 CO + #.6 PROD2 + #.4 MACO3 + #-2.2 XC	Phot Set= MVK-06			
BP64	IPRD + OH = #.289 MACO3 + #.67 {RO2C + xHO2} + #.041 {RO2XC + zRNO3} + #.336 xCO + #.055 xHCHO + #.129 xCCHO + #.013 xRCHO + #.15 xMEK + #.332 xPROD2 + #.15 xGLY + #.174 xMGLY + #-0.504 XC + #.711 yR6OOH	6.19E-11			
BP65	IPRD + O3 = #.285 OH + #.4 HO2 + #.048 {RO2C + xRCO3} + #.498 CO + #.14 CO2 + #.124 HCHO + #.21 MEK + #.023 GLY + #.742 MGLY + #.1 HCOOH + #.372 RCOOH + #.047 xCCHO + #.001 xHCHO + #.048 yR6OOH + #-.329 XC	4.18E-18			
BP66	IPRD + NO3 = #.15 {MACO3 + HNO3} + #.799 {RO2C + xHO2} + #.051 {RO2XC + zRNO3} + #.572 xCO + #.227 xHCHO + #.218 xRCHO + #.008 xMGLY + #.572 xRNO3 + #.85 yR6OOH + #.278 XN + #-.815 XC	1.00E-13			
BP67	IPRD + HV = #1.233 HO2 + #.467 MECO3 + #.3 RCO3 + #1.233 CO + #.3 HCHO + #.467 CCHO + #.233 MEK + #-.233 XC	Phot Set= MACR-06			
<u>Lumped Parameter Organic Products</u>					
BP68	PROD2 + OH = #.472 HO2 + #.379 xHO2 + #.029 xMECO3 + #.049 xRCO3 + #.473 RO2C + #.071 RO2XC + #.071 zRNO3 + #.002 HCHO + #.211 xHCHO + #.001 CCHO + #.083 xCCHO + #.143 RCHO + #.402 xRCHO + #.115 xMEK + #.329 PROD2 + #.007 xPROD2 + #.528 yR6OOH + #.877 XC	1.55E-11			
BP69	PROD2 + HV = #.913 xHO2 + #.4 MECO3 + #.6 RCO3 + #1.59 RO2C + #.087 RO2XC + #.087 zRNO3 + #.303 xHCHO + #.163 xCCHO + #.78 xRCHO + yR6OOH + #-.091 XC	Phot Set= MEK-06, qy= 4.86e-3			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BP70	RNO3 + OH = #.189 HO2 + #.305 xHO2 + #.019 NO2 + #.313 xNO2 + #.976 RO2C + #.175 RO2XC + #.175 zRNO3 + #.011 xHCHO + #.429 xCCHO + #.001 RCHO + #.036 xRCHO + #.004 xACET + #.01 MEK + #.17 xMEK + #.008 PROD2 + #.031 xPROD2 + #.189 RNO3 + #.305 xRNO3 + #.157 yROOH + #.636 yR6OOH + #.174 XN + #.04 XC	7.20E-12			
BP71	RNO3 + HV = #.344 HO2 + #.554 xHO2 + NO2 + #.721 RO2C + #.102 RO2XC + #.102 zRNO3 + #.074 HCHO + #.061 xHCHO + #.214 CCHO + #.23 xCCHO + #.074 RCHO + #.063 xRCHO + #.008 xACET + #.124 MEK + #.083 xMEK + #.19 PROD2 + #.261 xPROD2 + #.066 yROOH + #.591 yR6OOH + #.396 XC	Phot Set= IC3ONO2			

Steady-State Peroxy Radical operators (for formation of organic product species)

PO01	xHCHO = HCHO	k is variable parameter: RO2RO
PO02	xHCHO = XC	k is variable parameter: RO2XRO
PO03	xCCHO = CCHO	k is variable parameter: RO2RO
PO04	xCCHO = #2 XC	k is variable parameter: RO2XRO
PO05	xRCHO = RCHO	k is variable parameter: RO2RO
PO06	xRCHO = #3 XC	k is variable parameter: RO2XRO
PO07	xACET = ACET	k is variable parameter: RO2RO
PO08	xACET = #3 XC	k is variable parameter: RO2XRO
PO09	xMEK = MEK	k is variable parameter: RO2RO
PO10	xMEK = #4 XC	k is variable parameter: RO2XRO
PO11	xPROD2 = PROD2	k is variable parameter: RO2RO
PO12	xPROD2 = #6 XC	k is variable parameter: RO2XRO
PO13	xGLY = GLY	k is variable parameter: RO2RO
PO14	xGLY = #2 XC	k is variable parameter: RO2XRO
PO15	xMGLY = MGLY	k is variable parameter: RO2RO
PO16	xMGLY = #3 XC	k is variable parameter: RO2XRO
PO17	xBACL = BACL	k is variable parameter: RO2RO
PO18	xBACL = #4 XC	k is variable parameter: RO2XRO
PO19	xBALD = BALD	k is variable parameter: RO2RO
PO20	xBALD = #7 XC	k is variable parameter: RO2XRO
PO21	xAFG1 = AFG1	k is variable parameter: RO2RO
PO22	xAFG1 = #5 XC	k is variable parameter: RO2XRO
PO23	xAFG2 = AFG2	k is variable parameter: RO2RO
PO24	xAFG2 = #5 XC	k is variable parameter: RO2XRO
PO25	xAFG3 = AFG3	k is variable parameter: RO2RO
PO26	xAFG3 = #7 XC	k is variable parameter: RO2XRO
PO27	xMACR = MACR	k is variable parameter: RO2RO
PO28	xMACR = #4 XC	k is variable parameter: RO2XRO
PO29	xMVK = MVK	k is variable parameter: RO2RO
PO30	xMVK = #4 XC	k is variable parameter: RO2XRO
PO31	xIPRD = IPRD	k is variable parameter: RO2RO
PO32	xIPRD = #5 XC	k is variable parameter: RO2XRO

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
PO33	xRNO3 = RNO3	k is variable parameter: RO2RO			
PO34	xRNO3 = #6 XC + XN	k is variable parameter: RO2XRO			
Steady-State Peroxy Radical Operator (for formation of organic nitrates in peroxy + NO reactions) [d]					
PO35	zRNO3 = RNO3 + #-1 XN	k is variable parameter: RO2NO			
PO36	zRNO3 = PROD2 + HO2	k is variable parameter: RO22NN			
PO37	zRNO3 = #6 XC	k is variable parameter: RO2XRO			
PO38	yROOH = ROOH + #-3 XC	k is variable parameter: RO2HO2			
Steady-State Peroxy Radical Operators (for formation of hydroperoxides in peroxy + HO2 reactions) [e]					
PO39	yROOH = MEK + #-4 XC	k is variable parameter: RO2RO2M			
PO40	yROOH =	k is variable parameter: RO2RO			
PO41	yR6OOH = R6OOH + #-6 XC	k is variable parameter: RO2HO2			
PO42	yR6OOH = PROD2 + #-6 XC	k is variable parameter: RO2RO2M			
PO43	yR6OOH =	k is variable parameter: RO2RO			
PO44	yRAOOH = RAOOH + #-8 XC	k is variable parameter: RO2HO2			
PO45	yRAOOH = PROD2 + #-6 XC	k is variable parameter: RO2RO2M			
PO46	yRAOOH =	k is variable parameter: RO2RO			
Explicitly Represented Primary Organics					
BE01	CH4 + OH = H2O + MEO2	6.62E-15	1.85E-12	3.36	
BE02	ETHENE + OH = RO2C + xHO2 + #1.61 xHCHO + #.195 xCCHO + yROOH	8.15E-12	Falloff, F=0.60, N=1.00		
			0: 1.00E-28	0.00	-4.50
			inf: 8.80E-12	0.00	-0.85
BE03	ETHENE + O3 = #.16 OH + #.16 HO2 + #.51 CO + #.12 CO2 + HCHO + #.37 HCOOH	1.68E-18	9.14E-15	5.13	
BE04	ETHENE + NO3 = RO2C + xHO2 + xRCHO + yROOH + #-1 XC + XN	2.24E-16	3.30E-12	5.72	2.00
BE05	ETHENE + O3P = #.8 HO2 + #.51 MEO2 + #.29 RO2C + #.51 CO + #.1 CCHO + #.29 xHO2 + #.278 xCO + #.278 xHCHO + #.012 xGLY + #.29 yROOH + #.2 XC	7.43E-13	1.07E-11	1.59	
BE06	ISOPRENE + OH = #.986 RO2C + #.093 {RO2XC + zRNO3} + #.907 xHO2 + #.624 xHCHO + #.23 xMACR + #.32 xMVK + #.357 xIPRD + yR6OOH + #-0.167 XC	9.96E-11	2.54E-11	-0.81	
BE07	ISOPRENE + O3 = #.266 OH + #.066 HO2 + #.192 RO2C + #.008 {RO2XC + zRNO3} + #.275 CO + #.122 CO2 + #.4 HCHO + #.1 PROD2 + #.39 MACR + #.16 MVK + #.15 IPRD + #.204 HCOOH + #.192 {xMACO3 + xHCHO} + #.2 yR6OOH + #-0.559 XC	1.34E-17	7.86E-15	3.80	
BE08	ISOPRENE + NO3 = #.936 RO2C + #.064 {RO2XC + zRNO3} + #.749 xHO2 + #.187 xNO2 + #.936 xIPRD + yR6OOH + #-0.064 XC + #.813 XN	6.81E-13	3.03E-12	0.89	
BE09	ISOPRENE + O3P = #.25 MEO2 + #.24 RO2C + #.01 {RO2XC + zRNO3} + #.75 PROD2 + #.24 xMACO3 + #.24 xHCHO + #.25 yR6OOH + #-1.01 XC	3.50E-11			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BE10	ACETYLEN + OH = #.7 OH + #.3 HO2 + #.3 CO + #.7 GLY + #.3 HCOOH	7.56E-13	Falloff, F=0.60, N=1.00		
BE11	ACETYLEN + O3 = #.5 OH + #1.5 HO2 + #1.5 CO + #.5 CO2	1.16E-20	1.00E-14	8.15	
BE12	BENZENE + OH = #.116 OH + #.29 {RO2C + xHO2} + #.024 {RO2XC + zRNO3} + #.57 {HO2 + CRES} + #.116 AFG3 + #.290 xGLY + #.029 xAFG1 + #.261 xAFG2 + #.314 yRAOOH + #-.976 XC	1.22E-12	2.33E-12	0.38	
Reactions of Lumped Model Species Used to Represent Emitted VOCs [f]					
BL01	ALK1 + OH = xHO2 + RO2C + xCCHO + yROOH	2.54E-13	1.34E-12	0.99	2.00
BL02	ALK2 + OH = #.965 xHO2 + #.965 RO2C + #.035 RO2XC + #.035 zRNO3 + #.261 xRCHO + #.704 xACET + yROOH + #-.105 XC	1.11E-12	1.49E-12	0.17	2.00
BL03	ALK3 + OH = #.695 xHO2 + #.236 xTBUO + #1.253 RO2C + #.07 RO2XC + #.07 zRNO3 + #.026 xHCHO + #.445 xCCHO + #.122 xRCHO + #.024 xACET + #.332 xMEK + #.983 yROOH + #.017 yR6OOH + #-.046 XC	2.31E-12	1.51E-12	-0.25	
BL04	ALK4 + OH = #.83 xHO2 + #.01 xMEO2 + #.011 xMECO3 + #1.763 RO2C + #.149 RO2XC + #.149 zRNO3 + #.002 xCO + #.029 xHCHO + #.438 xCCHO + #.236 xRCHO + #.426 xACET + #.106 xMEK + #.146 xPROD2 + yR6OOH + #-.119 XC	4.34E-12	3.75E-12	-0.09	
BL05	ALK5 + OH = #.647 xHO2 + #1.605 RO2C + #.353 RO2XC + #.353 zRNO3 + #.04 xHCHO + #.106 xCCHO + #.209 xRCHO + #.071 xACET + #.086 xMEK + #.407 xPROD2 + yR6OOH + #2.004 XC	9.40E-12	2.70E-12	-0.74	
BL06	OLE1 + OH = #.904 xHO2 + #.001 xMEO2 + #1.138 RO2C + #.095 RO2XC + #.095 zRNO3 + #.7 xHCHO + #.301 xCCHO + #.47 xRCHO + #.005 xACET + #.026 xMACR + #.008 xMVK + #.006 xIPRD + #.119 xPROD2 + #.413 yROOH + #.587 yR6OOH + #.822 XC	3.29E-11	6.18E-12	-1.00	
BL07	OLE1 + O3 = #.116 HO2 + #.04 xHO2 + #.193 OH + #.104 MEO2 + #.063 RO2C + #.004 RO2XC + #.004 zRNO3 + #.368 CO + #.125 CO2 + #.5 HCHO + #.147 CCHO + #.007 xCCHO + #.353 RCHO + #.031 xRCHO + #.002 xACET + #.006 MEK + #.185 HCOOH + #.022 CCOOH + #.112 RCOOH + #.189 PROD2 + #.007 yROOH + #.037 yR6OOH + #.69 XC	1.09E-17	3.15E-15	3.38	
BL08	OLE1 + NO3 = #.824 xHO2 + #1.312 RO2C + #.176 RO2XC + #.176 zRNO3 + #.009 xCCHO + #.002 xRCHO + #.024 xACET + #.546 xRNO3 + #.413 yROOH + #.587 yR6OOH + #.454 XN + #.572 XC	1.44E-14	4.73E-13	2.08	
BL09	OLE1 + O3P = #.45 RCHO + #.437 MEK + #.113 PROD2 + #1.224 XC	5.02E-12	1.49E-11	0.65	

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BL10	OLE2 + OH = #.914 xHO2 + #.966 RO2C + #.086 RO2XC + #.086 zRNO3 + #.209 xHCHO + #.788 xCCHO + #.481 xRCHO + #.136 xACET + #.076 xMEK + #.027 xMACR + #.002 xMVK + #.037 xIPRD + #.022 xPROD2 + #.357 yROOH + #.643 yR6OOH + #.111 XC	6.42E-11	1.26E-11	-0.97	
BL11	OLE2 + O3 = #.093 HO2 + #.039 xHO2 + #.423 OH + #.29 MEO2 + #.147 xMECO3 + #.008 xRCO3 + #.2 RO2C + #.003 RO2XC + #.003 zRNO3 + #.297 CO + #.162 CO2 + #.152 HCHO + #.108 xHCHO + #.428 CCHO + #.067 xCCHO + #.315 RCHO + #.018 xRCHO + #.048 ACET + #.031 MEK + #.001 xMEK + #.033 HCOOH + #.061 CCOOH + #.222 RCOOH + #.028 MACR + #.021 MVK + #.042 PROD2 + #.069 yROOH + #.128 yR6OOH + #.125 XC	1.24E-16	8.14E-15	2.49	
BL12	OLE2 + NO3 = #.423 xHO2 + #.409 xNO2 + #.033 xMEO2 + #1.185 RO2C + #.136 RO2XC + #.136 zRNO3 + #.074 xHCHO + #.546 xCCHO + #.154 xRCHO + #.11 xACET + #.002 xMEK + #.026 xMVK + #.007 xIPRD + #.322 xRNO3 + #.357 yROOH + #.643 yR6OOH + #.269 XN + #.114 XC	7.85E-13	2.20E-13	-0.76	
BL13	OLE2 + O3P = #.014 HO2 + #.007 xHO2 + #.007 xMACO3 + #.013 RO2C + #.001 RO2XC + #.001 zRNO3 + #.006 xCO + #.074 RCHO + #.709 MEK + #.006 xMACR + #.202 PROD2 + #.014 yROOH + #.666 XC	2.07E-11	1.43E-11	-0.22	
BL14	ARO1 + OH = #.166 HO2 + #.482 xHO2 + #.284 OH + #.482 RO2C + #.068 RO2XC + #.068 zRNO3 + #.218 xGLY + #.138 xMGLY + #.166 CRES + #.049 xBALD + #.164 xAFG1 + #.193 xAFG2 + #.284 AFG3 + #.077 xPROD2 + #.403 yRAOOH + #.147 yR6OOH + #.002 XC	6.15E-12			
BL15	ARO2 + OH = #.108 HO2 + #.58 xHO2 + #.202 OH + #.58 RO2C + #.11 RO2XC + #.11 zRNO3 + #.116 xGLY + #.286 xMGLY + #.104 xBACL + #.108 CRES + #.039 xBALD + #.217 xAFG1 + #.21 xAFG2 + #.202 AFG3 + #.08 xAFG3 + #.035 xPROD2 + #.089 yR6OOH + #.601 yRAOOH + #1.486 XC	2.57E-11			
BL16	TERP + OH = #.759 xHO2 + #.042 xRCO3 + #1.147 RO2C + #.2 RO2XC + #.2 zRNO3 + #.001 xCO + #.264 xHCHO + #.533 xRCHO + #.036 xACET + #.005 xMEK + #.009 xMGLY + #.014 xBACL + #.002 xMVK + #.001 xIPRD + #.255 xPROD2 + yR6OOH + #5.056 XC	7.98E-11	1.87E-11	-0.86	

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BL17	TERP + O3 = #.052 HO2 + #.067 xHO2 + #.585 OH + #.126 xMECO3 + #.149 xRCO3 + #.875 RO2C + #.203 RO2XC + #.203 zRNO3 + #.166 CO + #.019 xCO + #.045 CO2 + #.079 HCHO + #.15 xHCHO + #.22 xRCHO + #.165 xACET + #.004 MEK + #.107 HCOOH + #.043 RCOOH + #.001 xGLY + #.002 xMGLY + #.055 xBACL + #.001 xMACR + #.001 xIPRD + #.409 PROD2 + #.545 yR6OOH + #3.526 XC	6.99E-17	9.57E-16	1.56	
BL18	TERP + NO3 = #.162 xHO2 + #.421 xNO2 + #.019 xRCO3 + #1.509 RO2C + #.397 RO2XC + #.397 zRNO3 + #.01 xCO + #.017 xHCHO + #.001 xCCHO + #.509 xRCHO + #.175 xACET + #.001 xMGLY + #.003 xMACR + #.001 xMVK + #.002 xIPRD + #.163 xRNO3 + yR6OOH + #.416 XN + #4.473 XC	6.53E-12	1.28E-12	-0.97	
BL19	TERP + O3P = #.147 RCHO + #.853 PROD2 + #4.441 XC	3.71E-11			
	Chlorine Mechanism				
	Base Chlorine Mechanism				
CI01	CL2 + HV = #2 CL	Phot Set= CL2			
	CL + O2 + M = CLO2. + M	(Ignored)			
	CLO2. + M = CL + O2 + M	(Ignored)			
CI02	CL + NO + M = CLNO + M	7.60E-32	7.60E-32	0.00	-1.80
CI03	CLNO + HV = CL + NO	Phot Set= CLNO-06			
CI04	CL + NO2 = CLONO	1.60E-11	Falloff, F=0.60, N=1.00		
		0:	1.30E-30	0.00	-2.00
		inf:	1.00E-10	0.00	-1.00
CI05	CL + NO2 = CLNO2	3.52E-12	Falloff, F=0.60, N=1.00		
		0:	1.80E-31	0.00	-2.00
		inf:	1.00E-10	0.00	-1.00
CI06	CLONO + HV = CL + NO2	Phot Set= CLONO			
CI07	CLNO2 + HV = CL + NO2	Phot Set= CLNO2			
CI08	CL + HO2 = HCL + O2	3.44E-11	3.44E-11	0.00	-0.56
CI09	CL + HO2 = CLO + OH	9.41E-12	9.41E-12	0.00	2.10
CI10	CL + O3 = CLO + O2	1.22E-11	2.80E-11	0.50	
CI11	CL + NO3 = CLO + NO2	2.40E-11			
CI12	CLO + NO = CL + NO2	1.66E-11	6.20E-12	-0.59	
CI13	CLO + NO2 = CLONO2	2.29E-12	Falloff, F=0.60, N=1.00		
		0:	1.80E-31	0.00	-3.40
		inf:	1.50E-11	0.00	-1.90
CI14	CLONO2 + HV = CLO + NO2	Phot Set= CLONO2-1			
CI15	CLONO2 + HV = CL + NO3	Phot Set= CLONO2-2			
CI16	CLONO2 = CLO + NO2	4.12E-04	Falloff, F=0.60, N=1.00		
		0:	4.48E-05	24.90	-1.00
		inf:	3.71E+15	24.90	3.50
CI17	CL + CLONO2 = CL2 + NO3	1.01E-11	6.20E-12	-0.29	
CI18	CLO + HO2 = HOCL + O2	6.83E-12	2.20E-12	-0.68	
CI19	HOCL + HV = OH + CL	Phot Set= HOCL-06			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
CI20	CLO + CLO = #.29 CL2 + #1.42 CL + O2	1.82E-14	1.25E-11	3.89	
CI21	OH + HCL = H2O + CL	7.90E-13	1.70E-12	0.46	
CI22	CL + H2 = HCL + HO2	1.77E-14	3.90E-11	4.59	
Chlorine reactions with common organic products					
CP01	HCHO + CL = HCL + HO2 + CO	7.33E-11	8.10E-11	0.06	
CP02	CCHO + CL = HCL + MECO3	8.00E-11	8.00E-11		
CP03	MEOH + CL = HCL + HCHO + HO2	5.50E-11	5.50E-11	0.00	
CP04	RCHO + CL = HCL + #.9 RCO3 + #.1 {RO2C + xCCHO + xCO + xHO2 + yROOH}	1.23E-10			
CP05	ACET + CL = HCL + RO2C + xHCHO + xMECO3 + yROOH	2.75E-12	7.70E-11	1.99	
CP06	MEK + CL = HCL + #.975 RO2C + #.039 RO2XC + #.039 zRNO3 + #.84 xHO2 + #.085 xMECO3 + #.036 xRCO3 + #.065 xHCHO + #.07 xCCHO + #.84 xRCHO + yROOH + #.763 XC	3.60E-11			
CP07	RNO3 + CL = HCL + #.038 NO2 + #.055 HO2 + #1.282 RO2C + #.202 RO2XC + #.202 zRNO3 + #.009 RCHO + #.018 MEK + #.012 PROD2 + #.055 RNO3 + #.159 xNO2 + #.547 xHO2 + #.045 xHCHO + #.300 xCCHO + #.020 xRCHO + #.003 xACET + #.041 xMEK + #.046 xPROD2 + #.547 xRNO3 + #.908 yR6OOH + #.201 XN + #-.149 XC	1.92E-10			
CP08	PROD2 + CL = HCL + #.314 HO2 + #.680 RO2C + #.116 RO2XC + #.116 zRNO3 + #.198 RCHO + #.116 PROD2 + #.541 xHO2 + #.007 xMECO3 + #.022 xRCO3 + #.237 xHCHO + #.109 xCCHO + #.591 xRCHO + #.051 xMEK + #.040 xPROD2 + #.686 yR6OOH + #1.262 XC	2.00E-10			
CP09	GLY + CL = HCL + #.63 HO2 + #1.26 CO + #.37 RCO3 + #-.37 XC	7.33E-11	8.10E-11	0.06	
CP10	MGLY + CL = HCL + CO + MECO3	8.00E-11			
CP11	CRES + CL = HCL + xHO2 + xBALD + yR6OOH	6.20E-11			
CP12	BALD + CL = HCL + BZCO3	8.00E-11			
CP13	ROOH + CL = HCL + #.414 OH + #.588 RO2C + #.414 RCHO + #.104 xOH + #.482 xHO2 + #.106 xHCHO + #.104 xCCHO + #.197 xRCHO + #.285 xMEK + #.586 yROOH + #-0.287 XC	1.66E-10			
CP14	R6OOH + CL = HCL + #.145 OH + #1.078 RO2C + #.117 {RO2XC + zRNO3} + #.145 PROD2 + #.502 xOH + #.237 xHO2 + #.186 xCCHO + #.676 xRCHO + #.28 xPROD2 + #.855 yR6OOH + #.348 XC	3.00E-10			
CP15	RAOOH + CL = #.404 HCL + #.139 OH + #.148 HO2 + #.589 RO2C + #.124 RO2XC + #.124 zRNO3 + #.074 PROD2 + #.147 MGLY + #.139 IPRD + #.565 xHO2 + #.024 xOH + #.448 xRCHO + #.026 xGLY + #.030 xMEK + #.252 xMGLY + #.073 xAFG1 + #.073 xAFG2 + #.713 yR6OOH + #2.674 XC	4.29E-10			

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
CP16	MACR + CL = #.25 HCL + #.165 MACO3 + #.802 RO2C + #.033 RO2XC + #.033 zRNO3 + #.802 xHO2 + #.541 xCO + #.082 xIPRD + #.18 xCLCCHO + #.541 xCLACET + #.835 yROOH + #.208 XC	3.85E-10			
CP17	MVK + CL = #1.283 RO2C + #.053 {RO2XC + zRNO3} + #.322 xHO2 + #.625 xMECO3 + #.947 xCLCCHO + yROOH + #.538 XC	2.32E-10			
CP18	IPRD + CL = #.401 HCL + #.084 HO2 + #.154 MACO3 + #.73 RO2C + #.051 RO2XC + #.051 zRNO3 + #.042 AFG1 + #.042 AFG2 + #.712 xHO2 + #.498 xCO + #.195 xHCHO + #.017 xMGLY + #.009 xAFG1 + #.009 xAFG2 + #.115 xIPRD + #.14 xCLCCHO + #.42 xCLACET + #.762 yR6OOH + #.709 XC	4.12E-10			
Reactions of Chlorinated Organic Product Species					
CP19	CLCCHO + HV = HO2 + CO + RO2C + xCL + xHCHO + yROOH	Phot Set= CLCCHO			
CP20	CLCCHO + OH = RCO3 + #-1 XC	3.10E-12			
CP21	CLCCHO + CL = HCL + RCO3 + #-1 XC	1.29E-11			
CP22	CLACET + HV = MECO3 + RO2C + xCL + xHCHO + yROOH	Phot Set= CLACET, qy= 0.50			
Steady-State Peroxy Radical operators (for formation of chlorine radical and product species) [c]					
CP23	xCL = CL	k is variable parameter: RO2RO			
CP24	xCL =	k is variable parameter: RO2XRO			
CP25	xCLCCHO = CLCCHO	k is variable parameter: RO2RO			
CP26	xCLCCHO = #2 XC	k is variable parameter: RO2XRO			
CP27	xCLACET = CLACET	k is variable parameter: RO2RO			
CP28	xCLACET = #3 XC	k is variable parameter: RO2XRO			
Chlorine Reactions with Explicitly Represented Primary Organics					
CE01	CH4 + CL = HCL + MEO2	1.02E-13	7.30E-12	2.54	
CE02	ETHENE + CL = #2 RO2C + xHO2 + xHCHO + CLCHO	1.04E-10	Falloff, F=0.60, N=1.00		
CE03	ISOPRENE + CL = #.15 HCL + #1.168 RO2C + #.085 RO2XC + #.085 zRNO3 + #.738 xHO2 + #.177 xCL + #.275 xHCHO + #.177 xMVK + #.671 xIPRD + #.067 xCLCCHO + yR6OOH + #.018 XC	4.80E-10			
CE04	ACETYLEN + CL = HO2 + CO + XC	4.97E-11	Falloff, F=0.60, N=1.00		
			0:	5.20E-30	0.00 -2.40
			inf:	2.20E-10	0.00 0.00
Chlorine Reactions of Lumped Model Species Used to Represent Emitted VOCs [f]					
BC01	ALK1 + CL = xHO2 + RO2C + HCL + xCCHO + yROOH	5.95e-11	8.30e-11	0.20	
BC02	ALK2 + CL = #.97 xHO2 + #.97 RO2C + #.03 RO2XC + #.03 zRNO3 + HCL + #.482 xRCHO + #.488 xACET + yROOH + #-.09 XC	1.37e-10	1.20e-10	-0.08	

Table A-2 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BC03	ALK3 + CL = #.835 xHO2 + #.094 xTBUO + #1.361 RO2C + #.07 RO2XC + #.07 zRNO3 + HCL + #.078 xHCHO + #.34 xCCHO + #.343 xRCHO + #.075 xACET + #.253 xMEK + #.983 yROOH + #.017 yR6OOH + #.18 XC	1.86e-10			
BC04	ALK4 + CL = #.827 xHO2 + #.003 xMEO2 + #.004 xMECO3 + #1.737 RO2C + #.165 RO2XC + #.165 zRNO3 + HCL + #.003 xCO + #.034 xHCHO + #.287 xCCHO + #.412 xRCHO + #.247 xACET + #.076 xMEK + #.13 xPROD2 + yR6OOH + #.327 XC	2.63e-10			
BC05	ALK5 + CL = #.647 xHO2 + #1.541 RO2C + #.352 RO2XC + #.352 zRNO3 + HCL + #.022 xHCHO + #.08 xCCHO + #.258 xRCHO + #.044 xACET + #.041 xMEK + #.378 xPROD2 + yR6OOH + #2.368 XC	4.21e-10			
BC06	OLE1 + CL = #.902 xHO2 + #1.42 RO2C + #.098 RO2XC + #.098 zRNO3 + #.308 HCL + #.025 xHCHO + #.146 xCCHO + #.051 xRCHO + #.188 xMACR + #.014 xMVK + #.027 xIPRD + #.225 xCLCCHO + #.396 xCLACET + #.413 yROOH + #.587 yR6OOH + #1.361 XC	3.55e-10			
BC07	OLE2 + CL = #.447 xHO2 + #.448 xCL + #.001 xMEO2 + #1.514 RO2C + #.104 RO2XC + #.104 zRNO3 + #.263 HCL + #.228 xHCHO + #.361 xCCHO + #.3 xRCHO + #.081 xACET + #.04 xMEK + #.049 xMACR + #.055 xMVK + #.179 xIPRD + #.012 xCLCCHO + #.18 xCLACET + #.357 yROOH + #.643 yR6OOH + #.247 XC	3.83e-10			
BC08	ARO1 + CL = #.88 xHO2 + #.88 RO2C + #.12 RO2XC + #.12 zRNO3 + #.671 xBALD + #.21 xPROD2 + #.323 XC	1.00e-10			
BC09	ARO2 + CL = #.842 xHO2 + #.842 RO2C + #.158 RO2XC + #.158 zRNO3 + #.618 xBALD + #.224 xPROD2 + #2.382 XC	2.18e-10			
BC10	TERP + CL = #.252 xHO2 + #.068 xCL + #.034 xMECO3 + #.05 xRCO3 + #.016 xMACO3 + #2.258 RO2C + #.582 RO2XC + #.582 zRNO3 + #.548 HCL + #.035 xCO + #.158 xHCHO + #.185 xRCHO + #.274 xACET + #.007 xGLY + #.003 xBACL + #.003 xMVK + #.158 xIPRD + #.006 xAFG1 + #.006 xAFG2 + #.001 xAFG3 + #.109 xCLCCHO + yR6OOH + #3.543 XC	5.46e-10			
	Reactions of Chloroform (used for test calculations only)				
TS01	CHCL3 + OH = xCL + RO2C + yROOH + XC	1.06e-13	5.67e-13	1.00	2.00
TS02	CHCL3 + CL = HCL + xCL + RO2C + yROOH + XC	1.22e-13	3.30e-12	1.97	

Table A-2 (continued)

[a] Format of reaction listing: "=" separates reactants from products; "*#number*" indicates stoichiometric coefficient, "*#coefficient* {*product list*}" means that the stoichiometric coefficient is applied to all the products listed.

[b] Except as indicated, the rate constants are given by $k(T) = A \cdot (T/300)^{B} \cdot e^{-Ea/RT}$, where the units of k and A are cm^3 $molec^{-1}$ s^{-1}, Ea are kcal mol^{-1}, T is ^oK, and R=0.0019872 kcal mol^{-1} deg^{-1}. The following special rate constant expressions are used:

Phot Set = *name*: The absorption cross sections and (if applicable) quantum yields for the photolysis reaction are documented by Carter (2010a) and are available at http://www.cert.ucr.edu/~carter/SAPRC, where "*name*" indicates the photolysis set used. If a "qy=*number*" notation is given, the number given is the overall quantum yield, which is assumed to be wavelength independent.

Falloff: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = \{k0(T)\cdot[M]/[1 + k0(T)\cdot[M]/kinf(T)]\}\cdot F^{Z}$, where $Z = \{1 + [\log10\{k0(T)\cdot[M])/kinf(T)\}/N]^2\}^{-1}$, [M] is the total pressure in molecules cm^{-3}, F and N are as indicated on the table, and the temperature dependences of k0 and kinf are as indicated on the table.

k = k0+k3M(1+k3M/k2): The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k0(T) + k3(T)\cdot[M] \cdot(1 + k3(T)\cdot[M]/k2(T))$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k0, k2 and k3 are as indicated on the table.

k = k1 + k2 [M]: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k1(T) + k2(T)\cdot[M]$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k1, and k2 are as indicated on the table.

Same K as Rxn xx: Uses the same rate constant as the reaction in the base mechanism with the same label.

[c] The xPROD chemical operator species are used to represent the formation of radicals and products from alkoxy radicals formed in the reactions of peroxy radicals with NO, NO_3, acyl peroxy radicals, and, in ~50% yields, with other peroxy radicals. These products are not formed when peroxy radicals react with HO_2, and, in ~50% yields, with other peroxy radicals, since those reactions are assumed not form alkoxy radicals, but instead form hydroperoxides or H-shift disproportion products that are represented by separate yROOH chemical operator species, discussed in a separate footnote. The reactions of peroxy radicals with other peroxy radicals are assumed to form alkoxy radicals 50% of the time, so the products from alkoxy radical reactions are represented as being formed in 50% yields in these reactions. The consumption and products formed from these species can be represented in several ways. The most straightforward method is to include a reaction for each of the types of peroxy radical reactions, as follows:

xPROD + NO → NO + PROD
xPROD + HO2 → HO2
xPROD + NO3 → NO3 + PROD
xPROD + MECO3 → MECO3 + PROD (& similar reactions for RCO3, BZCO3, and MACO3)
xPROD + MEO2 → MEO2 + 1/2 PROD
xPROD + RO2C → RO2C + 1/2 PROD (& a similar reaction for RO2XC)

where "PROD" represents the product species for the operator (e.g., HO2 for xHO2). The rate constants for these reactions should be the same as the rate constant for the corresponding reactions of RO2C or RO2XC. This is a somewhat cumbersome method because it requires 9 reactions for each of the many xPROD species. An alternative method, implemented in this table, uses the coefficient "RO2RO" to determine the rate of formation of the product species and "RO2XRO" to represent processes where the product is not formed. These are calculated as follows, where the k(RO2+..)'s refer to the rate constants for the reactions of RO2C or RO2XC with the indicated reactant.

Table A-2 (continued)

RO2RO = k(RO2+NO)[NO] + k(RO2+NO3)[NO3] + k(RO2+MECO3){[MECO3]+[RCO3]+ [BZCO3]+[MACO3]) + 0.5 k(RO2+MEO2)[MEO2] + 0.5 k(RO2+RO2) {[RO2C]+[RO2XC])
RO2XRO = k(RO2+HO2)[HO2] + 0.5 k(RO2+MEO2)[MEO2] + 0.5 k(RO2+RO2){[RO2C]+ [RO2XC])

The steady state approximation must be used for these operators when this representation is used, and the operators must not be allowed to be diluted or transported.

[d] The zRNO3 chemical operator species is used to represent the formation organic nitrates formed when peroxy radicals react with NO, or formation of radicals and products from alkoxy radicals formed in the reactions of peroxy radicals with NO_3, acyl peroxy radicals, and (in ~50% yields) with other peroxy radicals. These products are not formed when peroxy radicals react with HO_2 and (in the other ~50% of the time) with other peroxy radicals, since those reactions are assumed not form organic nitrates or alkoxy radicals, but instead form hydroperoxides or H-shift disproportion products that are represented by separate yROOH chemical operator species, discussed in a separate footnote. At present the mechanism has only one zRNO3 operator to correspond to the single lumped organic nitrate model species, but other such operators can be added if it is desired to have separate organic nitrate model species, such as, for example, those to represent semi-volatile organic nitrates that may contribute to SOA. In the case of zRNO3, the products resulting if alkoxy radicals are formed in the RCO3 or RO2 reactions would depend on reactant and individual radicals, and are approximated by PROD2 and HO2 (as might occur following the reaction of a peroxy radical with O_2 to form HO_2 and a ketone species). As with the xPROD species, the consumption and products formed from these species can be represented in several ways, with the most straightforward method being to include a reaction for each of the types of peroxy radical reactions, as follows:

zRNO3 + NO → NO + RNO3
zRNO3 + HO2 → HO2
zRNO3 + NO3 → NO3 + PROD2 + HO2
zRNO3 + MECO3 → MECO3 + PROD2 + HO2 (& similar reactions for RCO3, BZCO3, and MACO3)
zRNO3 + MEO2 → MEO2 + 1/2 {PROD2 + HO2}
zRNO3 + RO2C → RO2C + 1/2 {PROD2 + HO2} (& a similar reaction for RO2XC)

The rate constants for these reactions should be the same as the rate constant for the corresponding reactions of RO2C or RO2XC. As with xPROD, an alternative method, requiring fewer reactions, is implemented in this table. In this case, the coefficient "RO2NO" is used to determine the rate of formation of organic nitrates, "RO22NN" is used to determine the rate of formation of the alkoxy radical products, and "RO2XRO" is used to represent processes where these products are is not formed, and is the same as used for xPROD. These are calculated as follows, where the k(RO2+..)'s refer to the rate constants for the reactions of RO2C or RO2XC with the indicated reactant.

RO2NO = k(RO2+NO)[NO]
RO22NN = k(RO2+NO3)[NO3] + k(RO2+MECO3){[MECO3]+[RCO3]+[BZCO3]+ [MACO3]) + 0.5 k(RO2+MEO2)[MEO2] + 0.5 k(RO2+RO2){[RO2C]+ [RO2XC])
RO2XRO = k(RO2+HO2)[HO2] + 0.5 k(RO2+MEO2)[MEO2] + 0.5 k(RO2+RO2){[RO2C]+ [RO2XC]) (same as used for xPROD)

The steady state approximation must be used for these operators when this representation is used, and the operators must not be allowed to be diluted or transported.

[e] The yROOH chemical operator species is used to represent the formation of organic hydroperoxides formed with peroxy radicals react with HO_2, or of H-shift disproportionation products formed when peroxy radicals react (in 50% yields) with other peroxy radicals. Note that the products formed when peroxy radicals react to form alkoxy radicals or organic nitrates (in the NO reaction) are represented using separate xPROD or zRNO3 species, and together these three types of operators represent all

Table A-2 (continued)

the products and radicals formed. Separate such yROOH species are used to represent formation of hydroperoxides or H-shift disproportion products in different molecular weight ranges or volatilities, and more can be added as needed for appropriate predictions of SOA formation. The hydroperoxide formed in the HO2 reaction is represented by either ROOH, R6OOH, or RAOOH, and the H-shift disproportion products are represented by either MEK (for yROOH) or PROD2 (for the others). As with the xPROD and zRNO3 species, the consumption and products formed from these species can be represented in several ways, with the most straightforward method being to include a reaction for each of the types of peroxy radical reactions, as follows for yROOH (the reactions for the other two are analogous).

yROOH + NO → NO
yROOH + HO2 → HO2 + ROOH
yROOH + NO3 → NO3
yROOH + MECO3 → MECO3 (& similar reactions for RCO3, BZCO3, and MACO3)
yROOH + MEO2 → MEO2 + 1/2 MEK
yROOH + RO2C → RO2C + 1/2 MEK (& a similar reaction for RO2XC)

The rate constants for these reactions should be the same as the rate constant for the corresponding reactions of RO2C or RO2XC. As with the other operators, an alternative method, requiring fewer reactions, is implemented in this table. In this case, the coefficient "RO2HO2" is used to determine the rate of formation of organic hydroperoxides, "RO2RO2M" to determine the rate of formation of H-shift disproportion products, and "RO2RO" is used to represent processes where these products are is not formed. Note that the latter is the same as the coefficient that is used to represent the formation products from the xPROD species. These are calculated as follows, where the k(RO2+..)'s refer to the rate constants for the reactions of RO2C or RO2XC with the indicated reactant.

RO2HO2 = k(RO2+HO2)[HO2]
RO2RO2M = 0.5 k(RO2+RO2){[RO2C]+ [RO2XC])
RO2RO = k(RO2+NO)[NO] + k(RO2+NO3)[NO3] + k(RO2+MECO3){[MECO3]+[RCO3]+ [BZCO3]+[MACO3]) + 0.5 k(RO2+MEO2) [MEO2] + 0.5 k(RO2+RO2) {[RO2C]+[RO2XC])

The steady state approximation must be used for these operators when this representation is used, and the operators must not be allowed to be diluted or transported.

[f] Mechanisms for these lumped model species were derived from the composition of the base ROG ambient mixture used in the reactivity simulations as documented by Carter (2010a).

Table A-3. Listing of reactions and rate parameters in the SAPRC-07A mechanism, the uncondensed SAPRC-07 mechanism using the more condensed SAPRC-99 peroxy radical representation.

Label	Reaction and Products [a]	Rate Parameters [b]			
		k(300)	A	Ea	B
1	NO2 + HV = NO + O3P	Phot Set= NO2-06			
2	O3P + O2 + M = O3 + M	5.68e-34	5.68e-34	0.00	-2.60
3	O3P + O3 = #2 O2	8.34e-15	8.00e-12	4.09	
4	O3P + NO = NO2	1.64e-12	Falloff, F=0.60, N=1.00		
			k0: 9.00e-32	0.00	-1.50
			inf: 3.00e-11	0.00	0.00
5	O3P + NO2 = NO + O2	1.03e-11	5.50e-12	-0.37	
6	O3P + NO2 = NO3	3.24e-12	Falloff, F=0.60, N=1.00		
			k0: 2.50e-31	0.00	-1.80
			inf: 2.20e-11	0.00	-0.70
7	O3 + NO = NO2 + O2	2.02e-14	3.00e-12	2.98	
8	O3 + NO2 = O2 + NO3	3.72e-17	1.40e-13	4.91	
9	NO + NO3 = #2 NO2	2.60e-11	1.80e-11	-0.22	
10	NO + NO + O2 = #2 NO2	1.93e-38	3.30e-39	-1.05	
11	NO2 + NO3 = N2O5	1.24e-12	Falloff, F=0.35, N=1.33		
			k0: 3.60e-30	0.00	-4.10
			inf: 1.90e-12	0.00	0.20
12	N2O5 = NO2 + NO3	5.69e-2	Falloff, F=0.35, N=1.33		
			k0: 1.30e-3	21.86	-3.50
			inf: 9.70e+14	22.02	0.10
13	N2O5 + H2O = #2 HNO3	2.50e-22			
14	N2O5 + H2O + H2O = #2 HNO3 + H2O	1.80e-39			
15	NO2 + NO3 = NO + NO2 + O2	6.75e-16	4.50e-14	2.50	
16	NO3 + HV = NO + O2	Phot Set= NO3NO-06			
17	NO3 + HV = NO2 + O3P	Phot Set= NO3NO2-6			
18	O3 + HV = O1D + O2	Phot Set= O3O1D-06			
19	O3 + HV = O3P + O2	Phot Set= O3O3P-06			
20	O1D + H2O = #2 OH	1.99e-10	1.63E-10	-0.12	
21	O1D + M = O3P + M	3.28e-11	2.38e-11	-0.19	
22	OH + NO = HONO	7.31e-12	Falloff, F=0.60, N=1.00		
			k0: 7.00e-31	0.00	-2.60
			inf: 3.60e-11	0.00	-0.10
23	HONO + HV = OH + NO	Phot Set= HONO-06			
24	OH + HONO = H2O + NO2	5.95e-12	2.50e-12	-0.52	
25	OH + NO2 = HNO3	1.05e-11	Falloff, F=0.60, N=1.00		
			k0: 1.80e-30	0.00	-3.00
			inf: 2.80e-11	0.00	0.00
26	OH + NO3 = HO2 + NO2	2.00e-11			
27	OH + HNO3 = H2O + NO3	1.51e-13	k = k0+k3M/(1+k3M/k2)		
			k0: 2.40e-14	-0.91	0.00
			k2: 2.70e-17	-4.37	0.00
			k3: 6.50e-34	-2.65	0.00
28	HNO3 + HV = OH + NO2	Phot Set= HNO3			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
29	OH + CO = HO2 + CO2	2.28e-13	k = k1 + k2 [M]		
		k1:	1.44e-13	0.00	0.00
		k2:	3.43e-33	0.00	0.00
30	OH + O3 = HO2 + O2	7.41e-14	1.70e-12	1.87	
31	HO2 + NO = OH + NO2	8.85e-12	3.60e-12	-0.54	
32	HO2 + NO2 = HNO4	1.12e-12	Falloff, F=0.60, N=1.00		
		k0:	2.00e-31	0.00	-3.40
		inf:	2.90e-12	0.00	-1.10
33	HNO4 = HO2 + NO2	1.07e-1	Falloff, F=0.60, N=1.00		
		k0:	3.72e-5	21.16	-2.40
		inf:	5.42e+15	22.20	-2.30
34	HNO4 + HV = #.61 {HO2 + NO2} + #.39 {OH + NO3}	Phot Set= HNO4-06			
35	HNO4 + OH = H2O + NO2 + O2	4.61e-12	1.30e-12	-0.76	
36	HO2 + O3 = OH + #2 O2	2.05e-15	2.03e-16	-1.38	4.57
37	HO2 + HO2 = HO2H + O2	2.84e-12	k = k1 + k2 [M]		
		k1:	2.20e-13	-1.19	0.00
		k2:	1.90e-33	-1.95	0.00
38	HO2 + HO2 + H2O = HO2H + O2 + H2O	6.09e-30	k = k1 + k2 [M]		
		k1:	3.08e-34	-5.56	0.00
		k2:	2.66e-54	-6.32	0.00
39	NO3 + HO2 = #.8 {OH + NO2 + O2} + #.2 {HNO3 + O2}	4.00e-12			
40	NO3 + NO3 = #2 NO2 + O2	2.41e-16	8.50e-13	4.87	
41	HO2H + HV = #2 OH	Phot Set= H2O2			
42	HO2H + OH = HO2 + H2O	1.80e-12	1.80e-12	0.00	
43	OH + HO2 = H2O + O2	1.10e-10	4.80e-11	-0.50	
44	OH + SO2 = HO2 + SULF	9.49e-13	Falloff, F=0.60, N=1.00		
		k0:	3.30e-31	0.00	-4.30
		inf:	1.60e-12	0.00	0.00
45	OH + H2 = HO2 + H2O	7.02e-15	7.70e-12	4.17	
BR01	MEO2 + NO = NO2 + HCHO + HO2	7.64e-12	2.30e-12	-0.72	
BR02	MEO2 + HO2 = COOH + O2	4.65e-12	3.46e-13	-1.55	0.36
BR03	MEO2 + HO2 = HCHO + O2 + H2O	4.50e-13	3.34e-14	-1.55	-3.53
BR04	MEO2 + NO3 = HCHO + HO2 + NO2	1.30e-12			
BR05	MEO2 + MEO2 = MEOH + HCHO + O2	2.16e-13	6.39e-14	-0.73	-1.80
BR06	MEO2 + MEO2 = #2 {HCHO + HO2}	1.31e-13	7.40e-13	1.03	
BR07	RO2R + NO = NO2 + HO2	9.23e-12	2.60e-12	-0.76	
BR08	RO2R + HO2 = XOOH + O2	7.63e-12	3.80e-13	-1.79	
BR09	RO2R + NO3 = NO2 + O2 + HO2	2.30e-12			
BR10	RO2R + MEO2 = HO2 + #.75 HCHO + #.25 MEOH	2.00e-13			
BR11	RO2R + RO2R = HO2	3.50e-14			
BR12	RO2N + NO = RNO3	Same k as rxn BR07			
BR13	RO2N + HO2 = XOOH + PROD2	Same k as rxn BR08			
BR14	RO2N + NO3 = NO2 + O2 + HO2 + PROD2	Same k as rxn BR09			
BR15	RO2N + MEO2 = HO2 + #.25 MEOH + PROD2 + #.75 HCHO	Same k as rxn BR10			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BR16	RO2N + RO2R = HO2 + PROD2 + O2	Same k as rxn BR11			
BR17	RO2N + RO2N = HO2 + #2 PROD2 + O2	Same k as rxn BR11			
BR18	MECO3 + NO2 = PAN	9.37e-12	Falloff, F=0.30, N=1.41		
			k0: 2.70e-28	0.00	-7.10
			inf: 1.21e-11	0.00	-0.90
BR19	PAN = MECO3 + NO2	6.27e-4	Falloff, F=0.30, N=1.41		
			k0: 4.90e-3	24.05	0.00
			inf: 4.00e+16	27.03	0.00
BR20	PAN + HV = #.6 {MECO3 + NO2} + #.4 {MEO2 + CO2 + NO3}	Phot Set= PAN			
BR21	MECO3 + NO = MEO2 + CO2 + NO2	1.97e-11	7.50e-12	-0.58	
BR22	MECO3 + HO2 = CCOOH + #.7 O2 + #.3 O3	1.36e-11	5.20e-13	-1.95	
BR23	MECO3 + NO3 = MEO2 + CO2 + NO2 + O2	Same k as rxn BR09			
BR24	MECO3 + MEO2 = #.1 {CCOOH + HCHO + O2} + #.9 {HCHO + HO2 + MEO2 + CO2}	1.06e-11	2.00e-12	-0.99	
BR25	MECO3 + RO2R = MEO2 + CO2	1.56e-11	4.40e-13	-2.13	
BR26	MECO3 + RO2N = MEO2 + CO2 + HO2 + PROD2	Same k as rxn BR25			
BR27	MECO3 + MECO3 = #2 {MEO2 + CO2} + O2	1.54e-11	2.90e-12	-0.99	
BR28	RCO3 + NO2 = PAN2	1.21e-11	1.21e-11	0.00	-1.07
BR29	PAN2 = RCO3 + NO2	5.48e-4	8.30e+16	27.70	
BR30	PAN2 + HV = #.6 {RCO3 + NO2} + #.4 {CCHO + RO2R + CO2 + NO3}	Phot Set= PAN			
BR31	RCO3 + NO = NO2 + CCHO + RO2R + CO2	2.08e-11	6.70e-12	-0.68	
BR32	RCO3 + HO2 = RCOOH + #.75 O2 + #.25 O3	1.36e-11	5.20e-13	-1.95	
BR33	RCO3 + NO3 = NO2 + CCHO + RO2R + CO2 + O2	Same k as rxn BR09			
BR34	RCO3 + MEO2 = CO2 + RO2R + CCHO + HCHO + HO2	1.06e-11	2.00e-12	-0.99	
BR35	RCO3 + RO2R = CO2 + RO2R + CCHO	1.56e-11	4.40e-13	-2.13	
BR36	RCO3 + RO2N = RO2R + CCHO + CO2 + HO2 + PROD2	Same k as rxn BR35			
BR37	RCO3 + MECO3 = #2 CO2 + MEO2 + CCHO + RO2R + O2	1.54e-11	2.90e-12	-0.99	
BR38	RCO3 + RCO3 = #2 {CCHO + RO2R + CO2}	Same k as rxn BR37			
BR39	BZCO3 + NO2 = PBZN	1.37e-11			
BR40	PBZN = BZCO3 + NO2	4.27e-4	7.90e+16	27.82	
BR41	PBZN + HV = #.6 {BZCO3 + NO2} + #.4 {CO2 + BZO + R2O2 + NO3}	Phot Set= PAN			
BR42	BZCO3 + NO = NO2 + CO2 + BZO + R2O2	Same k as rxn BR31			
BR43	BZCO3 + HO2 = RCOOH + #.75 O2 + #.25 O3 + #4 XC	Same k as rxn BR32			
BR44	BZCO3 + NO3 = NO2 + CO2 + BZO + R2O2 + O2	Same k as rxn BR09			
BR45	BZCO3 + MEO2 = CO2 + BZO + R2O2 + HCHO + HO2	Same k as rxn BR34			
BR46	BZCO3 + RO2R = CO2 + BZO + R2O2	Same k as rxn BR35			
BR47	BZCO3 + RO2N = CO2 + BZO + R2O2 + HO2 + PROD2	Same k as rxn BR35			
BR48	BZCO3 + MECO3 = #2 CO2 + MEO2 + BZO + R2O2	Same k as rxn BR37			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BR49	BZCO3 + RCO3 = #2 CO2 + CCHO + RO2R + BZO + R2O2	Same k as rxn BR37			
BR50	BZCO3 + BZCO3 = #2 {BZO + R2O2 + CO2}	Same k as rxn BR37			
BR51	MACO3 + NO2 = MAPAN	Same k as rxn BR28			
BR52	MAPAN = MACO3 + NO2	4.79e-4	1.60e+16	26.80	
BR53	MAPAN + HV = #.6 {MACO3 + NO2} + #.4 {CO2 + HCHO + MECO3 + NO3}	Phot Set= PAN			
BR54	MACO3 + NO = NO2 + CO2 + HCHO + MECO3	Same k as rxn BR31			
BR55	MACO3 + HO2 = RCOOH + #.75 O2 + #.25 O3 + XC	Same k as rxn BR32			
BR56	MACO3 + NO3 = NO2 + CO2 + HCHO + MECO3 + O2	Same k as rxn BR09			
BR57	MACO3 + MEO2 = #2 HCHO + HO2 + CO2 + MECO3	Same k as rxn BR34			
BR58	MACO3 + RO2R = CO2 + HCHO + MECO3	Same k as rxn BR35			
BR59	MACO3 + RO2N = CO2 + HCHO + MECO3 + HO2 + PROD2	Same k as rxn BR35			
BR60	MACO3 + MECO3 = #2 CO2 + MEO2 + HCHO + MECO3 + O2	Same k as rxn BR37			
BR61	MACO3 + RCO3 = HCHO + MECO3 + CCHO + RO2R + #2 CO2	Same k as rxn BR37			
BR62	MACO3 + BZCO3 = HCHO + MECO3 + BZO + R2O2 + #2 CO2	Same k as rxn BR37			
BR63	MACO3 + MACO3 = #2 {HCHO + MECO3 + CO2}	Same k as rxn BR37			
BR64	TBUO + NO2 = RNO3 + #-2 XC	2.40e-11			
BR65	TBUO = ACET + MEO2	1.18e+3	7.50e+14	16.20	
BR66	BZO + NO2 = NPHE	3.79e-11	2.30e-11	-0.30	
BR67	BZO + HO2 = CRES + #-1 XC	Same k as rxn BR08			
BR68	BZO = CRES + RO2R + #-1 XC	1.00e-3			
BR69	R2O2 + NO = NO2	Same k as rxn BR07			
BR70	R2O2 + HO2 = HO2	Same k as rxn BR08			
BR71	R2O2 + NO3 = NO2	Same k as rxn BR09			
BR72	R2O2 + MEO2 = MEO2	Same k as rxn BR10			
BR73	R2O2 + RO2R = RO2R	Same k as rxn BR11			
BR74	R2O2 + RO2N = RO2N	Same k as rxn BR11			
BR75	R2O2 + R2O2 =	Same k as rxn BR11			
BR76	R2O2 + MECO3 = MECO3	Same k as rxn BR25			
BR77	R2O2 + RCO3 = RCO3	Same k as rxn BR35			
BR78	R2O2 + BZCO3 = BZCO3	Same k as rxn BR35			
BR79	R2O2 + MACO3= MACO3	Same k as rxn BR35			
BP01	HCHO + HV = #2 HO2 + CO	Phot Set= HCHOR-06			
BP02	HCHO + HV = H2 + CO	Phot Set= HCHOM-06			
BP03	HCHO + OH = HO2 + CO + H2O	8.47e-12	5.40e-12	-0.27	
BP07	HCHO + NO3 = HNO3 + HO2 + CO	6.06e-16	2.00e-12	4.83	
BP08	CCHO + OH = MECO3	1.49e-11	4.40e-12	-0.73	
BP09	CCHO + HV = HO2 + MEO2 + CO	Phot Set= CCHO_R			
BP10	CCHO + NO3 = MECO3 + HNO3	2.84e-15	1.40e-12	3.70	

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BP11	RCHO + OH = #.035 RO2R + #.965 RCO3 + #.035 CO + #.035 CCHO	1.97e-11	5.10e-12	-0.80	
BP12	RCHO + HV = HO2 + RO2R + CO + CCHO	Phot Set= C2CHO			
BP13	RCHO + NO3 = RCO3 + HNO3	6.74e-15	1.40e-12	3.18	
BP14	ACET + OH = MECO3 + R2O2 + HCHO	1.91e-13	4.56e-14	-0.85	3.65
BP15	ACET + HV = #1.38 MEO2 + #.62 MECO3 + #.38 CO	Phot Set= ACET-06, qy= 0.5			
BP16	MEK + OH = #.376 RO2R + #.51 MECO3 + #.074 RCO3 + #.039 RO2N + #.591 R2O2 + #.088 HCHO + #.504 CCHO + #.376 RCHO + #.3 XC	1.20e-12	1.30e-12	0.05	2.00
BP17	MEK + HV = RO2R + MECO3 + CCHO	Phot Set= MEK-06, qy= 0.175			
BP18	MEOH + OH = HO2 + HCHO	9.02e-13	2.85e-12	0.69	
BP19	HCOOH + OH = HO2 + CO2	4.50e-13			
BP20	CCOOH + OH = #.491 RO2R + #.509 MEO2 + #.509 CO2 + #.491 MGLY + #-.491 XC	7.26e-13	4.20e-14	-1.70	
BP21	RCOOH + OH = RO2R + #.143 CO2 + #.142 CCHO + #.4 RCHO + #.457 BACL + #-.455 XC	1.20e-12			
BP22	COOH + OH = #.3 OH + #.7 MEO2 + #.3 HCHO	7.40e-12	3.80e-12	-0.40	
BP23	COOH + HV = HO2 + OH + HCHO	Phot Set= COOH			
BP24	XOOH + OH = OH	2.50e-11			
BP25	XOOH + HV = HO2 + OH	Phot Set= COOH			
BP30	GLY + HV = #2 HO2 + #2 CO	Phot Set= GLY-07R			
BP31	GLY + HV = HCHO + CO	Phot Set= GLY-07M			
BP32	GLY + OH = #.63 HO2 + #.37 RCO3 + #1.26 CO + #-.37 XC	1.10e-11			
BP33	GLY + NO3 = #.63 HO2 + #.37 RCO3 + HNO3 + #1.26 CO + #-.37 XC	1.02e-15	2.80e-12	4.72	
BP34	MGLY + HV = HO2 + MECO3 + CO	Phot Set= MGLY-06			
BP35	MGLY + OH = MECO3 + CO	1.50e-11			
BP36	MGLY + NO3 = MECO3 + HNO3 + CO	2.53e-15	1.40e-12	3.77	
BP37	BACL + HV = #2 MECO3	Phot Set= BACL-07			
BP38	CRES + OH = #.8 RO2R + #.2 BZO + #.25 MGLY + #5.05 XC	4.03e-11	1.70e-12	-1.89	
BP39	CRES + NO3 = BZO + HNO3 + XC	1.40e-11			
BP40	NPHE + OH = BZO + XN	3.50e-12			
BP41	NPHE + HV = HONO + #6 XC	Phot Set= NO2-06, qy= 1.5e-3			
BP42	NPHE + HV = XN + #6 XC	Phot Set= NO2-06, qy= 1.5e-2			
BP43	BALD + OH = BZCO3	1.20e-11			
BP44	BALD + HV = #7 XC	Phot Set= BALD-06, qy= 0.06			
BP45	BALD + NO3 = BZCO3 + HNO3	2.73e-15	1.34e-12	3.70	
BP46	AFG1 + OH = #.521 RO2R + #.201 MECO3 + #.217 MACO3 + #.06 RO2N + #.202 R2O2 + #.334 CO + #.407 RCHO + #.129 MEK + #.107 GLY + #.267 MGLY + #.284 XC	7.40e-11			
BP47	AFG1 + O3 = #.522 HO2 + #.826 OH + #.652 RCO3 + #.652 R2O2 + #.522 CO + #.174 CO2 + #.652 HCHO + #.432 GLY + #.568 MGLY + #-.872 XC	9.66e-18			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BP48	AFG1 + HV = #1.023 HO2 + #.173 MEO2 + #.305 MECO3 + #.5 MACO3 + #.695 CO + #.195 GLY + #.305 MGLY + #.217 XC	Phot Set= AFG1			
BP49	AFG2 + OH = #.521 RO2R + #.201 MECO3 + #.217 MACO3 + #.06 RO2N + #.202 R2O2 + #.334 CO + #.407 RCHO + #.129 MEK + #.107 GLY + #.267 MGLY + #.284 XC	7.40e-11			
BP50	AFG2 + O3 = #.522 HO2 + #.826 OH + #.652 RCO3 + #.652 R2O2 + #.522 CO + #.174 CO2 + #.652 HCHO + #.432 GLY + #.568 MGLY + #-.872 XC	9.66e-18			
BP51	AFG2 + HV = PROD2 + #-1 XC	Phot Set= AFG1			
BP52	AFG3 + OH = #.561 RO2R + #.117 MECO3 + #.206 MACO3 + #.117 RO2N + #.172 R2O2 + #.114 CO + #.274 GLY + #.153 MGLY + #.019 BACL + #.231 IPRD + #.195 AFG1 + #.195 AFG2 + #.938 XC	9.35e-11			
BP53	AFG3 + O3 = #.554 HO2 + #.095 RO2R + #.471 OH + #.013 MECO3 + #.163 RCO3 + #.007 RO2N + #.163 R2O2 + #.58 CO + #.19 CO2 + #.163 HCHO + #.366 GLY + #.279 MGLY + #.003 MACR + #.004 MVK + #.003 IPRD + #.35 AFG1 + #.35 AFG2 + #.139 AFG3 + #-.575 XC	1.43e-17			
BP54	MACR + OH = #.5 RO2R + #.5 MACO3 + #.416 CO + #.084 HCHO + #.416 MEK + #.084 MGLY + #-.416 XC	2.84e-11	8.00e-12	-0.76	
BP55	MACR + O3 = #.108 HO2 + #.208 OH + #.1 RCO3 + #.1 R2O2 + #.45 CO + #.117 CO2 + #.2 HCHO + #.333 HCOOH + #.9 MGLY + #-.1 XC	1.28e-18	1.40e-15	4.17	
BP56	MACR + NO3 = #.5 RO2R + #.5 MACO3 + #.5 HNO3 + #.5 CO + #.5 XN + #1.5 XC	3.54e-15	1.50e-12	3.61	
BP57	MACR + O3P = RCHO + XC	6.34e-12			
BP58	MACR + HV = #.67 HO2 + #.33 OH + #.67 MECO3 + #.33 MACO3 + #.33 R2O2 + #.67 CO + #.67 HCHO	Phot Set= MACR-06			
BP59	MVK + OH = #.3 RO2R + #.675 MECO3 + #.025 RO2N + #.675 R2O2 + #.3 HCHO + #.675 RCHO + #.3 MGLY + #-.725 XC	1.99e-11	2.60e-12	-1.21	
BP60	MVK + O3 = #.064 HO2 + #.05 RO2R + #.164 OH + #.05 RCO3 + #.475 CO + #.124 CO2 + #.1 HCHO + #.351 HCOOH + #.95 MGLY + #-.05 XC	5.36e-18	8.50e-16	3.02	
BP62	MVK + O3P = #.45 RCHO + #.55 MEK + #.45 XC	4.32e-12			
BP63	MVK + HV = #.4 MEO2 + #.4 MACO3 + #.6 CO + #.6 PROD2 + #-2.2 XC	Phot Set= MVK-06			
BP64	IPRD + OH = #.67 RO2R + #.289 MACO3 + #.041 RO2N + #.336 CO + #.055 HCHO + #.129 CCHO + #.013 RCHO + #.15 MEK + #.332 PROD2 + #.15 GLY + #.174 MGLY + #-.504 XC	6.19e-11			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BP65	IPRD + O3 = #.4 HO2 + #.285 OH + #.048 RCO3 + #.048 R2O2 + #.498 CO + #.14 CO2 + #.125 HCHO + #.047 CCHO + #.21 MEK + #.1 HCOOH + #.372 RCOOH + #.023 GLY + #.742 MGLY + #-.329 XC	4.18e-18			
BP66	IPRD + NO3 = #.799 RO2R + #.15 MACO3 + #.051 RO2N + #.15 HNO3 + #.572 CO + #.227 HCHO + #.218 RCHO + #.008 MGLY + #.572 RNO3 + #.278 XN + #-.815 XC	1.00e-13			
BP67	IPRD + HV = #1.233 HO2 + #.467 MECO3 + #.3 RCO3 + #1.233 CO + #.3 HCHO + #.467 CCHO + #.233 MEK + #-.233 XC	Phot Set= MACR-06			
BP68	PROD2 + OH = #.472 HO2 + #.379 RO2R + #.029 MECO3 + #.049 RCO3 + #.071 RO2N + #.094 R2O2 + #.213 HCHO + #.084 CCHO + #.545 RCHO + #.115 MEK + #.336 PROD2 + #.877 XC	1.55e-11			
BP69	PROD2 + HV = #.913 RO2R + #.4 MECO3 + #.6 RCO3 + #.087 RO2N + #.677 R2O2 + #.303 HCHO + #.163 CCHO + #.78 RCHO + #-.091 XC	Phot Set= MEK-06, qy= 4.86e-3			
BP70	RNO3 + OH = #.189 HO2 + #.305 RO2R + #.332 NO2 + #.175 RO2N + #.671 R2O2 + #.011 HCHO + #.429 CCHO + #.037 RCHO + #.004 ACET + #.18 MEK + #.039 PROD2 + #.494 RNO3 + #.174 XN + #.04 XC	7.20e-12			
BP71	RNO3 + HV = #.344 HO2 + #.554 RO2R + NO2 + #.102 RO2N + #.167 R2O2 + #.135 HCHO + #.444 CCHO + #.137 RCHO + #.008 ACET + #.207 MEK + #.451 PROD2 + #.396 XC	Phot Set= IC3ONO2			
BE01	CH4 + OH = MEO2	6.62e-15	1.85e-12	3.36	
BE02	ETHENE + OH = RO2R + #1.61 HCHO + #.195 CCHO	8.15e-12	Falloff, F=0.60, N=1.00		
		k0:	1.00e-28	0.00	-4.50
		inf:	8.80e-12	0.00	-0.85
BE03	ETHENE + O3 = #.16 HO2 + #.16 OH + #.51 CO + #.12 CO2 + HCHO + #.37 HCOOH	1.68e-18	9.14e-15	5.13	
BE04	ETHENE + NO3 = RO2R + RCHO + XN + #-1 XC	2.24e-16	3.30e-12	5.72	2.00
BE05	ETHENE + O3P = #.8 HO2 + #.29 RO2R + #.51 MEO2 + #.788 CO + #.278 HCHO + #.1 CCHO + #.012 GLY + #.2 XC	7.43e-13	1.07e-11	1.59	
BE06	ISOPRENE + OH = #.907 RO2R + #.093 RO2N + #.079 R2O2 + #.624 HCHO + #.23 MACR + #.32 MVK + #.357 IPRD + #-.167 XC	9.96e-11	2.54e-11	-0.81	
BE07	ISOPRENE + O3 = #.066 HO2 + #.266 OH + #.192 MACO3 + #.008 RO2N + #.192 R2O2 + #.275 CO + #.122 CO2 + #.592 HCHO + #.1 PROD2 + #.204 HCOOH + #.39 MACR + #.16 MVK + #.15 IPRD + #-.559 XC	1.34e-17	7.86e-15	3.80	

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BE08	ISOPRENE + NO3 = #.749 RO2R + #.187 NO2 + #.064 RO2N + #.187 R2O2 + #.936 IPRD + #.813 XN + #-.064 XC	6.81e-13	3.03e-12	0.89	
BE09	ISOPRENE + O3P = #.25 MEO2 + #.24 MACO3 + #.01 RO2N + #.24 R2O2 + #.24 HCHO + #.75 PROD2 + #-1.01 XC	3.50e-11			
BE10	ACETYLEN + OH = #.3 HO2 + #.7 OH + #.3 CO + #.3 HCOOH + #.7 GLY	7.56e-13	Falloff, F=0.60, N=1.00		
		k0:	5.50e-30	0.00	-2.00
		inf:	8.30e-13	0.00	0.00
BE11	ACETYLEN + O3 = #1.5 HO2 + #.5 OH + #1.5 CO + #.5 CO2	1.16e-20	1.00e-14	8.15	
BE12	BENZENE + OH = #.57 HO2 + #.29 RO2R + #.116 OH + #.024 RO2N + #.29 GLY + #.57 CRES + #.029 AFG1 + #.261 AFG2 + #.116 AFG3 + #-.976 XC	1.22e-12	2.33e-12	0.38	
BL01	ALK1 + OH = RO2R + CCHO	2.54e-13	1.34e-12	0.99	2.00
BL02	ALK2 + OH = #.965 RO2R + #.035 RO2N + #.261 RCHO + #.704 ACET + #-.105 XC	1.11e-12	1.49e-12	0.17	2.00
BL03	ALK3 + OH = #.695 RO2R + #.236 TBUO + #.07 RO2N + #.558 R2O2 + #.026 HCHO + #.445 CCHO + #.122 RCHO + #.024 ACET + #.332 MEK + #-.046 XC	2.31e-12	1.51e-12	-0.25	
BL04	ALK4 + OH = #.83 RO2R + #.01 MEO2 + #.011 MECO3 + #.149 RO2N + #.933 R2O2 + #.002 CO + #.029 HCHO + #.438 CCHO + #.236 RCHO + #.426 ACET + #.106 MEK + #.146 PROD2 + #-.119 XC	4.34e-12	3.75e-12	-0.09	
BL05	ALK5 + OH = #.647 RO2R + #.353 RO2N + #.958 R2O2 + #.04 HCHO + #.106 CCHO + #.209 RCHO + #.071 ACET + #.086 MEK + #.407 PROD2 + #2.004 XC	9.40e-12	2.70e-12	-0.74	
BL06	OLE1 + OH = #.904 RO2R + #.001 MEO2 + #.095 RO2N + #.234 R2O2 + #.7 HCHO + #.301 CCHO + #.47 RCHO + #.005 ACET + #.119 PROD2 + #.026 MACR + #.008 MVK + #.006 IPRD + #.822 XC	3.29e-11	6.18e-12	-1.00	
BL07	OLE1 + O3 = #.116 HO2 + #.04 RO2R + #.193 OH + #.104 MEO2 + #.004 RO2N + #.023 R2O2 + #.368 CO + #.125 CO2 + #.5 HCHO + #.154 CCHO + #.384 RCHO + #.002 ACET + #.006 MEK + #.189 PROD2 + #.185 HCOOH + #.022 CCOOH + #.112 RCOOH + #.69 XC	1.09e-17	3.15e-15	3.38	
BL08	OLE1 + NO3 = #.824 RO2R + #.176 RO2N + #.488 R2O2 + #.009 CCHO + #.002 RCHO + #.024 ACET + #.546 RNO3 + #.454 XN + #.572 XC	1.44e-14	4.73e-13	2.08	
BL09	OLE1 + O3P = #.45 RCHO + #.437 MEK + #.113 PROD2 + #1.224 XC	5.02e-12	1.49e-11	0.65	

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BL10	OLE2 + OH = #.914 RO2R + #.086 RO2N + #.052 R2O2 + #.209 HCHO + #.788 CCHO + #.481 RCHO + #.136 ACET + #.076 MEK + #.022 PROD2 + #.027 MACR + #.002 MVK + #.037 IPRD + #.111 XC	6.42e-11	1.26e-11	-0.97	
BL11	OLE2 + O3 = #.093 HO2 + #.039 RO2R + #.423 OH + #.29 MEO2 + #.147 MECO3 + #.008 RCO3 + #.003 RO2N + #.161 R2O2 + #.297 CO + #.162 CO2 + #.26 HCHO + #.495 CCHO + #.333 RCHO + #.048 ACET + #.032 MEK + #.042 PROD2 + #.033 HCOOH + #.061 CCOOH + #.222 RCOOH + #.028 MACR + #.021 MVK + #.125 XC	1.24e-16	8.14e-15	2.49	
BL12	OLE2 + NO3 = #.423 RO2R + #.409 NO2 + #.033 MEO2 + #.136 RO2N + #.762 R2O2 + #.074 HCHO + #.546 CCHO + #.154 RCHO + #.11 ACET + #.002 MEK + #.026 MVK + #.007 IPRD + #.322 RNO3 + #.269 XN + #.114 XC	7.85e-13	2.20e-13	-0.76	
BL13	OLE2 + O3P = #.014 HO2 + #.007 RO2R + #.007 MACO3 + #.001 RO2N + #.006 R2O2 + #.006 CO + #.074 RCHO + #.709 MEK + #.202 PROD2 + #.006 MACR + #.666 XC	2.07e-11	1.43e-11	-0.22	
BL14	ARO1 + OH = #.166 HO2 + #.482 RO2R + #.284 OH + #.068 RO2N + #.077 PROD2 + #.218 GLY + #.138 MGLY + #.166 CRES + #.049 BALD + #.164 AFG1 + #.193 AFG2 + #.284 AFG3 + #.002 XC	6.15e-12			
BL15	ARO2 + OH = #.108 HO2 + #.58 RO2R + #.202 OH + #.11 RO2N + #.035 PROD2 + #.116 GLY + #.286 MGLY + #.104 BACL + #.108 CRES + #.039 BALD + #.217 AFG1 + #.21 AFG2 + #.282 AFG3 + #1.486 XC	2.57e-11			
BL16	TERP + OH = #.759 RO2R + #.042 RCO3 + #.2 RO2N + #.388 R2O2 + #.001 CO + #.264 HCHO + #.533 RCHO + #.036 ACET + #.005 MEK + #.255 PROD2 + #.009 MGLY + #.014 BACL + #.002 MVK + #.001 IPRD + #5.056 XC	7.98e-11	1.87e-11	-0.86	
BL17	TERP + O3 = #.052 HO2 + #.067 RO2R + #.585 OH + #.126 MECO3 + #.149 RCO3 + #.203 RO2N + #.808 R2O2 + #.185 CO + #.045 CO2 + #.229 HCHO + #.22 RCHO + #.165 ACET + #.004 MEK + #.409 PROD2 + #.107 HCOOH + #.043 RCOOH + #.001 GLY + #.002 MGLY + #.055 BACL + #.001 MACR + #.001 IPRD + #3.526 XC	6.99e-17	9.57e-16	1.56	
BL18	TERP + NO3 = #.162 RO2R + #.421 NO2 + #.019 RCO3 + #.397 RO2N + #1.347 R2O2 + #.01 CO + #.017 HCHO + #.001 CCHO + #.509 RCHO + #.175 ACET + #.001 MGLY + #.003 MACR + #.001 MVK + #.002 IPRD + #.163 RNO3 + #.416 XN + #4.473 XC	6.53e-12	1.28e-12	-0.97	
BL19	TERP + O3P = #.147 RCHO + #.853 PROD2 + #4.441 XC	3.71e-11			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
	Chlorine Mechanism				
CI01	CL2 + HV = #2 CL	Phot Set= CL2			
CI02	CL + NO + M = CLNO + M	7.60e-32	7.60e-32	0.00	-1.80
CI03	CLNO + HV = CL + NO	Phot Set= CLNO-06			
CI04	CL + NO2 = CLONO	1.60e-11	Falloff, F=0.60, N=1.00		
			k0: 1.30e-30	0.00	-2.00
			inf: 1.00e-10	0.00	-1.00
CI05	CL + NO2 = CLNO2	3.52e-12	Falloff, F=0.60, N=1.00		
			k0: 1.80e-31	0.00	-2.00
			inf: 1.00e-10	0.00	-1.00
CI06	CLONO + HV = CL + NO2	Phot Set= CLONO			
CI07	CLNO2 + HV = CL + NO2	Phot Set= CLNO2			
CI08	CL + HO2 = HCL + O2	3.44e-11	3.44e-11	0.00	-0.56
CI09	CL + HO2 = CLO + OH	9.41e-12	9.41e-12	0.00	2.10
CI10	CL + O3 = CLO + O2	1.22e-11	2.80e-11	0.50	
CI11	CL + NO3 = CLO + NO2	2.40e-11			
CI12	CLO + NO = CL + NO2	1.66e-11	6.20e-12	-0.59	
CI13	CLO + NO2 = CLONO2	2.29e-12	Falloff, F=0.60, N=1.00		
			k0: 1.80e-31	0.00	-3.40
			inf: 1.50e-11	0.00	-1.90
CI14	CLONO2 + HV = CLO + NO2	Phot Set= CLONO2-1			
CI15	CLONO2 + HV = CL + NO3	Phot Set= CLONO2-2			
CI16	CLONO2 = CLO + NO2	4.12e-4	Falloff, F=0.60, N=1.00		
			k0: 4.48e-5	24.90	-1.00
			inf: 3.71e+15	24.90	3.50
CI17	CL + CLONO2 = CL2 + NO3	1.01e-11	6.20e-12	-0.29	
CI18	CLO + HO2 = HOCL + O2	6.83e-12	2.20e-12	-0.68	
CI19	HOCL + HV = OH + CL	Phot Set= HOCL-06			
CI20	CLO + CLO = #.29 CL2 + #1.42 CL + O2	1.82e-14	1.25e-11	3.89	
CI21	OH + HCL = H2O + CL	7.90e-13	1.70e-12	0.46	
CI22	CL + H2 = HCL + HO2	1.77e-14	3.90e-11	4.59	
CP01	HCHO + CL = HCL + HO2 + CO	7.33e-11	8.10e-11	0.06	
CP02	CCHO + CL = HCL + MECO3	8.00e-11	8.00e-11		
CP03	MEOH + CL = HCL + HO2 + HCHO	5.50e-11	5.50e-11	0.00	
CP04	RCHO + CL = HCL + #.1 RO2R + #.9 RCO3 + #.1 CO + #.1 CCHO	1.23e-10			
CP05	ACET + CL = HCL + MECO3 + R2O2 + HCHO	2.75e-12	7.70e-11	1.99	
CP06	MEK + CL = HCL + #.84 RO2R + #.085 MECO3 + #.036 RCO3 + #.039 RO2N + #.135 R2O2 + #.065 HCHO + #.07 CCHO + #.84 RCHO + #.763 XC	3.60e-11			
CP07	RNO3 + CL = HCL + #.055 HO2 + #.547 RO2R + #.197 NO2 + #.202 RO2N + #.735 R2O2 + #.045 HCHO + #.3 CCHO + #.029 RCHO + #.003 ACET + #.059 MEK + #.058 PROD2 + #.602 RNO3 + #.201 XN + #-.149 XC	1.92e-10			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
CP08	PROD2 + CL = HCL + #.314 HO2 + #.541 RO2R + #.007 MECO3 + #.022 RCO3 + #.116 RO2N + #.138 R2O2 + #.237 HCHO + #.109 CCHO + #.789 RCHO + #.051 MEK + #.156 PROD2 + #1.262 XC	2.00e-10			
CP09	GLY + CL = HCL + #.63 HO2 + #.37 RCO3 + #1.26 CO + #-.37 XC	7.33e-11	8.10e-11	0.06	
CP10	MGLY + CL = HCL + MECO3 + CO	8.00e-11			
CP11	CRES + CL = HCL + RO2R + #-1 R2O2 + BALD	6.20e-11			
CP12	BALD + CL = HCL + BZCO3	8.00e-11			
CP13	XOOH + CL = CL	1.66e-10			
CP16	MACR + CL = #.25 HCL + #.802 RO2R + #.165 MACO3 + #.033 RO2N + #.541 CO + #.082 IPRD + #.18 CLCCHO + #.541 CLACET + #.208 XC	3.85e-10			
CP17	MVK + CL = #.322 RO2R + #.625 MECO3 + #.053 RO2N + #.961 R2O2 + #.947 CLCCHO + #.538 XC	2.32e-10			
CP18	IPRD + CL = #.401 HCL + #.084 HO2 + #.712 RO2R + #.154 MACO3 + #.051 RO2N + #.018 R2O2 + #.498 CO + #.195 HCHO + #.017 MGLY + #.115 IPRD + #.051 AFG1 + #.051 AFG2 + #.14 CLCCHO + #.42 CLACET + #.709 XC	4.12e-10			
CP19	CLCCHO + HV = HO2 + RO2CL + CO + HCHO	Phot Set= CLCCHO			
CP20	CLCCHO + OH = RCO3 + #-1 XC	3.10e-12			
CP21	CLCCHO + CL = HCL + RCO3 + #-1 XC	1.29e-11			
CP22	CLACET + HV = RO2CL + MECO3 + HCHO	Phot Set= CLACET, qy= 0.50			
CR01	RO2CL + NO = NO2 + CL	Same k as rxn BR07			
CR02	RO2CL + HO2 = XOOH + O2	Same k as rxn BR08			
CR03	RO2CL + NO3 = NO2 + O2 + CL	Same k as rxn BR09			
CR04	RO2CL + MEO2 = #.5 {CL + HO2} + #.75 HCHO + #.25 MEOH	Same k as rxn BR10			
CR05	RO2CL + RO2R = #.5 {CL + HO2}	Same k as rxn BR11			
CR06	RO2CL + R2O2 = RO2CL	Same k as rxn BR11			
CR07	RO2CL + RO2N = #.5 {CL + HO2 + MEK + PROD2} + O2 + XC	Same k as rxn BR11			
CR08	RO2CL + RO2CL = CL	Same k as rxn BR11			
CR09	RO2CL + MECO3 = MEO2 + CO2	Same k as rxn BR35			
CR10	RO2CL + RCO3 = CO2 + RO2R + CCHO	Same k as rxn BR35			
CR11	RO2CL + BZCO3 = CO2 + BZO + R2O2	Same k as rxn BR35			
CR12	RO2CL + MACO3 = CO2 + HCHO + MECO3	Same k as rxn BR35			
CE01	CH4 + CL = HCL + MEO2	1.02e-13	7.30e-12	2.54	
CE02	ETHENE + CL = RO2R + R2O2 + HCHO + CLCHO	1.04e-10	Falloff, F=0.60, N=1.00		
		k0:	1.60e-29	0.00	-3.30
		inf:	3.10e-10	0.00	-1.00
CE03	ISOPRENE + CL = #.15 HCL + #.738 RO2R + #.177 RO2CL + #.085 RO2N + #.253 R2O2 + #.275 HCHO + #.177 MVK + #.671 IPRD + #.067 CLCCHO + #.018 XC	4.80e-10			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
CE04	ACETYLEN + CL = HO2 + CO + XC	4.97e-11	Falloff, F=0.60, N=1.00		
			k0: 5.20e-30	0.00	-2.40
			inf: 2.20e-10	0.00	0.00
BC01	ALK1 + CL = HCL + RO2R + CCHO	5.95e-11	5.95e-11	0.00	
BC02	ALK2 + CL = HCL + #.97 RO2R + #.03 RO2N + #.482 RCHO + #.488 ACET + #-.09 XC	1.37e-10	1.37e-10	0.00	
BC03	ALK3 + CL = HCL + #.835 RO2R + #.094 TBUO + #.07 RO2N + #.526 R2O2 + #.078 HCHO + #.34 CCHO + #.343 RCHO + #.075 ACET + #.253 MEK + #.18 XC	1.86e-10			
BC04	ALK4 + CL = HCL + #.827 RO2R + #.003 MEO2 + #.004 MECO3 + #.165 RO2N + #.91 R2O2 + #.003 CO + #.034 HCHO + #.287 CCHO + #.412 RCHO + #.247 ACET + #.076 MEK + #.13 PROD2 + #.327 XC	2.63e-10			
BC05	ALK5 + CL = HCL + #.647 RO2R + #.352 RO2N + #.894 R2O2 + #.022 HCHO + #.08 CCHO + #.258 RCHO + #.044 ACET + #.041 MEK + #.378 PROD2 + #2.368 XC	4.21e-10			
BC06	OLE1 + CL = #.308 HCL + #.902 RO2R + #.098 RO2N + #.518 R2O2 + #.025 HCHO + #.146 CCHO + #.051 RCHO + #.188 MACR + #.014 MVK + #.027 IPRD + #.225 CLCCHO + #.396 CLACET + #1.361 XC	3.55e-10			
BC07	OLE2 + CL = #.263 HCL + #.447 RO2R + #.448 RO2CL + #.001 MEO2 + #.104 RO2N + #.619 R2O2 + #.228 HCHO + #.361 CCHO + #.3 RCHO + #.081 ACET + #.04 MEK + #.049 MACR + #.055 MVK + #.179 IPRD + #.012 CLCCHO + #.18 CLACET + #.247 XC	3.83e-10			
BC08	ARO1 + CL = #.88 RO2R + #.12 RO2N + #.21 PROD2 + #.671 BALD + #.323 XC	1.00e-10			
BC09	ARO2 + CL = #.842 RO2R + #.158 RO2N + #.224 PROD2 + #.618 BALD + #2.382 XC	2.18e-10			
BC10	TERP + CL = #.548 HCL + #.252 RO2R + #.068 RO2CL + #.034 MECO3 + #.05 RCO3 + #.016 MACO3 + #.582 RO2N + #1.938 R2O2 + #.035 CO + #.158 HCHO + #.185 RCHO + #.274 ACET + #.007 GLY + #.003 BACL + #.003 MVK + #.158 IPRD + #.006 AFG1 + #.006 AFG2 + #.001 AFG3 + #.109 CLCCHO + #3.543 XC	5.46e-10			
	<u>Reactions of Chloroform (used for test calculations only)</u>				
TS01	CHCL3 + OH = RO2CL + XC	1.06e-13	5.67e-13	1.00	2.00
TS02	CHCL3 + CL = HCL + RO2CL + XC	1.22e-13	3.30e-12	1.97	

[a] Format of reaction listing: "=" separates reactants from products; "*#number*" indicates stoichiometric coefficient, "*#coefficient* {*product list*}" means that the stoichiometric coefficient is applied to all the products listed.

Table A-3 (continued)

[b] Except as indicated, the rate constants are given by $k(T) = A \cdot (T/300)^B \cdot e^{-Ea/RT}$, where the units of k and A are cm^3 $molec^{-1}$ s^{-1}, Ea are kcal mol^{-1}, T is ^oK, and R=0.0019872 kcal mol^{-1} deg^{-1}. The following special rate constant expressions are used:

Phot Set = *name*: The absorption cross sections and (if applicable) quantum yields for the photolysis reaction are documented by Carter (2010a) and are available at http://www.cert.ucr.edu/~carter/SAPRC, where "*name*" indicates the photolysis set used. If a "qy=*number*" notation is given, the number given is the overall quantum yield, which is assumed to be wavelength independent.

Falloff: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = \{k0(T)\cdot[M]/[1 + k0(T)\cdot[M]/kinf(T)]\}\cdot F^Z$, where $Z = \{1 + [\log10\{k0(T)\cdot[M])/kinf(T)\}/N]^2\}^{-1}$, [M] is the total pressure in molecules cm^{-3}, F and N are as indicated on the table, and the temperature dependences of k0 and kinf are as indicated on the table.

k = k0+k3M(1+k3M/k2): The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k0(T) + k3(T)\cdot[M] \cdot(1 + k3(T)\cdot[M]/k2(T))$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k0, k2 and k3 are as indicated on the table.

k = k1 + k2 [M]: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k1(T) + k2(T)\cdot[M]$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k1, and k2 are as indicated on the table.

Same K as Rxn xx: Uses the same rate constant as the reaction in the base mechanism with the same label.

Table A-4. Listing of reactions and rate parameters in the CS07A mechanism, the condensed SAPRC-07 mechanism using the SAPRC-99 peroxy radical representation method "A".

Label	Reaction and Products [a]	Rate Parameters [b]			
		k(300)	A	Ea	B
1	NO2 + HV = NO + O3P	Phot Set= NO2-06			
2	O3P + O2 + M = O3 + M	5.68e-34	5.68e-34	0.00	-2.60
3	O3P + O3 = #2 O2	8.34e-15	8.00e-12	4.09	
4	O3P + NO = NO2	1.64e-12	Falloff, F=0.60, N=1.00		
			k0: 9.00e-32	0.00	-1.50
			inf: 3.00e-11	0.00	0.00
5	O3P + NO2 = NO + O2	1.03e-11	5.50e-12	-0.37	
6	O3P + NO2 = NO3	3.24e-12	Falloff, F=0.60, N=1.00		
			k0: 2.50e-31	0.00	-1.80
			inf: 2.20e-11	0.00	-0.70
7	O3 + NO = NO2 + O2	2.02e-14	3.00e-12	2.98	
8	O3 + NO2 = O2 + NO3	3.72e-17	1.40e-13	4.91	
9	NO + NO3 = #2 NO2	2.60e-11	1.80e-11	-0.22	
10	NO + NO + O2 = #2 NO2	1.93e-38	3.30e-39	-1.05	
11	NO2 + NO3 = N2O5	1.24e-12	Falloff, F=0.35, N=1.33		
			k0: 3.60e-30	0.00	-4.10
			inf: 1.90e-12	0.00	0.20
12	N2O5 = NO2 + NO3	5.69e-2	Falloff, F=0.35, N=1.33		
			k0: 1.30e-3	21.86	-3.50
			inf: 9.70e+14	22.02	0.10
13	N2O5 + H2O = #2 HNO3	2.50e-22			
14	N2O5 + H2O + H2O = #2 HNO3 + H2O	1.80e-39			
15	NO2 + NO3 = NO + NO2 + O2	6.75e-16	4.50e-14	2.50	
16	NO3 + HV = NO + O2	Phot Set= NO3NO-06			
17	NO3 + HV = NO2 + O3P	Phot Set= NO3NO2-6			
18	O3 + HV = O1D + O2	Phot Set= O3O1D-06			
19	O3 + HV = O3P + O2	Phot Set= O3O3P-06			
20	O1D + H2O = #2 OH	1.99e-10	1.63E-10	-0.12	
21	O1D + M = O3P + M	3.28e-11	2.38e-11	-0.19	
22	OH + NO = HONO	7.31e-12	Falloff, F=0.60, N=1.00		
			k0: 7.00e-31	0.00	-2.60
			inf: 3.60e-11	0.00	-0.10
23	HONO + HV = OH + NO	Phot Set= HONO-06			
24	OH + HONO = H2O + NO2	5.95e-12	2.50e-12	-0.52	
25	OH + NO2 = HNO3	1.05e-11	Falloff, F=0.60, N=1.00		
			k0: 1.80e-30	0.00	-3.00
			inf: 2.80e-11	0.00	0.00
26	OH + NO3 = HO2 + NO2	2.00e-11			
27	OH + HNO3 = H2O + NO3	1.51e-13	k = k0+k3M/(1+k3M/k2)		
			k0: 2.40e-14	-0.91	0.00
			k2: 2.70e-17	-4.37	0.00
			k3: 6.50e-34	-2.65	-4.37
28	HNO3 + HV = OH + NO2	Phot Set= HNO3			

Table A-4 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
29	OH + CO = HO2 + CO2	2.28e-13	k = k1 + k2 [M]		
		k1:	1.44e-13	0.00	0.00
		k2:	3.43e-33	0.00	0.00
30	OH + O3 = HO2 + O2	7.41e-14	1.70e-12	1.87	
31	HO2 + NO = OH + NO2	8.85e-12	3.60e-12	-0.54	
32	HO2 + NO2 = HNO4	1.12e-12	Falloff, F=0.60, N=1.00		
		k0:	2.00e-31	0.00	-3.40
		inf:	2.90e-12	0.00	-1.10
33	HNO4 = HO2 + NO2	1.07e-1	Falloff, F=0.60, N=1.00		
		k0:	3.72e-5	21.16	-2.40
		inf:	5.42e+15	22.20	-2.30
34	HNO4 + HV = #.61 {HO2 + NO2} + #.39 {OH + NO3}	Phot Set= HNO4-06			
35	HNO4 + OH = H2O + NO2 + O2	4.61e-12	1.30e-12	-0.76	
36	HO2 + O3 = OH + #2 O2	2.05e-15	2.03e-16	-1.38	4.57
37	HO2 + HO2 = HO2H + O2	2.84e-12	k = k1 + k2 [M]		
		k1:	2.20e-13	-1.19	0.00
		k2:	1.90e-33	-1.95	0.00
38	HO2 + HO2 + H2O = HO2H + O2 + H2O	6.09e-30	k = k1 + k2 [M]		
		k1:	3.08e-34	-5.56	0.00
		k2:	2.66e-54	-6.32	0.00
39	NO3 + HO2 = #.8 {OH + NO2 + O2} + #.2 {HNO3 + O2}	4.00e-12			
40	NO3 + NO3 = #2 NO2 + O2	2.41e-16	8.50e-13	4.87	
41	HO2H + HV = #2 OH	Phot Set= H2O2			
42	HO2H + OH = HO2 + H2O	1.80e-12	1.80e-12	0.00	
43	OH + HO2 = H2O + O2	1.10e-10	4.80e-11	-0.50	
44	OH + SO2 = HO2 + SULF	9.49e-13	Falloff, F=0.60, N=1.00		
		k0:	3.30e-31	0.00	-4.30
		inf:	1.60e-12	0.00	0.00
45	OH + H2 = HO2 + H2O	7.02e-15	7.70e-12	4.17	
BR07	RO2R + NO = NO2 + HO2	9.23e-12	2.60e-12	-0.76	
BR08	RO2R + HO2 = XOOH + O2	7.63e-12	3.80e-13	-1.79	
BR09	RO2R + NO3 = NO2 + O2 + HO2	2.30e-12			
BR11	RO2R + RO2R = HO2	3.50e-14			
BR12	RO2N + NO = RNO3	Same k as rxn BR07			
BR13	RO2N + HO2 = XOOH + PROD2	Same k as rxn BR08			
BR14	RO2N + NO3 = NO2 + O2 + HO2 + PROD2	Same k as rxn BR09			
BR16	RO2N + RO2R = HO2 + PROD2 + O2	Same k as rxn BR11			
BR17	RO2N + RO2N = HO2 + #2 PROD2 + O2	Same k as rxn BR11			
BR18	MECO3 + NO2 = PAN	9.37e-12	Falloff, F=0.30, N=1.41		
		k0:	2.70e-28	0.00	-7.10
		inf:	1.21e-11	0.00	-0.90
BR19	PAN = MECO3 + NO2	6.27e-4	Falloff, F=0.30, N=1.41		
		k0:	4.90e-3	24.05	0.00
		inf:	4.00e+16	27.03	0.00

Table A-4 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BR20	PAN + HV = #.6 {MECO3 + NO2} + #.4 {RO2R + HCHO + CO2 + NO3}	Phot Set= PAN			
BR21	MECO3 + NO = RO2R + HCHO + CO2 + NO2	1.97e-11	7.50e-12	-0.58	
BR22	MECO3 + HO2 = #.243 ALK3 + #.086 CCHO + #.7 O2 + #.3 O3 + #.856 XC	1.36e-11	5.20e-13	-1.95	
BR23	MECO3 + NO3 = RO2R + HCHO + CO2 + NO2 + O2	Same k as rxn BR09			
BR25	MECO3 + RO2R = HCHO + RO2R + CO2	1.56e-11	4.40e-13	-2.13	
BR26	MECO3 + RO2N = RO2R + HCHO + CO2 + HO2 + PROD2	Same k as rxn BR25			
BR27	MECO3 + MECO3 = #2 {RO2R + HCHO + CO2} + O2	1.54e-11	2.90e-12	-0.99	
BR28	RCO3 + NO2 = PAN2	1.21e-11	1.21e-11	0.00	-1.07
BR29	PAN2 = RCO3 + NO2	5.48e-4	8.30e+16	27.70	
BR30	PAN2 + HV = #.6 {RCO3 + NO2} + #.4 {CCHO + RO2R + CO2 + NO3}	Phot Set= PAN			
BR31	RCO3 + NO = NO2 + CCHO + RO2R + CO2	2.08e-11	6.70e-12	-0.68	
BR32	RCO3 + HO2 = #.526 ALK3 + #.190 CCHO + #.75 O2 + #.25 O3 + #.516 XC	1.36e-11	5.20e-13	-1.95	
BR33	RCO3 + NO3 = NO2 + CCHO + RO2R + CO2 + O2	Same k as rxn BR09			
BR35	RCO3 + RO2R = CO2 + RO2R + CCHO	1.56e-11	4.40e-13	-2.13	
BR36	RCO3 + RO2N = RO2R + CCHO + CO2 + HO2 + PROD2	Same k as rxn BR35			
BR37	RCO3 + MECO3 = #2 CO2 + HCHO + CCHO + #2 RO2R + O2	1.54e-11	2.90e-12	-0.99	
BR38	RCO3 + RCO3 = #2 {CCHO + RO2R + CO2}	Same k as rxn BR37			
BR66	BZO + NO2 = #.5 CRES + #2.5 XC + XN	3.79e-11	2.30e-11	-0.30	
BR67	BZO + HO2 = CRES + #-1 XC	Same k as rxn BR08			
BR68	BZO = CRES + RO2R + #-1 XC	1.00e-3			
BR69	R2O2 + NO = NO2	Same k as rxn BR07			
BR70	R2O2 + HO2 = HO2	Same k as rxn BR08			
BR71	R2O2 + NO3 = NO2	Same k as rxn BR09			
BR73	R2O2 + RO2R = RO2R	Same k as rxn BR11			
BR74	R2O2 + RO2N = RO2N	Same k as rxn BR11			
BR75	R2O2 + R2O2 =	Same k as rxn BR11			
BR76	R2O2 + MECO3 = MECO3	Same k as rxn BR25			
BR77	R2O2 + RCO3 = RCO3	Same k as rxn BR35			
BP01	HCHO + HV = #2 HO2 + CO	Phot Set= HCHOR-06			
BP02	HCHO + HV = H2 + CO	Phot Set= HCHOM-06			
BP03	HCHO + OH = HO2 + CO + H2O	8.47e-12	5.40e-12	-0.27	
BP07	HCHO + NO3 = HNO3 + HO2 + CO	6.06e-16	2.00e-12	4.83	
BP08	CCHO + OH = MECO3	1.49e-11	4.40e-12	-0.73	
BP09	CCHO + HV = HO2 + RO2R + CO + HCHO	Phot Set= CCHO_R			
BP10	CCHO + NO3 = MECO3 + HNO3	2.84e-15	1.40e-12	3.70	
BP11	RCHO + OH = #.035 RO2R + #.965 RCO3 + #.035 CO + #.035 CCHO	1.97e-11	5.10e-12	-0.80	
BP12	RCHO + HV = HO2 + RO2R + CO + CCHO	Phot Set= C2CHO			
BP13	RCHO + NO3 = RCO3 + HNO3	6.74e-15	1.40e-12	3.18	

Table A-4 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BP24	XOOH + OH = OH	2.50e-11			
BP25	XOOH + HV = HO2 + OH	Phot Set= COOH			
BP34	MGLY + HV = HO2 + MECO3 + CO	Phot Set= MGLY-06			
BP35	MGLY + OH = MECO3 + CO	1.50e-11			
BP36	MGLY + NO3 = MECO3 + HNO3 + CO	2.53e-15	1.40e-12	3.77	
BP38	CRES + OH = #.8 RO2R + #.2 BZO + #.25 MGLY + #5.05 XC	4.03e-11	1.70e-12	-1.89	
BP39	CRES + NO3 = BZO + HNO3 + XC	1.40e-11			
BP46	AFG1 + OH = #.521 RO2R + #.201 MECO3 + #.217 RCO3 + #.06 RO2N + #.202 R2O2 + #.334 CO + #.407 RCHO + #.048 PROD2 + #.329 MGLY + #.002 AFG1 + #.747 XC	7.40e-11			
BP47	AFG1 + O3 = #.522 HO2 + #.826 OH + #.652 RCO3 + #.652 R2O2 + #.522 CO + #.174 CO2 + #.652 HCHO + #.819 MGLY + #.007 AFG1 + #-.796 XC	9.66e-18			
BP48	AFG1 + HV = #1.023 HO2 + #.173 RO2R + #.305 MECO3 + #.5 RCO3 + #.695 CO + #.173 HCHO + #.418 MGLY + #.003 AFG1 + #.753 XC	Phot Set= AFG1			
BP49	AFG2 + OH = #.521 RO2R + #.201 MECO3 + #.217 RCO3 + #.06 RO2N + #.202 R2O2 + #.334 CO + #.407 RCHO + #.048 PROD2 + #.329 MGLY + #.002 AFG1 + #.747 XC	7.40e-11			
BP50	AFG2 + O3 = #.522 HO2 + #.826 OH + #.652 RCO3 + #.652 R2O2 + #.522 CO + #.174 CO2 + #.652 HCHO + #.819 MGLY + #.007 AFG1 + #-.796 XC	9.66e-18			
BP51	AFG2 + HV = PROD2 + #-1 XC	Phot Set= AFG1			
BP64	IPRD + OH = #.496 RO2R + #.238 MECO3 + #.241 RCO3 + #.025 RO2N + #.238 R2O2 + #.238 CO + #.149 HCHO + #.051 CCHO + #.243 RCHO + #.192 PROD2 + #.23 MGLY + #.001 AFG1 + #.586 XC	6.19e-11			
BP65	IPRD + O3 = #.211 HO2 + #.025 RO2R + #.219 OH + #.053 RCO3 + #.028 R2O2 + #.483 CO + #.13 CO2 + #.119 HCHO + #.05 CCHO + #.033 PROD2 + #.095 ALK3 + #.863 MGLY + #.842 XC	4.18e-18			
BP66	IPRD + NO3 = #.792 RO2R + #.158 RCO3 + #.05 RO2N + #.158 HNO3 + #.57 CO + #.222 HCHO + #.213 RCHO + #.008 MGLY + #.559 RNO3 + #.283 XN + #-.583 XC	1.00e-13			
BP67	IPRD + HV = #.655 HO2 + #.141 RO2R + #.084 OH + #.354 MECO3 + #.343 RCO3 + #.084 R2O2 + #.867 CO + #.429 HCHO + #.184 CCHO + #.246 PROD2 + #.123 XC	Phot Set= MACR-06			
BP68	PROD2 + OH = #.472 HO2 + #.379 RO2R + #.029 MECO3 + #.049 RCO3 + #.071 RO2N + #.094 R2O2 + #.213 HCHO + #.084 CCHO + #.545 RCHO + #.378 PROD2 + #1.085 XC	1.55e-11			

Table A-4 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BP69	PROD2 + HV = #.913 RO2R + #.4 MECO3 + #.6 RCO3 + #.087 RO2N + #.677 R2O2 + #.303 HCHO + #.163 CCHO + #.78 RCHO + #-.091 XC	Phot Set= MEK-06, qy= 4.86e-3			
BP70	RNO3 + OH = #.189 HO2 + #.305 RO2R + #.332 NO2 + #.175 RO2N + #.671 R2O2 + #.011 HCHO + #.429 CCHO + #.037 RCHO + #.106 PROD2 + #.494 RNO3 + #.174 XN + #.37 XC	7.20e-12			
BP71	RNO3 + HV = #.344 HO2 + #.554 RO2R + NO2 + #.102 RO2N + #.167 R2O2 + #.135 HCHO + #.444 CCHO + #.137 RCHO + #.528 PROD2 + #.786 XC	Phot Set= IC3ONO2			
BE01	CH4 + OH = RO2R + HCHO	6.62e-15	1.85e-12	3.36	
BE02	ETHENE + OH = RO2R + #1.61 HCHO + #.195 CCHO	8.15e-12	Falloff, F=0.60, N=1.00		
		k0:	1.00e-28	0.00	-4.50
		inf:	8.80e-12	0.00	-0.85
BE03	ETHENE + O3 = #.16 HO2 + #.16 OH + #.51 CO + #.12 CO2 + HCHO + #.018 ALK3 + #.298 XC	1.68e-18	9.14e-15	5.13	
BE04	ETHENE + NO3 = RO2R + RCHO + XN + #-1 XC	2.24e-16	3.30e-12	5.72	2.00
BE05	ETHENE + O3P = #.8 HO2 + #.8 RO2R + #.788 CO + #.788 HCHO + #.1 CCHO + #.007 MGLY + #.203 XC	7.43e-13	1.07e-11	1.59	
BE06	ISOPRENE + OH = #.907 RO2R + #.093 RO2N + #.079 R2O2 + #.624 HCHO + #.907 IPRD + #-.717 XC	9.96e-11	2.54e-11	-0.81	
BE07	ISOPRENE + O3 = #.066 HO2 + #.266 OH + #.192 RCO3 + #.008 RO2N + #.192 R2O2 + #.275 CO + #.122 CO2 + #.592 HCHO + #.1 PROD2 + #.01 ALK3 + #.7 IPRD + #-.753 XC	1.34e-17	7.86e-15	3.80	
BE08	ISOPRENE + NO3 = #.749 RO2R + #.187 NO2 + #.064 RO2N + #.187 R2O2 + #.936 IPRD + #.813 XN + #-.064 XC	6.81e-13	3.03e-12	0.89	
BE09	ISOPRENE + O3P = #.25 RO2R + #.24 RCO3 + #.01 RO2N + #.24 R2O2 + #.49 HCHO + #.75 PROD2 + #-.77 XC	3.50e-11			
BL03	ALK3 + OH = #.931 RO2R + #.07 RO2N + #.558 R2O2 + #.262 HCHO + #.445 CCHO + #.122 RCHO + #.141 PROD2 + #1.216 XC	2.31e-12	1.51e-12	-0.25	
BLC4	ALK4 + OH = #.766 RO2R + #.007 MECO3 + #.227 RO2N + #.943 R2O2 + #.001 CO + #.039 HCHO + #.31 CCHO + #.226 RCHO + #.303 PROD2 + #.468 XC	6.16e-12			
BL06	OLE1 + OH = #.905 RO2R + #.095 RO2N + #.234 R2O2 + #.701 HCHO + #.301 CCHO + #.47 RCHO + #.119 PROD2 + #.04 IPRD + #.803 XC	3.29e-11	6.18e-12	-1.00	
BL07	OLE1 + O3 = #.116 HO2 + #.144 RO2R + #.193 OH + #.004 RO2N + #.023 R2O2 + #.368 CO + #.125 CO2 + #.604 HCHO + #.177 CCHO + #.384 RCHO + #.191 PROD2 + #.073 ALK3 + #.935 XC	1.09e-17	3.15e-15	3.38	

Table A-4 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BL08	OLE1 + NO3 = #.824 RO2R + #.176 RO2N + #.488 R2O2 + #.009 CCHO + #.002 RCHO + #.002 PROD2 + #.546 RNO3 + #.454 XN + #.632 XC	1.44e-14	4.73e-13	2.08	
BL09	OLE1 + O3P = #.45 RCHO + #.274 PROD2 + #2.006 XC	5.02e-12	1.49e-11	0.65	
BL10	OLE2 + OH = #.914 RO2R + #.086 RO2N + #.052 R2O2 + #.209 HCHO + #.788 CCHO + #.481 RCHO + #.06 PROD2 + #.066 IPRD + #.566 XC	6.42e-11	1.26e-11	-0.97	
BL11	OLE2 + O3 = #.093 HO2 + #.329 RO2R + #.423 OH + #.147 MECO3 + #.008 RCO3 + #.003 RO2N + #.161 R2O2 + #.297 CO + #.162 CO2 + #.55 HCHO + #.542 CCHO + #.333 RCHO + #.057 PROD2 + #.133 ALK3 + #.049 IPRD + #.453 XC	1.24e-16	8.14e-15	2.49	
BL12	OLE2 + NO3 = #.456 RO2R + #.409 NO2 + #.136 RO2N + #.762 R2O2 + #.107 HCHO + #.546 CCHO + #.154 RCHO + #.009 PROD2 + #.033 IPRD + #.322 RNO3 + #.269 XN + #.372 XC	7.85e-13	2.20e-13	-0.76	
BL13	OLE2 + O3P = #.014 HO2 + #.007 RO2R + #.007 RCO3 + #.001 RO2N + #.006 R2O2 + #.006 CO + #.074 RCHO + #.464 PROD2 + #.006 IPRD + #1.931 XC	2.07e-11	1.43e-11	-0.22	
BL14	ARO1 + OH = #.166 HO2 + #.482 RO2R + #.284 OH + #.068 RO2N + #.077 PROD2 + #.47 MGLY + #.166 CRES + #.167 AFG1 + #.454 AFG2 + #.453 XC	6.15e-12			
BL15	ARO2 + OH = #.108 HO2 + #.58 RO2R + #.202 OH + #.11 RO2N + #.035 PROD2 + #.709 MGLY + #.108 CRES + #.219 AFG1 + #.469 AFG2 + #1.807 XC	2.57e-11			
BL16	TERP + OH = #.759 RO2R + #.042 RCO3 + #.2 RO2N + #.388 R2O2 + #.001 CO + #.264 HCHO + #.533 RCHO + #.259 PROD2 + #.029 MGLY + #.003 IPRD + #5.154 XC	7.98e-11	1.87e-11	-0.86	
BL17	TERP + O3 = #.052 HO2 + #.067 RO2R + #.585 OH + #.126 MECO3 + #.149 RCO3 + #.203 RO2N + #.808 R2O2 + #.185 CO + #.045 CO2 + #.229 HCHO + #.008 CCHO + #.22 RCHO + #.422 PROD2 + #.028 ALK3 + #.083 MGLY + #.002 IPRD + #4.045 XC	6.99e-17	9.57e-16	1.56	
BL18	TERP + NO3 = #.162 RO2R + #.421 NO2 + #.019 RCO3 + #.397 RO2N + #1.347 R2O2 + #.01 CO + #.017 HCHO + #.001 CCHO + #.509 RCHO + #.012 PROD2 + #.001 MGLY + #.006 IPRD + #.163 RNO3 + #.416 XN + #4.922 XC	6.53e-12	1.28e-12	-0.97	
BL19	TERP + O3P = #.147 RCHO + #.853 PROD2 + #4.441 XC	3.71e-11			

Table A-4 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
	Chlorine Mechanism				
CI01	CL2 + HV = #2 CL	Phot Set= CL2			
CI08	CL + HO2 = HCL + O2	3.44e-11	3.44e-11	0.00	-0.56
CI09	CL + HO2 = CLO + OH	9.41e-12	9.41e-12	0.00	2.10
CI10	CL + O3 = CLO + O2	1.22e-11	2.80e-11	0.50	
CI11	CL + NO3 = CLO + NO2	2.40e-11			
CI12	CLO + NO = CL + NO2	1.66e-11	6.20e-12	-0.59	
CI13	CLO + NO2 = CLONO2	2.29e-12	Falloff, F=0.60, N=1.00		
		k0:	1.80e-31	0.00	-3.40
		inf:	1.50e-11	0.00	-1.90
CI14	CLONO2 + HV = CLO + NO2	Phot Set= CLONO2-1			
CI15	CLONO2 + HV = CL + NO3	Phot Set= CLONO2-2			
CI16	CLONO2 = CLO + NO2	4.12e-4	Falloff, F=0.60, N=1.00		
		k0:	4.48e-5	24.90	-1.00
		inf:	3.71e+15	24.90	3.50
CI17	CL + CLONO2 = CL2 + NO3	1.01e-11	6.20e-12	-0.29	
CI20	CLO + CLO = #.29 CL2 + #1.42 CL + O2	1.82e-14	1.25e-11	3.89	
CI21	OH + HCL = H2O + CL	7.90e-13	1.70e-12	0.46	
CI22	CL + H2 = HCL + HO2	1.77e-14	3.90e-11	4.59	
CP01	HCHO + CL = HCL + HO2 + CO	7.33e-11	8.10e-11	0.06	
CP02	CCHO + CL = HCL + MECO3	8.00e-11	8.00e-11		
CP04	RCHO + CL = HCL + #.1 RO2R + #.9 RCO3 + #.1 CO + #.1 CCHO	1.23e-10			
CP07	RNO3 + CL = HCL + #.055 HO2 + #.547 RO2R + #.197 NO2 + #.202 RO2N + #.735 R2O2 + #.045 HCHO + #.3 CCHO + #.029 RCHO + #.08 PROD2 + #.602 RNO3 + #.201 XN + #-.036 XC	1.92e-10			
CP08	PROD2 + CL = HCL + #.314 HO2 + #.541 RO2R + #.007 MECO3 + #.022 RCO3 + #.116 RO2N + #.138 R2O2 + #.237 HCHO + #.109 CCHO + #.789 RCHO + #.175 PROD2 + #1.352 XC	2.00e-10			
CP10	MGLY + CL = HCL + MECO3 + CO	8.00e-11			
CP11	CRES + CL = HCL + RO2R + #-1 R2O2 + #7 XC	6.20e-11			
CP13	XOOH + CL = CL	1.66e-10			
CP18	IPRD + CL = #.221 HCL + #.033 HO2 + #.597 RO2R + #.221 MECO3 + #.102 RCO3 + #.047 RO2N + #.346 R2O2 + #.333 CO + #.077 HCHO + #.235 RCHO + #.494 MGLY + #.066 IPRD + #.021 AFG1 + #.021 AFG2 + #.833 XC	4.12e-10			
CE01	CH4 + CL = HCL + RO2R + HCHO	1.02e-13	7.30e-12	2.54	
CE02	ETHENE + CL = RO2R + R2O2 + HCHO + XC	1.04e-10	Falloff, F=0.60, N=1.00		
		k0:	1.60e-29	0.00	-3.30
		inf:	3.10e-10	0.00	-1.00
CE03	ISOPRENE + CL = #.15 HCL + #.738 RO2R + #.177 CL + #.085 RO2N + #.43 R2O2 + #.275 HCHO + #.017 RCHO + #.048 MGLY + #.848 IPRD + #-.22 XC	4.80e-10			

Table A-4 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B
BC03	ALK3 + CL = HCL + #.929 RO2R + #.07 RO2N + #.526 R2O2 + #.172 HCHO + #.34 CCHO + #.343 RCHO + #.105 PROD2 + #1.069 XC	1.86e-10			
CLC4	ALK4 + CL = HCL + #.76 RO2R + #.002 MECO3 + #.237 RO2N + #.904 R2O2 + #.002 CO + #.031 HCHO + #.207 CCHO + #.353 RCHO + #.26 PROD2 + #.508 XC	3.20e-10			
BC06	OLE1 + CL = #.308 HCL + #.902 RO2R + #.098 RO2N + #.518 R2O2 + #.025 HCHO + #.146 CCHO + #.268 RCHO + #.391 MGLY + #.229 IPRD + #.973 XC	3.55e-10			
BC07	OLE2 + CL = #.263 HCL + #.448 RO2R + #.448 CL + #.104 RO2N + #1.067 R2O2 + #.229 HCHO + #.361 CCHO + #.375 RCHO + #.021 PROD2 + #.113 MGLY + #.283 IPRD + #.42 XC	3.83e-10			
BC08	ARO1 + CL = #.88 RO2R + #.12 RO2N + #.21 PROD2 + #5.02 XC	1.00e-10			
BC09	ARO2 + CL = #.842 RO2R + #.158 RO2N + #.224 PROD2 + #6.708 XC	2.18e-10			
BC10	TERP + CL = #.548 HCL + #.252 RO2R + #.068 CL + #.034 MECO3 + #.066 RCO3 + #.582 RO2N + #2.006 R2O2 + #.035 CO + #.158 HCHO + #.213 RCHO + #.019 PROD2 + #.087 MGLY + #.161 IPRD + #.006 AFG1 + #.007 AFG2 + #4.165 XC	5.46e-10			
	Reactions of Chloroform (used for test calculations only)				
TS01	CHCL3 + OH = CL + R2O2 + XC	1.06e-13	5.67e-13	1.00	2.00
TS02	CHCL3 + CL = HCL + CL + R2O2 + XC	1.22e-13	3.30e-12	1.97	

[a] Format of reaction listing: "=" separates reactants from products; "*#number*" indicates stoichiometric coefficient, "*#coefficient* {*product list*}" means that the stoichiometric coefficient is applied to all the products listed.

[b] Except as indicated, the rate constants are given by $k(T) = A \cdot (T/300)^B \cdot e^{-Ea/RT}$, where the units of k and A are cm^3 $molec^{-1}$ s^{-1}, Ea are kcal mol^{-1}, T is ^oK, and R=0.0019872 kcal mol^{-1} deg^{-1}. The following special rate constant expressions are used:

Phot Set = *name*: The absorption cross sections and (if applicable) quantum yields for the photolysis reaction are documented by Carter (2010a) and are available at http://www.cert.ucr.edu/~carter/SAPRC, where "*name*" indicates the photolysis set used. If a "qy=*number*" notation is given, the number given is the overall quantum yield, which is assumed to be wavelength independent.

Falloff: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = \{k0(T)\cdot[M]/[1 + k0(T)\cdot[M]/kinf(T)]\}\cdot F^Z$, where $Z = \{1 + [\log10\{k0(T)\cdot[M])/kinf(T)\}/N]^2\}^{-1}$, [M] is the total pressure in molecules cm^{-3}, F and N are as indicated on the table, and the temperature dependences of k0 and kinf are as indicated on the table.

k = k0+k3M(1+k3M/k2): The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k0(T) + k3(T)\cdot[M] \cdot(1 + k3(T)\cdot[M]/k2(T))$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k0, k2 and k3 are as indicated on the table.

Table A-4 (continued)

k = k1 + k2 [M]: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k1(T) + k2(T)\cdot[M]$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k1, and k2 are as indicated on the table.

Same K as Rxn xx: Uses the same rate constant as the reaction in the base mechanism with the same label.

Table A-5. Listing of reactions and rate parameters in the CS07B mechanism, the condensed SAPRC-07 mechanism using the standard SAPRC-07 peroxy radical representation Method "B".

Label	Reaction and Products [a]	Rate Parameters [b,c]			
		k(300)	A	Ea	B
1	NO2 + HV = NO + O3P	Phot Set= NO2-06			
2	O3P + O2 + M = O3 + M	5.68e-34	5.68e-34	0.00	-2.60
3	O3P + O3 = #2 O2	8.34e-15	8.00e-12	4.09	
4	O3P + NO = NO2	1.64e-12	Falloff, F=0.60, N=1.00		
			k0: 9.00e-32	0.00	-1.50
			inf: 3.00e-11	0.00	0.00
5	O3P + NO2 = NO + O2	1.03e-11	5.50e-12	-0.37	
6	O3P + NO2 = NO3	3.24e-12	Falloff, F=0.60, N=1.00		
			k0: 2.50e-31	0.00	-1.80
			inf: 2.20e-11	0.00	-0.70
7	O3 + NO = NO2 + O2	2.02e-14	3.00e-12	2.98	
8	O3 + NO2 = O2 + NO3	3.72e-17	1.40e-13	4.91	
9	NO + NO3 = #2 NO2	2.60e-11	1.80e-11	-0.22	
10	NO + NO + O2 = #2 NO2	1.93e-38	3.30e-39	-1.05	
11	NO2 + NO3 = N2O5	1.24e-12	Falloff, F=0.35, N=1.33		
			k0: 3.60e-30	0.00	-4.10
			inf: 1.90e-12	0.00	0.20
12	N2O5 = NO2 + NO3	5.69e-2	Falloff, F=0.35, N=1.33		
			k0: 1.30e-3	21.86	-3.50
			inf: 9.70e+14	22.02	0.10
13	N2O5 + H2O = #2 HNO3	2.50e-22			
14	N2O5 + H2O + H2O = #2 HNO3 + H2O	1.80e-39			
15	NO2 + NO3 = NO + NO2 + O2	6.75e-16	4.50e-14	2.50	
16	NO3 + HV = NO + O2	Phot Set= NO3NO-06			
17	NO3 + HV = NO2 + O3P	Phot Set= NO3NO2-6			
18	O3 + HV = O1D + O2	Phot Set= O3O1D-06			
19	O3 + HV = O3P + O2	Phot Set= O3O3P-06			
20	O1D + H2O = #2 OH	1.99e-10	1.63E-10	-0.12	
21	O1D + M = O3P + M	3.28e-11	2.38e-11	-0.19	
22	OH + NO = HONO	7.31e-12	Falloff, F=0.60, N=1.00		
			k0: 7.00e-31	0.00	-2.60
			inf: 3.60e-11	0.00	-0.10
23	HONO + HV = OH + NO	Phot Set= HONO-06			
24	OH + HONO = H2O + NO2	5.95e-12	2.50e-12	-0.52	
25	OH + NO2 = HNO3	1.05e-11	Falloff, F=0.60, N=1.00		
			k0: 1.80e-30	0.00	-3.00
			inf: 2.80e-11	0.00	0.00
26	OH + NO3 = HO2 + NO2	2.00e-11			
27	OH + HNO3 = H2O + NO3	1.51e-13	k = k0+k3M/(1+k3M/k2)		
			k0: 2.40e-14	-0.91	0.00
			k2: 2.70e-17	-4.37	0.00
			k3: 6.50e-34	-2.65	-4.37
28	HNO3 + HV = OH + NO2	Phot Set= HNO3			

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
29	OH + CO = HO2 + CO2	2.28e-13	k = k1 + k2 [M]		
		k1:	1.44e-13	0.00	0.00
		k2:	3.43e-33	0.00	0.00
30	OH + O3 = HO2 + O2	7.41e-14	1.70e-12	1.87	
31	HO2 + NO = OH + NO2	8.85e-12	3.60e-12	-0.54	
32	HO2 + NO2 = HNO4	1.12e-12	Falloff, F=0.60, N=1.00		
		k0:	2.00e-31	0.00	-3.40
		inf:	2.90e-12	0.00	-1.10
33	HNO4 = HO2 + NO2	1.07e-1	Falloff, F=0.60, N=1.00		
		k0:	3.72e-5	21.16	-2.40
		inf:	5.42e+15	22.20	-2.30
34	HNO4 + HV = #.61 {HO2 + NO2} + #.39 {OH + NO3}	Phot Set= HNO4-06			
35	HNO4 + OH = H2O + NO2 + O2	4.61e-12	1.30e-12	-0.76	
36	HO2 + O3 = OH + #2 O2	2.05e-15	2.03e-16	-1.38	4.57
37	HO2 + HO2 = HO2H + O2	2.84e-12	k = k1 + k2 [M]		
		k1:	2.20e-13	-1.19	0.00
		k2:	1.90e-33	-1.95	0.00
38	HO2 + HO2 + H2O = HO2H + O2 + H2O	6.09e-30	k = k1 + k2 [M]		
		k1:	3.08e-34	-5.56	0.00
		k2:	2.66e-54	-6.32	0.00
39	NO3 + HO2 = #.8 {OH + NO2 + O2} + #.2 {HNO3 + O2}	4.00e-12			
40	NO3 + NO3 = #2 NO2 + O2	2.41e-16	8.50e-13	4.87	
41	HO2H + HV = #2 OH	Phot Set= H2O2			
42	HO2H + OH = HO2 + H2O	1.80e-12	1.80e-12	0.00	
43	OH + HO2 = H2O + O2	1.10e-10	4.80e-11	-0.50	
44	OH + SO2 = HO2 + SULF	9.49e-13	Falloff, F=0.60, N=1.00		
		k0:	3.30e-31	0.00	-4.30
		inf:	1.60e-12	0.00	0.00
45	OH + H2 = HO2 + H2O	7.02e-15	7.70e-12	4.17	
BR07	RO2C + NO = NO2	9.23e-12	2.60e-12	-0.76	
BR08	RO2C + HO2 =	7.63e-12	3.80e-13	-1.79	
BR09	RO2C + NO3 = NO2	2.30e-12			
BR11	RO2C + RO2C =	3.50e-14			
BR12	RO2XC + NO = XN	Same k as rxn BR07			
BR13	RO2XC + HO2 =	Same k as rxn BR08			
BR14	RO2XC + NO3 = NO2	Same k as rxn BR09			
BR16	RO2XC + RO2C =	Same k as rxn BR11			
BR17	RO2XC + RO2XC =	Same k as rxn BR11			
BR18	MECO3 + NO2 = PAN	9.37e-12	Falloff, F=0.30, N=1.41		
		k0:	2.70e-28	0.00	-7.10
		inf:	1.21e-11	0.00	-0.90
BR19	PAN = MECO3 + NO2	6.27e-4	Falloff, F=0.30, N=1.41		
		k0:	4.90e-3	24.05	0.00
		inf:	4.00e+16	27.03	0.00

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
BR20	PAN + HV = #.6 {MECO3 + NO2} + #.4 {RO2C + xHO2 + xHCHO + yROOH + CO2 + NO3}	Phot Set= PAN			
BR21	MECO3 + NO = RO2C + xHO2 + xHCHO + yROOH + CO2 + NO2	1.97e-11	7.50e-12	-0.58	
BR22	MECO3 + HO2 = #.243 ALK3 + #.086 CCHO + #.7 O2 + #.3 O3 + #.856 XC	1.36e-11	5.20e-13	-1.95	
BR23	MECO3 + NO3 = RO2C + xHO2 + xHCHO + yROOH + CO2 + NO2 + O2	Same k as rxn BR09			
BR25	MECO3 + RO2C = RO2C + xHO2 + xHCHO + yROOH + CO2	1.56e-11	4.40e-13	-2.13	
BR26	MECO3 + RO2XC = RO2C + xHO2 + xHCHO + yROOH + CO2	Same k as rxn BR25			
BR27	MECO3 + MECO3 = #2 {RO2C + xHO2 + xHCHO + yROOH + CO2} + O2	1.54e-11	2.90e-12	-0.99	
BR28	RCO3 + NO2 = PAN2	1.21e-11	1.21e-11	0.00	-1.07
BR29	PAN2 = RCO3 + NO2	5.48e-4	8.30e+16	27.70	
BR30	PAN2 + HV = #.6 {RCO3 + NO2} + #.4 {RO2C + xHO2 + yROOH + xCCHO + CO2 + NO3}	Phot Set= PAN			
BR31	RCO3 + NO = NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2	2.08e-11	6.70e-12	-0.68	
BR32	RCO3 + HO2 = #.526 ALK3 + #.190 CCHO + #.75 O2 + #.25 O3 + #.516 XC	Same k as rxn BR22			
BR33	RCO3 + NO3 = NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2 + O2	Same k as rxn BR09			
BR35	RCO3 + RO2C = RO2C + xHO2 + xCCHO + yROOH + CO2	Same k as rxn BR25			
BR36	RCO3 + RO2XC = RO2C + xHO2 + xCCHO + yROOH + CO2	Same k as rxn BR25			
BR37	RCO3 + MECO3 = #2 CO2 + RO2C + xHO2 + xHCHO + yROOH + RO2C + xHO2 + yROOH + xCCHO + O2	Same k as rxn BR27			
BR38	RCO3 + RCO3 = #2 {RO2C + xHO2 + xCCHO + yROOH + CO2}	Same k as rxn BR27			
BR66	BZO + NO2 = #.5 CRES + #2.5 XC + XN	3.79e-11	2.30e-11	-0.30	
BR67	BZO + HO2 = CRES + #-1 XC	Same k as rxn BR08			
BR68	BZO = CRES + RO2C + xHO2 + #-1 XC	1.00e-3			
RO01	xHO2 = HO2	k is variable parameter: RO2RO			
RO02	xHO2 =	k is variable parameter: RO2XRO			
RO03	xOH = OH	k is variable parameter: RO2RO			
RO04	xOH =	k is variable parameter: RO2XRO			
RO05	xNO2 = NO2	k is variable parameter: RO2RO			
RO06	xNO2 = XN	k is variable parameter: RO2XRO			
RO09	xMECO3 = MECO3	k is variable parameter: RO2RO			
RO10	xMECO3 = #2 XC	k is variable parameter: RO2XRO			
RO11	xRCO3 = RCO3	k is variable parameter: RO2RO			
RO12	xRCO3 = #3 XC	k is variable parameter: RO2XRO			
BP01	HCHO + HV = #2 HO2 + CO	Phot Set= HCHOR-06			

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
BP02	HCHO + HV = H2 + CO	Phot Set= HCHOM-06			
BP03	HCHO + OH = HO2 + CO + H2O	8.47e-12	5.40e-12	-0.27	
BP07	HCHO + NO3 = HNO3 + HO2 + CO	6.06e-16	2.00e-12	4.83	
BP08	CCHO + OH = MECO3	1.49e-11	4.40e-12	-0.73	
BP09	CCHO + HV = HO2 + xHO2 + RO2C + CO + xHCHO + yROOH	Phot Set= CCHO_R			
BP10	CCHO + NO3 = MECO3 + HNO3	2.84e-15	1.40e-12	3.70	
BP11	RCHO + OH = #.035 xHO2 + #.965 RCO3 + #.035 RO2C + #.035 CO + #.035 xCCHO + #.035 yROOH	1.97e-11	5.10e-12	-0.80	
BP12	RCHO + HV = HO2 + xHO2 + RO2C + CO + xCCHO + yROOH	Phot Set= C2CHO			
BP13	RCHO + NO3 = RCO3 + HNO3	6.74e-15	1.40e-12	3.18	
BC24	ROOH + OH = #.156 xHO2 + #.798 OH + #.028 xOH + #.235 RO2C + #.018 RO2XC + #.018 zRNO3 + #.005 xHCHO + #.016 xCCHO + #.328 RCHO + #.132 xRCHO + #.469 PROD2 + #.062 xPROD2 + #.202 yROOH + #.289 XC	4.23e-11			
BP25	ROOH + HV = #.521 HO2 + #.437 xHO2 + OH + #.437 RO2C + #.043 RO2XC + #.043 zRNO3 + #.015 xCCHO + #.489 RCHO + #.032 xRCHO + #.079 PROD2 + #.39 xPROD2 + #.479 yROOH + #.335 XC	Phot Set= COOH			
BP28	RAOOH + OH = #.148 HO2 + #.565 xHO2 + #.139 OH + #.024 xOH + #.589 RO2C + #.124 RO2XC + #.124 zRNO3 + #.448 xRCHO + #.147 MGLY + #.26 xMGLY + #.139 IPRD + #.077 xAFG1 + #.147 xAFG2 + #.074 PROD2 + #.011 xPROD2 + #.713 yROOH + #2.366 XC	1.41e-10			
BP29	RAOOH + HV = HO2 + OH + #.661 MGLY + #.584 AFG1 + #1.01 AFG2 + #-1.951 XC	Phot Set= COOH			
BP34	MGLY + HV = HO2 + MECO3 + CO	Phot Set= MGLY-06			
BP35	MGLY + OH = MECO3 + CO	1.50e-11			
BP36	MGLY + NO3 = MECO3 + HNO3 + CO	2.53e-15	1.40e-12	3.77	
BP38	CRES + OH = #.8 xHO2 + #.2 BZO + #.8 RO2C + #.25 xMGLY + #.8 yROOH + #5.05 XC	4.03e-11	1.70e-12	-1.89	
BP39	CRES + NO3 = BZO + HNO3 + XC	1.40e-11			
BP46	AFG1 + OH = #.521 xHO2 + #.201 xMECO3 + #.217 RCO3 + #.723 RO2C + #.06 RO2XC + #.06 zRNO3 + #.334 CO + #.407 xRCHO + #.301 xMGLY + #.018 xAFG1 + #.048 xPROD2 + #.783 yROOH + #.753 XC	7.40e-11			
BP47	AFG1 + O3 = #.522 HO2 + #.826 OH + #.652 xRCO3 + #.652 RO2C + #.522 CO + #.174 CO2 + #.652 xHCHO + #.707 MGLY + #.072 AFG1 + #.652 yROOH + #-.786 XC	9.66e-18			
BP48	AFG1 + HV = #1.023 HO2 + #.173 xHO2 + #.305 MECO3 + #.5 RCO3 + #.173 RO2C + #.695 CO + #.173 xHCHO + #.368 MGLY + #.033 AFG1 + #.173 yROOH + #.756 XC	Phot Set= AFG1			

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
BP49	AFG2 + OH = #.521 xHO2 + #.201 xMECO3 + #.217 RCO3 + #.723 RO2C + #.06 RO2XC + #.06 zRNO3 + #.334 CO + #.407 xRCHO + #.301 xMGLY + #.018 xAFG1 + #.048 xPROD2 + #.783 yROOH + #.753 XC	7.40e-11			
BP50	AFG2 + O3 = #.522 HO2 + #.826 OH + #.652 xRCO3 + #.652 RO2C + #.522 CO + #.174 CO2 + #.652 xHCHO + #.707 MGLY + #.072 AFG1 + #.652 yROOH + #-.786 XC	9.66e-18			
BP51	AFG2 + HV = PROD2 + #-1 XC	Phot Set= AFG1			
BP64	IPRD + OH = #.496 xHO2 + #.238 xMECO3 + #.241 RCO3 + #.734 RO2C + #.025 RO2XC + #.025 zRNO3 + #.238 CO + #.149 xHCHO + #.051 xCCHO + #.243 xRCHO + #.215 xMGLY + #.01 xAFG1 + #.192 xPROD2 + #.76 yROOH + #.587 XC	6.19e-11			
BP65	IPRD + O3 = #.211 HO2 + #.025 xHO2 + #.219 OH + #.053 xRCO3 + #.053 RO2C + #.483 CO + #.13 CO2 + #.086 HCHO + #.033 xHCHO + #.051 CCHO + #.02 xCCHO + #.86 MGLY + #.002 AFG1 + #.033 PROD2 + #.095 ALK3 + #.053 yROOH + #.8 XC	4.18e-18			
BP66	IPRD + NO3 = #.792 xHO2 + #.158 RCO3 + #.792 RO2C + #.05 RO2XC + #.05 zRNO3 + #.158 HNO3 + #.57 CO + #.222 xHCHO + #.213 xRCHO + #.008 xMGLY + #.559 xRNO3 + #.842 yROOH + #.283 XN + #-.583 XC	1.00e-13			
BP67	IPRD + HV = #.655 HO2 + #.141 xHO2 + #.084 OH + #.27 MECO3 + #.084 xMECO3 + #.343 RCO3 + #.225 RO2C + #.867 CO + #.204 HCHO + #.225 xHCHO + #.184 CCHO + #.246 PROD2 + #.225 yROOH + #.123 XC	Phot Set= MACR-06			
BP68	PROD2 + OH = #.472 HO2 + #.379 xHO2 + #.029 xMECO3 + #.049 xRCO3 + #.473 RO2C + #.071 RO2XC + #.071 zRNO3 + #.002 HCHO + #.211 xHCHO + #.001 CCHO + #.083 xCCHO + #.143 RCHO + #.402 xRCHO + #.329 PROD2 + #.049 xPROD2 + #.528 yROOH + #1.082 XC	1.55e-11			
BP69	PROD2 + HV = #.913 xHO2 + #.4 MECO3 + #.6 RCO3 + #1.59 RO2C + #.087 RO2XC + #.087 zRNO3 + #.303 xHCHO + #.163 xCCHO + #.78 xRCHO + yROOH + #-.091 XC	Phot Set= MEK-06, qy= 4.86e-3			
BP70	RNO3 + OH = #.189 HO2 + #.305 xHO2 + #.019 NO2 + #.313 xNO2 + #.976 RO2C + #.175 RO2XC + #.175 zRNO3 + #.011 xHCHO + #.429 xCCHO + #.001 RCHO + #.036 xRCHO + #.012 PROD2 + #.094 xPROD2 + #.189 RNO3 + #.305 xRNO3 + #.793 yROOH + #.174 XN + #.372 XC	7.20e-12			

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
BP71	RNO3 + HV = #.344 HO2 + #.554 xHO2 + NO2 + #.721 RO2C + #.102 RO2XC + #.102 zRNO3 + #.074 HCHO + #.061 xHCHO + #.214 CCHO + #.23 xCCHO + #.074 RCHO + #.063 xRCHO + #.236 PROD2 + #.292 xPROD2 + #.657 yROOH + #.786 XC	Phot Set= IC3ONO2			
PO01	xHCHO = HCHO	k is variable parameter: RO2RO			
PO02	xHCHO = XC	k is variable parameter: RO2XRO			
PO03	xCCHO = CCHO	k is variable parameter: RO2RO			
PO04	xCCHO = #2 XC	k is variable parameter: RO2XRO			
PO05	xRCHO = RCHO	k is variable parameter: RO2RO			
PO06	xRCHO = #3 XC	k is variable parameter: RO2XRO			
PO11	xPROD2 = PROD2	k is variable parameter: RO2RO			
PO12	xPROD2 = #6 XC	k is variable parameter: RO2XRO			
PO15	xMGLY = MGLY	k is variable parameter: RO2RO			
PO16	xMGLY = #3 XC	k is variable parameter: RO2XRO			
PO21	xAFG1 = AFG1	k is variable parameter: RO2RO			
PO22	xAFG1 = #5 XC	k is variable parameter: RO2XRO			
PO23	xAFG2 = AFG2	k is variable parameter: RO2RO			
PO24	xAFG2 = #5 XC	k is variable parameter: RO2XRO			
PO31	xIPRD = IPRD	k is variable parameter: RO2RO			
PO32	xIPRD = #5 XC	k is variable parameter: RO2XRO			
PO33	xRNO3 = RNO3	k is variable parameter: RO2RO			
PO34	xRNO3 = #6 XC + XN	k is variable parameter: RO2XRO			
PO35	zRNO3 = RNO3 + #-1 XN	k is variable parameter: RO2NO			
PO36	zRNO3 = PROD2 + HO2	k is variable parameter: RO22NN			
PO37	zRNO3 = #6 XC	k is variable parameter: RO2XRO			
PO38	yROOH = ROOH + #-5 XC	k is variable parameter: RO2HO2			
PO39	yROOH = PROD2 + #-6 XC	k is variable parameter: RO2RO2M			
PO40	yROOH =	k is variable parameter: RO2RO			
PO44	yRAOOH = RAOOH + #-8 XC	k is variable parameter: RO2HO2			
PO45	yRAOOH = PROD2 + #-6 XC	k is variable parameter: RO2RO2M			
PO46	yRAOOH =	k is variable parameter: RO2RO			
BE01	CH4 + OH = xHO2 + RO2C + xHCHO + yROOH	6.62e-15	1.85e-12	3.36	
BE02	ETHENE + OH = xHO2 + RO2C + #1.61 xHCHO + #.195 xCCHO + yROOH	8.15e-12	Falloff, F=0.60, N=1.00		
		k0:	1.00e-28	0.00	-4.50
		inf:	8.80e-12	0.00	-0.85
BE03	ETHENE + O3 = #.16 HO2 + #.16 OH + #.51 CO + #.12 CO2 + HCHO + #.032 CCHO + #.018 ALK3 + #.235 XC	1.68e-18	9.14e-15	5.13	
BE04	ETHENE + NO3 = xHO2 + RO2C + xRCHO + yROOH + XN + #-1 XC	2.24e-16	3.30e-12	5.72	2.00
BE05	ETHENE + O3P = #.8 HO2 + #.8 xHO2 + #.8 RO2C + #.788 CO + #.788 xHCHO + #.1 CCHO + #.004 xMGLY + #.002 xAFG1 + #.8 yROOH + #.202 XC	7.43e-13	1.07e-11	1.59	

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
BE06	ISOPRENE + OH = #.907 xHO2 + #.986 RO2C + #.093 RO2XC + #.093 zRNO3 + #.624 xHCHO + #.907 xIPRD + yROOH + #-.717 XC	9.96e-11	2.54e-11	-0.81	
BE07	ISOPRENE + O3 = #.066 HO2 + #.266 OH + #.192 xRCO3 + #.192 RO2C + #.008 RO2XC + #.008 zRNO3 + #.275 CO + #.122 CO2 + #.4 HCHO + #.192 xHCHO + #.018 CCHO + #.7 IPRD + #.1 PROD2 + #.01 ALK3 + #.2 yROOH + #-.787 XC	1.34e-17	7.86e-15	3.80	
BE08	ISOPRENE + NO3 = #.749 xHO2 + #.187 xNO2 + #.936 RO2C + #.064 RO2XC + #.064 zRNO3 + #.936 xIPRD + yROOH + #.813 XN + #-.064 XC	6.81e-13	3.03e-12	0.89	
BE09	ISOPRENE + O3P = #.25 xHO2 + #.24 xRCO3 + #.49 RO2C + #.01 RO2XC + #.01 zRNO3 + #.49 xHCHO + #.75 PROD2 + #.5 yROOH + #-.77 XC	3.50e-11			
BL03	ALK3 + OH = #.931 xHO2 + #1.253 RO2C + #.07 RO2XC + #.07 zRNO3 + #.262 xHCHO + #.445 xCCHO + #.122 xRCHO + #.141 xPROD2 + #1.236 yROOH + #1.216 XC	2.31e-12	1.51e-12	-0.25	
BLC4	ALK4 + OH = #.766 xHO2 + #.007 xMECO3 + #1.708 RO2C + #.227 RO2XC + #.227 zRNO3 + #.001 CO + #.039 xHCHO + #.31 xCCHO + #.226 xRCHO + #.303 xPROD2 + #1.006 yROOH + #.469 XC	6.16e-12			
BL06	OLE1 + OH = #.905 xHO2 + #1.139 RO2C + #.095 RO2XC + #.095 zRNO3 + #.701 xHCHO + #.301 xCCHO + #.47 xRCHO + #.04 xIPRD + #.119 xPROD2 + #1.001 yROOH + #.801 XC	3.29e-11	6.18e-12	-1.00	
BL07	OLE1 + O3 = #.116 HO2 + #.144 xHO2 + #.193 OH + #.167 RO2C + #.004 RO2XC + #.004 zRNO3 + #.368 CO + #.125 CO2 + #.5 HCHO + #.104 xHCHO + #.184 CCHO + #.007 xCCHO + #.353 RCHO + #.031 xRCHO + #.191 PROD2 + #.073 ALK3 + #.148 yROOH + #.904 XC	1.09e-17	3.15e-15	3.38	
BL08	OLE1 + NO3 = #.824 xHO2 + #1.312 RO2C + #.176 RO2XC + #.176 zRNO3 + #.009 xCCHO + #.002 xRCHO + #.002 xPROD2 + #.546 xRNO3 + yROOH + #.454 XN + #.634 XC	1.44e-14	4.73e-13	2.08	
BL09	OLE1 + O3P = #.45 RCHO + #.274 PROD2 + #2.004 XC	5.02e-12	1.49e-11	0.65	
BL10	OLE2 + OH = #.914 xHO2 + #.966 RO2C + #.086 RO2XC + #.086 zRNO3 + #.209 xHCHO + #.788 xCCHO + #.481 xRCHO + #.066 xIPRD + #.06 xPROD2 + yROOH + #.568 XC	6.42e-11	1.26e-11	-0.97	

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
BL11	OLE2 + O3 = #.093 HO2 + #.329 xHO2 + #.423 OH + #.147 xMECO3 + #.008 xRCO3 + #.49 RO2C + #.003 RO2XC + #.003 zRNO3 + #.297 CO + #.162 CO2 + #.152 HCHO + #.398 xHCHO + #.473 CCHO + #.067 xCCHO + #.315 RCHO + #.018 xRCHO + #.049 IPRD + #.057 PROD2 + #.133 ALK3 + #.487 yROOH + #.455 XC	1.24e-16	8.14e-15	2.49	
BL12	OLE2 + NO3 = #.456 xHO2 + #.409 xNO2 + #1.218 RO2C + #.136 RO2XC + #.136 zRNO3 + #.107 xHCHO + #.546 xCCHO + #.154 xRCHO + #.033 xIPRD + #.009 xPROD2 + #.322 xRNO3 + #1.033 yROOH + #.269 XN + #.375 XC	7.85e-13	2.20e-13	-0.76	
BL13	OLE2 + O3P = #.014 HO2 + #.007 xHO2 + #.007 xRCO3 + #.013 RO2C + #.001 RO2XC + #.001 zRNO3 + #.006 CO + #.074 RCHO + #.006 xIPRD + #.464 PROD2 + #.014 yROOH + #1.933 XC	2.07e-11	1.43e-11	-0.22	
BL14	ARO1 + OH = #.166 HO2 + #.482 xHO2 + #.284 OH + #.482 RO2C + #.068 RO2XC + #.068 zRNO3 + #.201 MGLY + #.208 xMGLY + #.166 CRES + #.2 xAFG1 + #.39 xAFG2 + #.077 xPROD2 + #.147 yROOH + #.403 yRAOOH + #.789 XC	6.15e-12			
BL15	ARO2 + OH = #.108 HO2 + #.58 xHO2 + #.202 OH + #.58 RO2C + #.11 RO2XC + #.11 zRNO3 + #.143 MGLY + #.532 xMGLY + #.108 CRES + #.236 xAFG1 + #.424 xAFG2 + #.035 xPROD2 + #.089 yROOH + #.601 yRAOOH + #2.047 XC	2.57e-11			
BL16	TERP + OH = #.759 xHO2 + #.042 xRCO3 + #1.147 RO2C + #.2 RO2XC + #.2 zRNO3 + #.001 CO + #.264 xHCHO + #.533 xRCHO + #.029 xMGLY + #.003 xIPRD + #.259 xPROD2 + yROOH + #5.15 XC	7.98e-11	1.87e-11	-0.86	
BL17	TERP + O3 = #.052 HO2 + #.067 xHO2 + #.585 OH + #.126 xMECO3 + #.149 xRCO3 + #.875 RO2C + #.203 RO2XC + #.203 zRNO3 + #.185 CO + #.045 CO2 + #.079 HCHO + #.15 xHCHO + #.017 CCHO + #.22 xRCHO + #.083 xMGLY + #.002 xIPRD + #.41 PROD2 + #.012 xPROD2 + #.028 ALK3 + #.545 yROOH + #4.026 XC	6.99e-17	9.57e-16	1.56	
BL18	TERP + NO3 = #.162 xHO2 + #.421 xNO2 + #.019 xRCO3 + #1.509 RO2C + #.397 RO2XC + #.397 zRNO3 + #.01 CO + #.017 xHCHO + #.001 xCCHO + #.509 xRCHO + #.001 xMGLY + #.006 xIPRD + #.012 xPROD2 + #.163 xRNO3 + yROOH + #.416 XN + #4.919 XC	6.53e-12	1.28e-12	-0.97	
BL19	TERP + O3P = #.147 RCHO + #.853 PROD2 + #4.441 XC	3.71e-11			

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
	Chlorine Mechanism				
CI01	CL2 + HV = #2 CL	Phot Set= CL2			
CI08	CL + HO2 = HCL + O2	3.44e-11	3.44e-11	0.00	-0.56
CI09	CL + HO2 = CLO + OH	9.41e-12	9.41e-12	0.00	2.10
CI10	CL + O3 = CLO + O2	1.22e-11	2.80e-11	0.50	
CI11	CL + NO3 = CLO + NO2	2.40e-11			
CI12	CLO + NO = CL + NO2	1.66e-11	6.20e-12	-0.59	
CI13	CLO + NO2 = CLONO2	2.29e-12	Falloff, F=0.60, N=1.00		
		k0:	1.80e-31	0.00	-3.40
		inf:	1.50e-11	0.00	-1.90
CI14	CLONO2 + HV = CLO + NO2	Phot Set= CLONO2-1			
CI15	CLONO2 + HV = CL + NO3	Phot Set= CLONO2-2			
CI16	CLONO2 = CLO + NO2	4.12e-4	Falloff, F=0.60, N=1.00		
		k0:	4.48e-5	24.90	-1.00
		inf:	3.71e+15	24.90	3.50
CI17	CL + CLONO2 = CL2 + NO3	1.01e-11	6.20e-12	-0.29	
CI20	CLO + CLO = #.29 CL2 + #1.42 CL + O2	1.82e-14	1.25e-11	3.89	
CI21	OH + HCL = H2O + CL	7.90e-13	1.70e-12	0.46	
CI22	CL + H2 = HCL + HO2	1.77e-14	3.90e-11	4.59	
CP01	HCHO + CL = HCL + HO2 + CO	7.33e-11	8.10e-11	0.06	
CP02	CCHO + CL = HCL + MECO3	8.00e-11	8.00e-11		
CP04	RCHO + CL = HCL + #.1 xHO2 + #.9 RCO3 + #.1 RO2C + #.1 CO + #.1 xCCHO + #.1 yROOH	1.23e-10			
CP07	RNO3 + CL = HCL + #.055 HO2 + #.547 xHO2 + #.038 NO2 + #.159 xNO2 + #1.282 RO2C + #.202 RO2XC + #.202 zRNO3 + #.045 xHCHO + #.3 xCCHO + #.009 RCHO + #.02 xRCHO + #.019 PROD2 + #.061 xPROD2 + #.055 RNO3 + #.547 xRNO3 + #.907 yROOH + #.201 XN + #-.036 XC	1.92e-10			
CP08	PROD2 + CL = HCL + #.314 HO2 + #.541 xHO2 + #.007 xMECO3 + #.022 xRCO3 + #.679 RO2C + #.116 RO2XC + #.116 zRNO3 + #.237 xHCHO + #.109 xCCHO + #.198 RCHO + #.591 xRCHO + #.116 PROD2 + #.059 xPROD2 + #.686 yROOH + #1.353 XC	2.00e-10			
CP10	MGLY + CL = HCL + MECO3 + CO	8.00e-11			
CP11	CRES + CL = HCL + xHO2 + yROOH + #7 XC	6.20e-11			
CC13	ROOH + CL = HCL + #.345 xHO2 + #.264 OH + #.326 xOH + #.862 RO2C + #.065 RO2XC + #.065 zRNO3 + #.047 xHCHO + #.15 xCCHO + #.183 RCHO + #.465 xRCHO + #.081 PROD2 + #.202 xPROD2 + #.737 yROOH + #.618 XC	2.41e-10			

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
CP15	RAOOH + CL = #.404 HCL + #.148 HO2 + #.565 xHO2 + #.139 OH + #.024 xOH + #.589 RO2C + #.124 RO2XC + #.124 zRNO3 + #.448 xRCHO + #.147 MGLY + #.26 xMGLY + #.139 IPRD + #.077 xAFG1 + #.147 xAFG2 + #.074 PROD2 + #.011 xPROD2 + #.713 yROOH + #2.366 XC	4.29e-10			
CP18	IPRD + CL = #.221 HCL + #.033 HO2 + #.597 xHO2 + #.221 xMECO3 + #.102 RCO3 + #.943 RO2C + #.047 RO2XC + #.047 zRNO3 + #.333 CO + #.077 xHCHO + #.259 xRCHO + #.007 xMGLY + #.066 xIPRD + #.017 AFG1 + #.004 xAFG1 + #.034 AFG2 + #.008 xAFG2 + #.865 yROOH + #2.114 XC	4.12e-10			
CP23	xCL = CL	k is variable parameter: RO2RO			
CP24	xCL =	k is variable parameter: RO2XRO			
CE01	CH4 + CL = HCL + xHO2 + RO2C + xHCHO + yROOH	1.02e-13	7.30e-12	2.54	
CE02	ETHENE + CL = xHO2 + #2 RO2C + xHCHO + XC	1.04e-10	Falloff, F=0.60, N=1.00		
		k0:	1.60e-29	0.00	-3.30
		inf:	3.10e-10	0.00	-1.00
CE03	ISOPRENE + CL = #.15 HCL + #.738 xHO2 + #.177 xCL + #1.168 RO2C + #.085 RO2XC + #.085 zRNO3 + #.275 xHCHO + #.02 xRCHO + #.848 xIPRD + yROOH + #-.085 XC	4.80e-10			
BC03	ALK3 + CL = HCL + #.929 xHO2 + #1.361 RO2C + #.07 RO2XC + #.07 zRNO3 + #.172 xHCHO + #.34 xCCHO + #.343 xRCHO + #.105 xPROD2 + #1.094 yROOH + #1.067 XC	1.86e-10			
CLC4	ALK4 + CL = HCL + #.76 xHO2 + #.002 xMECO3 + #1.664 RO2C + #.237 RO2XC + #.237 zRNO3 + #.002 CO + #.031 xHCHO + #.207 xCCHO + #.353 xRCHO + #.26 xPROD2 + #1.002 yROOH + #.507 XC	3.20e-10			
BC06	OLE1 + CL = #.308 HCL + #.902 xHO2 + #1.42 RO2C + #.098 RO2XC + #.098 zRNO3 + #.025 xHCHO + #.146 xCCHO + #.287 xRCHO + #.229 xIPRD + yROOH + #2.09 XC	3.55e-10			
BC07	OLE2 + CL = #.263 HCL + #.448 xHO2 + #.448 xCL + #1.515 RO2C + #.104 RO2XC + #.104 zRNO3 + #.229 xHCHO + #.361 xCCHO + #.38 xRCHO + #.283 xIPRD + #.021 xPROD2 + #1.001 yROOH + #.747 XC	3.83e-10			
BC08	ARO1 + CL = #.88 xHO2 + #.88 RO2C + #.12 RO2XC + #.12 zRNO3 + #.21 xPROD2 + #5.02 XC	1.00e-10			
BC09	ARO2 + CL = #.842 xHO2 + #.842 RO2C + #.158 RO2XC + #.158 zRNO3 + #.224 xPROD2 + #6.708 XC	2.18e-10			

Table A-5 (continued)

Label	Reaction and Products [a]	Rate Parameters [b,c] k(300)	A	Ea	B
BC10	TERP + CL = #.548 HCL + #.252 xHO2 + #.068 xCL + #.034 xMECO3 + #.066 xRCO3 + #2.258 RO2C + #.582 RO2XC + #.582 zRNO3 + #.035 CO + #.158 xHCHO + #.218 xRCHO + #.007 xMGLY + #.161 xIPRD + #.007 xAFG1 + #.012 xAFG2 + #.019 xPROD2 + yROOH + #4.356 XC	5.46e-10			
	Reactions of Chloroform (used for test calculations only)				
TS01	CHCL3 + OH = xCL + RO2C + yROOH + XC	1.06e-13	5.67e-13	1.00	2.00
TS02	CHCL3 + CL = HCL + xCL + RO2C + yROOH + XC	1.22e-13	3.30e-12	1.97	

[a] Format of reaction listing: "=" separates reactants from products; "*#number*" indicates stoichiometric coefficient, "*#coefficient* {*product list*}" means that the stoichiometric coefficient is applied to all the products listed.

[b] Except as indicated, the rate constants are given by $k(T) = A \cdot (T/300)^B \cdot e^{-Ea/RT}$, where the units of k and A are cm^3 $molec^{-1}$ s^{-1}, Ea are kcal mol^{-1}, T is ^oK, and R=0.0019872 kcal mol^{-1} deg^{-1}. The following special rate constant expressions are used:

Phot Set = *name*: The absorption cross sections and (if applicable) quantum yields for the photolysis reaction are documented by Carter (2010a) and are available at http://www.cert.ucr.edu/~carter/SAPRC, where "*name*" indicates the photolysis set used. If a "qy=*number*" notation is given, the number given is the overall quantum yield, which is assumed to be wavelength independent.

Falloff: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = \{k0(T)\cdot[M]/[1 + k0(T)\cdot[M]/kinf(T)]\}\cdot F^Z$, where $Z = \{1 + [\log10\{k0(T)\cdot[M])/kinf(T)\}/N]^2\}^{-1}$, [M] is the total pressure in molecules cm^{-3}, F and N are as indicated on the table, and the temperature dependences of k0 and kinf are as indicated on the table.

k = k0+k3M(1+k3M/k2): The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k0(T) + k3(T)\cdot[M] \cdot(1 + k3(T)\cdot[M]/k2(T))$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k0, k2 and k3 are as indicated on the table.

k = k1 + k2 [M]: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k1(T) + k2(T)\cdot[M]$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k1, and k2 are as indicated on the table.

Same K as Rxn xx: Uses the same rate constant as the reaction in the base mechanism with the same label.

[c] See Footnotes [c], [d], and [e] in Table A-2 for methods used to calculate rates of the xPROD, zRNO3, and yROOH species.

APPENDIX B. CHANGE LOG

In this Appendix, the changes to the mechanisms and the mechanism documentation that have been made since the mechanism and this report were first distributed in July, 2008 are listed. If the mechanism needs to be changed or corrected in the future, this report and the supplementary material will be changed accordingly, and the modifications will be listed in this section.

3/13/09 Several corrections and revisions were made to the uncondensed SAPRC-07 mechanism as a result of problems discovered during the peer review of the mechanism. These are discussed in Appendix E of the updated SAPRC-07 mechanism documentation report (Carter, 2010a). The changes relevant to the condensed mechanisms documented here are as follows:

- An error in the activation energy for the $HO_2 + O_3$ reaction was corrected. This resulted in 20% increase in this rate constant at 300^oK.
- The rate constant expression for the reaction of OH radicals with methyl hydroperoxide was changed to that recommended by the NASA (2006) evaluation. This gives a 300^oK rate constant that is 35% higher than that previously used, which was from the IUPAC (2006) evaluation. The branching ratios for the two competing reactions were also changed slightly to be consistent with the NASA (2006) recommendation.
- The group additivity parameters used in the mechanism generation system to estimate rate constants for reactions of OH radicals with organic hydroperoxides were modified to be consistent with the revised rate constant and branching ratio used for OH + methyl hydroperoxide. The parameters used in the previous version of the mechanism were in error. The revised group additivity parameters resulted in changes in the rate constants and the product distributions derived for the reactions of OH with the lumped higher hydroperoxide species ROOH, R6OOH, and RAOOH. The products of the CL + RAOOH reaction were also revised, since they were estimated based on those for the OH reaction.

4/7/09 The condensed mechanisms documented in this report, the report itself, and the files implementing the mechanisms were revised where needed to be consistent with the changes in the uncondensed mechanism discussed above. The $HO_2 + O_3$ and the OH + hydroperoxide rate constants were corrected, including the OH + XOOH rate constant, which is the average of those for ROOH and R6OOH, and the products for the affected hydroperoxide reactions were also corrected. The plots and tables in this report showing effects of condensations and other model simulation results have been updated to reflect the current versions of the uncondensed and condensed mechanisms.

Note that the data used to derive the incremental reactivities on Figure 2 and Figure 3 and the reactivity weighting factors derived from them, given on Table 1, were not recalculated using the revised mechanism. The differences are expected to be small, and this is consistent with the relatively small effects of the mechanism condensations resulting from using these unrevised factors with the updated mechanisms.

7/13/09 Methane was retained in the condensed versions of the mechanisms so they can be used in cleaner air scenarios where methane may be important. The recommended procedure for removing it is now to treat methane as a constant species.

Table A-5 (continued)

1/15/10 All mechanisms revised to be consistent with the current base SAPRC07 mechanism as of 12/31/09. See Appendix E of Carter (2010a) for a discussion of the updates made to the mechanism up to this time.

Condensation levels C1, C2, and C3 were revised so that the effect of removing MEO2 can be seen. This had no effect on the CS07A and CS07B mechanisms.

The reaction of Cl with methane was retained in the condensed mechanisms. This was omitted in previous versions even though methane was retained.

1/28/10 An error in the files implementing the mechanisms, resulting in the rate constant for the O^1D+H_2O reaction being low by ~18%, was corrected, and all calculations were redone. This had no significant effects on the evaluations, but had small but nonnegligible effects (on the order of ~10%) on ambient O_3 simulations Affected plots and mechanism listings (that previously did not give the temperature dependence for this reaction) were corrected.