IV. CONDENSATION OF THE MECHANISM

The detailed mechanism discussed in the previous sections, with its separate representation of over 100 detailed model species and its relatively large number of reactive product species, is clearly too large for use in most airshed models. For that reason, condensed versions of the mechanism were developed. The condensation of this mechanism involved two tasks: (1) reducing the number of species used to represent the reactive organic products, and (2) reducing the number of species used to represent the emitted primary organics. By "reactive organic products" we mean species such as formaldehyde, acetaldehyde, cresols, etc., which are formed from the reactions of other organics, and which are represented explicitly in the mechanism. By "primary emitted organics" we mean species such as alkanes, alkenes, aromatics, alcohols, etc., which are emitted and are not formed as a product from any other species, and which are represented in the mechanism with generalized reactions with variable mechanistic parameters. The methods used to reduce the number of species in the mechanism which represent each of these two types of reactant are different, and can be discussed and evaluated separately.

A number of options were examined both with regard to the number of reactive organic products and the number of lumped species used to represent the primary emitted organics. In both cases, the predictions of the condensed mechanisms were compared with more detailed versions of the mechanism in a series of test calculations. As a result of this evaluation, a condensed mechanism was developed where the number of active species used to represent the number of reactive organic products was reduced from 18 to 8, and where the emitted alkanes, aromatics, and alkenes can be represented by a variable number of lumped species with mechanistic parameters derived based on the distribution of species which they represent. Test calculations indicate that as few as four lumped species can be used to represent these emitted organics, though they indicate that use of at least six for this purpose is preferable. The condensed mechanisms, and the test calculations used to evaluate them, are documented in this section.

A. Summary of the Condensed Mechanisms

1. Condensation of Reactive Organic Product Species

The species used to represent the reactive organic product species in the detailed and the condensed mechanism developed in this program are summarized in Table 18. As indicated there, the detailed mechanism uses 18 model species to represent reactive organic products, and the condensed mechanism we recommend for use in airshed models, which is designated the "standard" condensed mechanism on the table, employs half this number. The condensation of the detailed mechanism to obtain the standard, or "level C" mechanism followed the same general approach as that employed in the condensation of the previous mechanism described by Lurmann et al. (1987a), though some of the assumptions and approaches employed by Lurmann et al. (1987a) were examined in test calculations, and some modifications were made. Among the modifications which were examined in the condensation test calculations was the use of alternative mechanisms where the species used to represent the aromatic ring fragmentation products were either kept at the same level as employed in the more detailed mechanism, or were reduced even further. The reactive organic product species used in these two alternative condensed mechanisms, which are designated as "Level B" and "Level D," respectively, are also listed in Table 18. A summary of the condensations which were made to the detailed mechanism, and a comparison of this condensed mechanism with the "condensed SAPRC/ERT" mechanism described by Lurmann et al. (1987a), is given below.

(1) As with the condensed SAPRC/ERT mechanism, the lumped higher aldehyde (RCHO), represented by propionaldehyde, was removed and is represented by acetaldehyde (CCHO). However, in order to determine whether a 1:1 representation, as incorporated in previous mechanisms was appropriate, we carried out calculations of the incremental reactivities of "pure product forming pseudo species" for these aldehydes for a variety of scenarios used in our previous reactivity studies (see Carter and Atkinson 1987 for a discussion of incremental reactivities, the "pure product pseudo-species" concept and the types of scenarios employed), and found that replacing RCHO by 1.5 CCHO was a better substitution, at least in terms of effects of predictions of maximum ozone yields. Thus the 1:1.5 substitution was used rather than the 1:1 ratio employed in the

Table 18. Species Used to Represent Reactive Organic Products in the Detailed and the Condensed Mechanisms

Model Species Name				Description
Level A (Detailed)	Level B	Level C (Standard Condensed)	Level D	
HCHO	HCHO	HCHO	HCHO	Formaldehyde
CCHO	CCHO	CCHO	CCHO	Acetaldehyde or higher aldehydes
RCHO				Higher aldehydes
ACET				Acetone
MEK	MEK	MEK	MEK	Higher ketones or all ketones
RNO3	RNO3	RNO3	RNO3	Alkyl nitrates
PAN	PAN	PAN	PAN	PAN or all PAN analogues
PPN				Higher PAN analogues
GPAN				PAN analogue formed from glyoxal
PBZN				Peroxy benzoyl nitrate
BALD				Aromatic aldehydes
PHEN				Phenol
CRES	CRES	CRES	CRES	Alkyl phenols or all phenols
NPHE				Nitrophenols
GLY	GLY			Glyoxal
MGLY	MGLY	MGLY		Methyl glyoxal
AFG1	AFG1			Uncharacterized aromatic fragmentation product #1
AFG2	AFG2	AFG2		Uncharacterized aromatic fragmentation product #2
			AFRG	Aromatic fragmentation products

condensed SAPRC/ERT mechanism. Note that this substitution has the additional advantage that the number of carbons are conserved. As with condensed SAPRC/ERT mechanism, removal of RCHO also resulted in removal of its corresponding PAN analogue.

(2) The condensed SAPRC/ERT mechanism also has acetone removed from the set of reactive product species, essentially assuming that its reactions are negligible. In order to examine whether this was appropriate, we compared the calculated incremental reactivities of "pure product forming pseudo-species" for acetone and MEK. We found that in terms of predictions of ozone, representing acetone by 0.33 MEK was a better approximation than ignoring it entirely. Therefore, in this version of the condensed mechanism, instead of neglecting the reactions of acetone, it is represented by 0.33 MEK.

(3) We were concerned about the neglect of the formation of benzaldehyde in the reactions of the aromatics in the condensed SAPRC/ERT mechanism, since benzaldehyde is actually a highly reactive species in a negative sense (Carter and Atkinson 1987), being an effective sink for both radicals and NO_x. Thus, again by calculating incremental reactivities of "pure product forming pseudo-species," we compared the contribution of benzaldehyde formation to formation of the other reactive aromatic products to the incremental reactivities of the aromatics. The results of this re-assured us that the neglect of benzaldehyde is indeed an acceptable approximation, since in all cases benzaldehyde had relatively small contributions to the reactivities of the aromatics, compared to the other products. Thus, as with condensed SAPRC/ERT, benzaldehyde was removed from the mechanism. Since none of the other reactive product species in the mechanism react in a manner very analogous to those of benzaldehyde, we did not consider it appropriate to represent benzaldehyde by any other reactive product species in the mechanism. In any case, it should be noted that any minor errors in the aromatic mechanisms introduced by neglecting benzaldehyde formation could be compensated for, at least in part, by the re-optimization of the aromatic mechanistic parameters we carried out as part of the re-formulation of the representation of the other aromatic products, discussed below.

(4) The phenolic products formed in the reactions of aromatic hydrocarbons represent significant NO_x sinks, and thus cannot be

neglected. In the detailed model, these phenolic products are represented by PHEN, CRES and NPHE (for phenol, cresol, and nitrophenol, respectively). In the condensed SAPRC/ERT mechanism, PHEN was eliminated because it is significant only in the photooxidation of benzene, which is relatively unreactive and whose reactions are ignored in the condensed SAPRC/ERT mechanism, but CRES and NPHE were retained. These species are consumed primarily by reaction with NO_3 radicals (though the CRES + OH reactions are also included in the mechanisms), with the main difference between them being the rate constant used for the NO_3 reactions, and the fact that it is assumed that CRES forms NPHE in its NO_3 reactions, while the product formed in the NPHE + NO_3 reaction is assumed to be too non-volatile to be reactive, and is thus ignored.

In view of the similarity between the reactions of CRES and NPHE, we investigated using CRES to represent the reactions of both. The NO_x that is tied up in the formation of NPHE is taken care of by adding a new steady-state pseudo-species "-NO2," which reacts with NO_2 to remove NO_x, or with HO_2 or unimolecularly in the absence of NO_x, with the same rate constants as used in the detailed model for phenoxy radicals, or "BZ-O." However, a simple substitution of CRES for NPHE would not be satisfactory, since the NO_3 reaction with CRES would then be represented as

NO3 + CRES = HNO3 + -NO2 + CRES,

with CRES being "recycled" to catalytically remove NO_x. This would result in significantly more NO_x removal than in the detailed mechanisms, where the mechanism is, in effect,

NO3 + CRES = HNO3 + -NO2 + (second phenolic product)

NO3 + (second phenolic product) = HONO2 + -NO2 + (unreactive product).

Thus the detailed mechanism has a limit of four moles of NO_x being removed for each mole of CRES formed, while there is no such limit if the simple substitution formulation were employed. On the other hand, the alternative of ignoring NPHE reactions entirely is also unacceptable, since the amount of NO_x removed by NPHE reactions in the detailed model can be

significant. However, these difficulties can be bypassed if the above reactions are represented by

NO3 + CRES = HNO3 + -NO2 + 0.5 CRES.

Under conditions where consumption by reaction with NO_3 is the dominant fate for phenolic species, it can be shown mathematically that this results in the same maximum amount of NO_x removal as the two-step process used by the more detailed mechanism. This approach was used to remove NPHE from the mechanism, while avoiding the possibility of catalytic NO_x removal which would be caused by a simple replacement of NPHE by CRES.

(5) The photooxidations of the aromatic hydrocarbons involve the formation of a number of aromatic ring-fragmentation products, most of which are poorly characterized. In the detailed mechanism, these products are represented by glyoxal and methylglyoxal (representing themselves), and the pseudo-species designated AFG1 and AFG2, used to represent all other fragmentation products. [AFG1 is used to represent those formed from benzene and naphthalene, and AFG2 is used to represent those formed from alkyl-substituted benzenes and naphthalenes.] The yields of AFG1 and AFG2 from the aromatics used in the detailed mechanism were adjusted using non-linear, least-squares optimization to fit the chamber data, as described previously (Carter et al. 1987, Lurmann et al. 1987a). The glyoxal and AFG1 were removed from the condensed SAPRC/ERT mechanism, based on the argument that benzene emissions do not contribute significantly to ozone formation. However, these species are also used in the mechanisms derived for the naphthalenes, which, in general, are much more reactive compounds (though their contributions to emissions are relatively minor.) To examine the impact of neglecting these species, glyoxal and AFG1 were retained in the "Level B" version of the new condensed mechanism, but were removed from the "Level C" version. This involved representing AFG1 by AFG2 (with the yields re-optimized as discussed below), and representing glyoxal by 0.4 formaldehyde + 0.3 acetaldehyde. The latter representation was derived based on incremental reactivity calculations of "pure product forming" species, as discussed above.

Methylglyoxal and AFG2 were retained in the condensed SAPRC/ERT mechanism, and also in both levels "B" and "C" of the new condensed mechanism.

However, these two species are similar in their reaction mechanisms, with the major difference between them (at least in the condensed mechanism, where all PAN species are lumped together) being that, in order to fit results of aromatic-NO_x-air chamber experiments carried out using black-light irradiations, we had to assume that AFG2 [and AFG1] photodecompose at significantly lower wavelengths than do the alpha-dicarbonyls. In view of the many other uncertainties and approximations involved in the current aromatic photooxidation mechanism, the retention of two separate species to represent this effect did not seem to be necessarily appropriate. Thus to investigate the effects of replacing these two with a single aromatic fragmentation species, in the "Level D" condensed mechanism both methylglyoxal and AFG2 were replaced by a single species designated "AFRG," for "aromatic fragmentation" product. This species was represented as reacting like methylglyoxal, with the same photodecomposition rate in sunlight for solar zenith angle of zero, with the only difference being that the ratio of its photolysis rate to that of NO_2 was assumed to be constant. NO_2 was used to define the zenith angle dependence of the photolysis of this species because the zenith angle dependence of the photolysis of NO_2 is intermediate in behavior between those for methylglyoxal and those for the "unknown" fragmentation products of the detailed mechanism.

Because of the changes in the representation of both the ring-fragmentation and the phenolic products in the three versions of the new condensed mechanism, for all three mechanisms the yields of the aromatic fragmentation product(s), which for the detailed mechanism were derived based on optimizations against chamber data (as described by Carter et al. 1987, and summarized in Table 7), were re-derived using optimizations with the formulations of the condensed mechanisms. The same general procedures were employed in the optimizations for the condensed mechanisms as used for the detailed mechanism, and the same sets of experimental data, as indicated in the comments in Table 7, were used in the optimization. We did not optimize against the predictions of the detailed mechanism because for the aromatics, even the "detailed" mechanism is condensed and approximate in its representation of the aromatic fragmentation products. For this reason, we considered it more appropriate to use the experimental

data, rather than the detailed mechanism, as the standard against which to derive the parameters for the condensed mechanisms.

(6) The condensed SAPRC/ERT mechanism also ignores the reactions of H_2O_2 and "-OOH," the pseudo-species used to represent radical formation due to photolysis of the organic hydroperoxide group. This is not an acceptable approximation for mechanisms to be used in acid deposition modeling, since H_2O_2 and hydroperoxides are believed to be important in the aqueous phase oxidation of SO_2. However, these species have relatively little effect on most other predictions, so for model applications not concerned with SO_2 oxidation and acid deposition, this may be a good approximation. The users of this mechanism have the option to include or exclude these reactions, and test calculations employing both options are presented here.

A complete listing of the reactions used in the standard, or "Level C" conversion mechanism is given in Table 19, and a listing of the mechanistic parameters derived for the aromatics for use with this mechanism is given in Table 20. This mechanism employs the same set of species as employed in the detailed mechanism (listed in Table 1), except for the smaller number of reactive organic product species, as indicated in Table 18. In addition, except for the condensations discussed above, the reactions, mechanisms, and rate constants are the same as employed in the detailed mechanism as documented in Section II. In particular, the condensed mechanism has the same inorganic and almost the same general peroxy radical reactions as used in the detailed mechanism. (The only difference in the general peroxy radical reactions is that since there is only one acyl peroxy radical species in the condensed mechanism, namely acetyl peroxy radicals, the general acyl peroxy radical species "RCO3." now refers specifically to acetyl peroxy radicals, and the separate steady state species, "CCO-O2.," used in the detailed mechanism to represent acetyl peroxy radicals, was eliminated.) The condensed mechanism also uses the same mechanistic parameters as the detailed mechanism for the alkane, alkene, and other types of detailed model species, which are listed in Tables 6, 9, and 8, respectively. The aromatic parameters are different only for those aspects, primarily yields of uncharacterized ring-opening products, which had to be optimized based on fits to chamber data, as indicated above.

Table 19. Listing of the Reactions in the Condensed Mechanism Recommended for Use in Airshed Model Applications

Rxn. Label	Kinetic Parameters[a] k(300)	A	Ea	B	Reactions[b]
		Inorganic Reactions			
1		PHOT=NO2			NO2 + HV = NO + O
2	2.16E-05	2.16E-05	0.00	-4.30	O + O2 + M = O3 + M
3A	1.42E+04	9.54E+03	-0.24	-1.00	O + NO2 = NO + O2
3B	2.28E+03	FALLOFF	0.60	1.00	O + NO2 = NO3 + M
		0.32E-02	0.00	-4.00	
		0.32E+05	0.00	-1.00	
4	2.76E+01	2.94E+03	2.78	-1.00	O3 + NO = NO2 + O2
5	4.94E-02	2.06E+02	4.97	-1.00	O3 + NO2 = O2 + NO3
6	4.11E+04	2.50E+04	-0.30	-1.00	NO + NO3 = #2 NO2
7	6.90E-10	1.19E-10	-1.05	-2.00	NO + NO + O2 = #2 NO2
8	1.84E+03	FALLOFF	0.60	1.00	NO2 + NO3 = N2O5
		0.79E-01	0.00	-6.30	
		0.22E+04	0.00	-1.50	
9	2.26E-03	3.72E+13	22.26	1.00	N2O5 + #RCON8 = NO2 + NO3
10	1.47E-06	1.47E-06	0.00	-1.00	N2O5 + H2O = #2 HNO3
11	6.13E-01	3.67E+01	2.44	-1.00	NO2 + NO3 = NO + NO2 + O2
12A		PHOT=NO3NO			NO3 + HV = NO + O2
12B		PHOT=NO3NO2			NO3 + HV = NO2 + O
13A		PHOT=O3O3P			O3 + HV = O + O2
13B		PHOT=O3O1D			O3 + HV = O*1D2 + O2
14	3.23E+05	3.23E+05	0.00	-1.00	O*1D2 + H2O = #2 HO.
15	4.29E+04	2.82E+04	-0.25	-1.00	O*1D2 + M = O + M
16	7.05E+03	FALLOFF	0.60	1.00	HO. + NO = HONO
		0.25E-01	0.00	-4.60	
		0.22E+05	0.00	-1.50	
17		PHOT=HONO			HONO + HV = HO. + NO
18	1.66E+04	FALLOFF	0.60	1.00	HO. + NO2 = HNO3
		0.93E-01	0.00	-5.20	
		0.35E+05	0.00	-2.30	
19	1.51E+02	9.47E+00	-1.65	-1.00	HO. + HNO3 = H2O + NO3
21	3.52E+02	3.52E+02	0.00	-1.00	HO. + CO = HO2. + CO2
22	1.02E+02	2.35E+03	1.87	-1.00	HO. + O3 = HO2. + O2
23	1.21E+04	5.43E+03	-0.48	-1.00	HO2. + NO = HO. + NO2
24	2.00E+03	FALLOFF	0.60	1.00	HO2. + NO2 = HNO4
		0.65E-02	0.00	-5.20	
		0.69E+04	0.00	-2.40	
25	3.24E-03	1.95E+13	21.66	1.00	HNO4 + #RCON24 = HO2. + NO2
27	6.77E+03	1.91E+03	-0.75	-1.00	HNO4 + HO. = H2O + NO2 + O2
28	3.05E+00	1.61E+01	0.99	-1.00	HO2. + O3 = HO. + #2 O2
29A	2.54E+03	3.23E+02	-1.23	-1.00	HO2. + HO2. = HO2H + O2
29B	1.80E-03	6.82E-05	-1.95	-2.00	HO2. + HO2. + M = HO2H + O2

(continued)

Table 19 (continued) - 2

Rxn. Label	Kinetic Parameters[a] k(300)	A	Ea	B	Reactions[b]
29C	1.34E-01	1.11E-05	-5.60	-2.00	HO2. + HO2. + H2O = HO2H + O2 + H2O
29D	9.52E-02	2.37E-06	-6.32	-2.00	HO2. + HO2. + H2O = HO2H + O2 + H2O
30A		K SAME AS RXN 29A			NO3 + HO2. = HNO3 + O2
30B		K SAME AS RXN 29B			NO3 + HO2. + M = HNO3 + O2
30C		K SAME AS RXN 29C			NO3 + HO2. + H2O = HNO3 + O2 + H2O
30A		K SAME AS RXN 29D			NO3 + HO2. + H2O = HNO3 + O2 + H2O
31		PHOT=H2O2			HO2H + HV = #2 HO.
32	2.49E+03	4.84E+03	0.40	-1.00	HO2H + HO. = HO2. + H2O
33	1.45E+05	6.75E+04	-0.46	-1.00	HO. + HO2. = H2O + O2
		Reactions of SO_2			
34	1.29E+03	FALLOFF	0.60	1.00	SO2 + HO. = HO2. + H2SO4
		0.11E-01	0.00	-5.30	
		0.22E+04	0.00	-1.00	
SR1	3.38E-02	3.38E-02	0.00	-1.00	O3OL-SB + H2O =
SR2	1.47E+02	1.47E+02	0.00	-1.00	O3OL-SB + SO2 = H2SO4
		General Peroxy Radical Reactions			
B1	1.13E+04	6.17E+03	-0.36	-1.00	RO2. + NO = NO
B5	7.20E+03	2.57E+02	-1.99	-1.00	RO2. + HO2. = HO2.
B8	1.47E+00	1.47E+00	0.00	-1.00	RO2. + RO2. =
B2	1.13E+04	6.17E+03	-0.36	-1.00	RCO3. + NO = CO2 + NO2 + HCHO + RO2-R. + RO2.
B4	6.68E+03	FALLOFF	0.19	1.00	RCO3. + NO2 = PAN
		0.18E+01	0.00	-6.10	
		0.87E+04	0.00	-4.60	
B6	7.20E+03	2.57E+02	-1.99	-1.00	RCO3. + HO2. = -OOH + CO2 + HCHO
B9	4.40E+03	4.40E+03	0.00	-1.00	RCO3. + RO2. = RO2. + #.5 HO2. + CO2 + HCHO
B10	7.78E+03	7.78E+03	0.00	-1.00	RCO3. + RCO3. = #2 "HO2. + CO2 + HCHO"
C18	3.51E-02	FALLOFF	0.27	1.47	PAN = RCO3. + NO2
		0.91E+14	25.40	-1.00	
		0.13E+19	26.70	0.00	
B11		K SAME AS RXN B1			RO2-R. + NO = NO2 + HO2.
B12		K SAME AS RXN B5			RO2-R. + HO2. = -OOH
B13		K SAME AS RXN B8			RO2-R. + RO2. = RO2. + #.5 HO2.
B14		K SAME AS RXN B9			RO2-R. + RCO3. = RCO3. + #.5 HO2.
B19		K SAME AS RXN B1			RO2-N. + NO = RNO3
B20		K SAME AS RXN B5			RO2-N. + HO2. = -OOH + MEK + #1.5 -C

(continued)

Table 19 (continued) - 3

Rxn. Label	Kinetic Parameters[a] k(300)	A	Ea	B	Reactions[b]
B21		K SAME AS RXN B8			RO2-N. + RO2. = RO2. + #.5 HO2. + MEK + #1.5 -C
B22		K SAME AS RXN B9			RO2-N. + RCO3. = RCO3. + #.5 HO2. + MEK + #1.5 -C
B15		K SAME AS RXN B1			R2O2. + NO = NO2
B16		K SAME AS RXN B5			R2O2. + HO2. =
B17		K SAME AS RXN B8			R2O2. + RO2. = RO2.
B18		K SAME AS RXN B9			R2O2. + RCO3. = RCO3.
G2		K SAME AS RXN B1			RO2-XN. + NO = -N
G3		K SAME AS RXN B5			RO2-XN. + HO2. = -OOH
G4		K SAME AS RXN B8			RO2-XN. + RO2. = RO2. + #.5 HO2.
G5		K SAME AS RXN B9			RO2-XN. + RCO3. = RCO3. + HO2.
		Lumped Organic Hydroperoxide Reactions			
B7		PHOT=CO2H			-OOH + HV = HO2. + HO.
B7A	7.34E+03	7.34E+03	0.00	-1.00	HO. + -OOH = HO.
B7B	7.34E+03	7.34E+03	0.00	-1.00	HO. + -OOH = RO2-R. + RO2.
		Reactions of Formaldehyde			
C1		PHOT=HCHOAVGR			HCHO + HV = #2 HO2. + CO
C2		PHOT=HCHOAVGM			HCHO + HV = H2 + CO
C3	1.63E+04	2.35E+04	0.22	-1.00	HCHO + HO. = HO2. + CO + H2O
C4	1.62E+02	1.62E+02	0.00	-1.00	HCHO + HO2. = HOCOO.
C4A	1.20E+03	1.20E+03	0.00	0.00	HOCOO. = HO2. + HCHO
C4B		K SAME AS RXN B1			HOCOO. + NO = -C + NO2 + HO2.
C9	9.36E-01	4.11E+03	5.00	-1.00	HCHO + NO3 = HNO3 + HO2. + CO
		Reactions of Acetaldehyde and Lumped Higher Aldehydes			
C10	2.31E+04	8.22E+03	-0.62	-1.00	CCHO + HO. = RCO3. + H2O
C11A		PHOT=CCHOR			CCHO + HV = CO + HO2. + HCHO + RO2-R. + RO2.
C12	4.17E+00	2.06E+03	3.70	-1.00	CCHO + NO3 = HNO3 + RCO3.
		Lumped Ketone Reactions			
C44	1.92E+03	3.38E+03	0.34	-1.00	MEK + HO. = H2O + #.5 "CCHO + HCHO" + RCO3. + #1.5 "R2O2. + RO2." + #.5 -C
C57		PHOT=KETONE			MEK + HV + #QY.MEK = RCO3. + CCHO + RO2-R. + RO2.

(continued)

Table 19 (continued) - 4

Rxn. Label	Kinetic Parameters[a] k(300)	A	Ea	B	Reactions[b]
					Lumped Alkyl Nitrate Reactions
C95	3.03E+03	3.22E+04	1.41	-1.00	RNO3 + HO. = NO2 + #.155 MEK + #2.055 CCHO + #.16 HCHO + #.11 -C + #1.39 "R2O2. + RO2."
					Reactions of Methyl Glyoxal
C68A		PHOT=MEGLYOX1			MGLY + HV = HO2. + CO + RCO3.
C68B		PHOT=MEGLYOX2			MGLY + HV + #.107 = HO2. + CO + RCO3.
C69	2.48E+04	2.48E+04	0.00	-1.00	MGLY + HO. = CO + RCO3.
C70		K SAME AS RXN C12			MGLY + NO3 = HNO3 + CO + RCO3.
					Reactions of Cresols and Phenols
G52	6.02E+04	6.02E+04	0.00	-1.00	HO. + CRES = #.15 RO2-XN. + #.85 RO2-R. + #.2 MGLY + #.085 CRES + RO2. + #5.805 -C
G57	3.08E+04	3.08E+04	0.00	-1.00	NO3 + CRES = HNO3 + -NO2 + #.5 CRES + #3.5 -C
G43	2.20E+04	2.20E+04	0.00	-1.00	-NO2 + NO2 = -N
G44	4.40E+03	4.40E+03	0.00	-1.00	-NO2 + HO2. =
G45	6.00E-02	6.00E-02	0.00	0.00	-NO2 =
					Reactions of Uncharacterized Aromatic Fragmentation Products
G9	2.48E+04	2.48E+04	0.00	-1.00	HO. + AFG2 = RCO3.
G10		PHOT=AROMUNKN			AFG2 + HV = HO2. + CO + RCO3.
					Reactions of the N'th Lumped Alkane/Aromatic Group[c]
AnOH	(Depends on compounds being represented)				HO. + AARn = #AnRR RO2-R. + #AnNR RO2-N. + #AnRXN RO2-XN + #AnRH HO2. + #AnR2 R2O2. + #AnRO2 RO2. + #AnA1X HCHO + #AnA2X CCHO + #AnK4X MEK + #AnCO CO + #AnC2 CO2 + #AnCRES CRES + #AnMG MGLY + #AnU2 AFG2 + #AnXC -C

(continued)

Table 19 (continued) - 5

Rxn. Label	Kinetic Parameters[a] k(300)	A	Ea	B	Reactions[b]
					Reactions of Ethene
D1	1.24E+04	3.16E+03	-0.82	-1.00	ETHE + HO. = #.22 CCHO + #1.56 HCHO + RO2-R. + RO2.
D6	2.75E-03	1.76E+01	5.23	-1.00	ETHE + O3 = HCHO + #.37 O3OL-SB + #.44 CO + #.56 -C + #.12 HO2.
D8	1.09E+03	1.53E+04	1.57	-1.00	ETHE + O = HCHO + CO + HO2. + RO2-R. + RO2.
D9	3.28E-01	3.16E+03	5.47	-1.00	ETHE + NO3 = NO2 + #2 HCHO + R2O2. + RO2.
					Reactions of the N'th Lumped Higher Alkene Groups[d]
OnOH	0.00E+00	0.00E+00	0.00	-1.00	OLE1 + HO. = #OnP1R HCHO + #OnP23R CCHO + #OnP45R MEK + #OnPR RO2-R. + #OnPN RO2-N. + RO2. + #OnOHXC -C
OnO3	0.00E+00	0.00E+00	0.00	-1.00	OLE1 + O3 = #OnO3A1 HCHO + #OnO3A2 CCHO + #OnO3K4 MEK + #OnO3MG MGLY + #OnO3CO CO + #OnO3SB O3OL-SB + #OnO3RH HO2. + #OnO3OH HO. + #OnO3RR RO2-R. + #OnO3R2 R2O2. + #OnO3RO2 RO2. + #OnO3PS RCO3. + #OnO3XC -C
OnOA	0.00E+00	0.00E+00	0.00	-1.00	OLE1 + O = #.4 HO2. + #.5 MEK + #.75 CCHO + #OnOAXC -C
OnN3	0.00E+00	0.00E+00	0.00	-1.00	OLE1 + NO3 = NO2 + #OnP1 HCHO + #OnP23 CCHO + #OnP45 MEK + R2O2. + RO2. + #OnN3XC -C

[a]The formats of the kinetic parameter input is the same as used in Table 2 except that the T = 300 K rate constant, k(300), is also given, and the rate constants and Arrhenius A factors are given in ppm, minute units. The absorption coefficients and quantum yields used for the photolysis reactions are the same as used in the detailed mechanism, and are listed in Table 3.

[b]The format of the reaction lists given in this table are the same as used in Table 2, and is described in footnotes to that table.

[c]The mechanistic parameters which must be specified for the lumped alkane/aromatic groups are the same as those listed in Table 4 for the detailed mechanism, except that the parameters "AnGL," "AnBZ,"

(continued)

Table 19 (continued) - 6

and "AnPH" and "AnU1" are not used. The other mechanistic parameters are derived from the specified values as follows:

```
AnA1X   = AnA1 + 0.4 AnGL
AnA2X   = AnA2 + 1.5 AnA3 + 0.3 AnGL
AnK4X   = 0.33 AnK3 + AnK4
AnCRES  = AnCR + AnNP + AnPH
AnRXN   = AnNP + AnXN
AnRO2   = AnRR + AnNR + AnRXN + AnR2
AnXC    = AnNC - 5 AnNR - AnA1X - 2 AnA2X - 4 AnK4X - AnCO - AnC2
          - 7 AnCRES - 3 AnMG - 3 AnU2
```

[d]The mechanistic parameters which must be specified for the lumped alkene groups are the same as those listed in Table 5 for the detailed mechanism. The other parameters are calculated from the specified parameters as indicated below:

```
OnP23   = OnP2 + 1.5 OnP3
OnP45   = 0.5 OnP4 + OnP5

OnPR    = 1 - OnPN
OnP1R   = ( OnPR x OnPN ) - 2 OnGA
OnP23R  = ( OnPN x OnP23 ) + OnGA
OnP45R  = OnPN x OnP45
OnOHXC  = OnNC - OnP1R - 2 OnP23R -4 OnP45R - 5 OnPN

OnO3A1  = 0.5 ( OnP1 + 0.3 OnP2 + 0.1 OnP5 ) + 0.75 OnP3
OnO3A2  = 0.5 ( OnP2 + 0.3 OnP3 + 0.1 OnP5 )
OnO3K4  = 0.25  OnP4 + 0.5 ( 0.28 OnP2 + 0.42 OnP3 + 0.8 OnP4
          + 0.8 OnP5)
OnO3MG  = 0.5 ( 0.2 OnP4)
OnO3CO  = 0.5 ( 0.44 OnP1 + 0.15 OnP2 + 0.15 OnP3)
OnO3SB  = 0.5 ( 0.37 OnP1 + 0.2 OnP2 + 0.2 OnP3)
OnO3PS  = 0.5 ( 0.2 OnP5)
OnO3RH  = 0.5 ( 0.12 OnP1 + 0.21 OnP2 + 0.21 OnP3)
OnO3OH  = 0.5 ( 0.12 OnP2 + 0.12 OnP3 + 0.2 OnP4 + 0.2 OnP5)
OnO3RR  = 0.5 ( 0.27 OnP2 + 0.27 OnP3 + 0.2 OnP4)
OnO3R2  = 0.5 ( 0.3 OnP5)
OnO3RO2 = OnO3RR + OnO3R2
OnO3XN  = OnNC - OnO3A1 - 2 OnO3A2 - 4 OnO3K4 - 3 OnO3MG - OnO3CO
          - 2 OnO3PS

OnOAXC  = OnNC - 3.5

OnN3XC  = OnNC - OnP1 - 2 OnP23 - 4 OnP45
```

Table 20. Listing of Mechanistic Parameters for the Aromatics for use with the Recommended Condensed Mechanism

Name	Rate Parameters[a]		Mechanistic Parameters[b]					
	A	Ea	Type	Value	Type	Value	Type	Value
BENZENE	2.50E-12	0.397	A1	0.083	A2	0.063	CR	0.270
			U2	0.105	RH	0.270		
TOLUENE	2.10E-12	-0.640	A1	0.050	A2	0.040	CR	0.240
			MG	0.131	U2	0.354	RH	0.240
			RR	0.760				
C2-BENZ	7.50E-12	0.000	A1	0.050	A2	0.040	CR	0.240
			MG	0.131	U2	0.354	RH	0.240
			RR	0.760				
I-C3-BEN	6.55E-12	0.000	A1	0.050	A2	0.040	CR	0.240
			MG	0.131	U2	0.354	RH	0.240
			RR	0.760				
N-C3-BEN	5.70E-12	0.000	A1	0.050	A2	0.040	CR	0.240
			MG	0.131	U2	0.354	RH	0.240
			RR	0.760				
S-C4-BEN	5.70E-12	0.000	A1	0.050	A2	0.040	CR	0.240
			MG	0.131	U2	0.354	RH	0.240
			RR	0.760				
M-XYLENE	1.66E-11	-0.231	A1	0.043	A2	0.032	CR	0.180
			MG	0.370	U2	0.573	RH	0.180
			RR	0.820				
O-XYLENE	1.47E-11	0.000	A1	0.043	A2	0.032	CR	0.180
			MG	0.370	U2	0.573	RH	0.180
			RR	0.820				
P-XYLENE	1.52E-11	0.000	A1	0.043	A2	0.032	CR	0.180
			MG	0.370	U2	0.573	RH	0.180
			RR	0.820				
135-TMB	5.80E-11	0.000	MG	0.620	CR	0.180	RH	0.180
			U2	0.570	RR	0.820		
123-TMB	3.30E-11	0.000	MG	0.620	CR	0.180	RH	0.180
			U2	0.570	RR	0.820		
124-TMB	3.30E-11	0.000	MG	0.620	CR	0.180	RH	0.180
			U2	0.570	RR	0.820		

(continued)

Table 20 (continued) - 2

Name	Rate Parameters[a]		Mechanistic Parameters[b]					
	A	Ea	Type	Value	Type	Value	Type	Value
NAPHTHAL	1.05E-12	-1.792	CR	0.130	NP	0.140	U2	0.080
			RH	0.170	RR	0.690		
23-DMN	7.70E-11	0.000	CR	0.040	NP	0.160	MG	0.870
			U2	0.150	RH	0.040	RR	0.800
ME-NAPH	5.20E-11	0.000	CR	0.085	NP	0.150	MG	0.435
			U2	0.115	RH	0.105	RR	0.745
TETRALIN	3.43E-11	0.000	CR	0.013	NP	0.120	U2	0.043
			RH	0.090	RR	0.790		

[a] A is the Arrhenius activation energy in cm^3 $molecule^{-1}$ sec^{-1}.
Ea is the activation energy in kcal $mole^{-1}$.

[b] The symbols used to indicate the types of aromatic mechanistic parameters are based on the nomenclature used in Tables 2 and 4.

Complete listings for the "Level B" and "Level D" condensed mechanisms are not given because the test calculations, discussed below, indicate that use of the standard, "Level C" mechanisms is to be preferred whenever condensation of the number of reactive organic products are needed. However, except for the reactions of the aromatic ring fragmentation products and the aromatic mechanistic parameters which were derived based on fits to chamber data, these mechanisms have the same sets of reactions and parameters as used in the standard condensed mechanism. The reactions in the "Level B" mechanism differs from the standard condensed mechanism only in that it includes the reactions of glyoxal, which are the same as those in the detailed mechanism, except that its PAN analogue, "GPAN," is represented by PAN itself. The reactions in the "Level D" mechanism differ only in that methyl glyoxal ("MGLY") and "AFG2" are replaced by "AFRG," which reacts like methyl glyoxal in the standard mechanism, except that its photolysis rate is assumed to be a constant fraction of that of NO_2, rather than being separately calculated as it is in the detailed and the standard condensed mechanism.

2. Lumping of the Primary Emitted Organics

The over 100 detailed model species used to represent the primary emitted organics are not intended to be represented explicitly in any airshed model calculation. Instead, they serve as a basis for deriving the kinetic and mechanistic parameters for the lumped species which are actually used in the model to represent them. Emissions processing software which has been developed for this program [described in detail in a separate report (Carter 1988)] can be used to derive the parameters for the lumped species in the mechanism, based on the distribution of species in a selected representative emissions profile, and on the degree of lumping of emitted organics considered appropriate for the particular airshed model application. To provide guidance on the appropriate degrees of lumping of emitted organics to use in airshed model applications, we carried out test calculations where the numbers of lumped species used to represent emitted alkanes (and other species which are lumped with them), aromatics, and alkenes were varied. The alternatives which were examined are summarized in this section.

As discussed elsewhere (Carter 1988), the degree of lumping of primary emitted organics can be controlled by input into the emissions

processing software which specify (1) groups of detailed model species that can be lumped together provided that their rates of OH radical reactions are sufficiently similar; (2) the number of lumped model species to use for each of these groups; and (3) for each lumped species, the range of OH radical rate constants for the detailed species they represent. There are a minimum of two types of groups of model species: (1) alkanes and aromatics, which are represented by generalized reactions of lumped species of the type "AARn," and (2) alkenes (other than ethene, which is represented explicitly), which are represented by generalized reactions of lumped species of the type "OLEn." (See the mechanism listings in Tables 2 and 19 for the generalized reactions used for these species.) For simple single-cell calculations where all species have the same emissions schedule, such as the condensation test calculations employed in this study, these two groups are all that are required. Thus, for the calculations aimed at examining effects of condensing the numbers of reactive organic product species, only these two groups were used. However, for multi-celled airshed model calculations, which can have different distributions of emitted species at different times or locations in the modeling region, it is generally advisable that alkanes and aromatics not be lumped together, since their mechanisms and reactivity characteristics are quite different. Thus, for the calculations aimed at examining the effects of varying degrees of lumping of the primary emitted organics, the alkanes (and alkane-like species), the aromatics, and the non-ethene alkenes were represented separately, with varying numbers of lumped model species being used to represent each group of compounds.

The various options with regard to the numbers of lumped model species used to represent primary emitted organics which were examined in the test calculations are summarized in Table 21. The test calculations comparing the condensation of the numbers of reactive organic products (for the calculations involving mixtures) used three lumped alkane/aromatic species and two lumped non-ethene alkenes. For the test calculations comparing the degree of lumping of primary emitted species, the numbers of lumped species used to represent alkanes, aromatics, and non-ethene alkenes were each varied from one to six, one to three, and one to two, respectively. A number of combinations of these lumpings were examined in the test calculations. In the presentation of the results,

Table 21. Summary of the Alternative Lumpings of Primary Emitted Organics Examined in the Condensation Evaluation Calculations

Type of Group	Number of Species in Group	Minimum kOH for Lumped Species (10^4 ppm^{-1} min^{-2})					
		1	2	3	4	5	6
	Lumping Used in Tests of Condensation of Reactive Organic Intermediates						
Alkanes and Aromatics	3	0.0[a]	1.0	2.0			
Non-Ethene Alkenes	2	0.0	7.5				
	Lumpings Used in Tests of Alternative Lumpings of Primary Emitted Organics						
Alkanes	1	0.0[a]					
	2	0.0[a]	1.0				
	3	0.0[a]	0.5	1.0			
	6	0.0[a]	0.5	0.75	1.0	1.5	2.0
Aromatics	1	0.0[a]					
	2	0.0[a]	2.0				
	3	0.0[a]	2.0	4.0			
Non-Ethene Alkenes	1	0.0					
	2	0.0	7.5				

[a]Contributions of species lumped into the least reactive of the alkane and aromatic groups were derived using "OH reactivity weighing," as discussed elsewhere (Carter 1988). In this method, the contribution of the individual species to the reactivity of the group, and in determining its kinetic and mechanistic parameters, is determined by the amount of the species estimated to react in the scenario, which is estimated using the formula

$$\text{Amount Reacting} = \text{Amount Emitted or Initially Present} \times [\, 1 - \exp(\text{kOH} \times \text{INTOH}) \,]$$

Where kOH is the OH radical rate constant, and INTOH is the integrated OH radical concentration, for which a value of 50 ppt-min was employed in all these calculations. For all other lumped groups, the contributions of the individual species were simply weighed by the amount emitted or initially present.

these combinations are identified by sets of three numbers, giving the numbers of lumped species used for alkanes, aromatics, and non-ethene alkenes, respectively. The test calculations are discussed in the following section.

B. Condensation Evaluation Calculations

1. Description of the Test Calculations Employed

The condensation evaluation calculations were carried out using a series of 70 test calculations, including NO_x-air irradiations of individual organic species in the mechanism, five mixtures of organics of varying composition, and of processed emissions data. All of the calculations with the individual organic reactants, and most of the calculations with the mixtures were "static" box model simulations, with all reactants present initially, and with no dilution of reactants after the simulation began, but with diurnally varying light intensity. In addition, to evaluate whether the results of the condensation tests might be any different if more complex test scenarios were employed, an additional eight sets of test calculations were carried out using the dynamic conditions of the "multi-day" scenario we employ in our reactivity assessment studies (e.g., as discussed in Carter and Atkinson 1987). These scenarios consist of two-day simulations with diurnally varying inversion and solar light intensity, and separate simulations of the aloft air mass to determine the composition of the pollutants aloft on day 2 which are entrained as the inversion height raises. The air is initially clean in these dynamic calculations, with the ground level receiving continuous daytime emissions for two consecutive days, and with significant carry-over of pollutants from day 1 to day 2.

The conditions used in these static and dynamic calculations are summarized in Table 22, and the initial or emitted reactant levels are summarized in Table 23. Table 23 also indicates the designations used to identify the calculations which are used in the tabulations summarizing their results. As indicated there, all the static calculations are indicated with the prefix "TST" in its designation, and all the multi-day dynamic calculations are indicated by the prefix "MD2."

As indicated in Table 23, the static test calculations employed six different mixtures of organics. The first five, designated mixtures "A"

Table 22. Conditions of the Test Calculations Used to Evaluate the Effects of Mechanism Condensation

	Static	Dynamic
Latitude (degrees N)	34.1	34.1
Date	June 21	June 21
Temperature (K)	300	300
Relative Humidity (%)	50	50
Calculated Sunrise (LDT)[a]	0552	0552
Sunset (LDT)	2008	2008
Rates of Photolysis Reactions:	Calculated for the date and latitude above using clear-sky actinic fluxes tabulated by Peterson (1976) for his "best estimate" surface albitos. See also Carter et al. (1986).	
Heterogeneous Reactions	Heterogeneous reactions assumed to be negligible.	
Simulation Start Time (LDT)	0700	0600
End time (LDT, Day 2)	0400 or 1900[b]	2100
Inversion Height Schedule, day 1:[c]	(not applicable)	(LDT) (meters) 0600 100 0880 100 1500 540 2100 540
day 2:		0800 100 (same as day 1)
Initial Pollutants	(See Table 23)	None
Initial NO_2/NO_x	0.25	(not applicable)
Emitted ROG (millimoles C m-2 day-1)	(none)	12.0[d]
ROG Composition	(See Table 23)	California Emissions[d]
Emitted NO_x (millimoles m-2 day-1)	(none)	Varied from 0.3 to 4.0[e]
Emitted NO_2/NO_x	(not applicable)	0.25
ROG and NO_x Emissions Schedule (both day 1 and day 2)	(not applicable)	(LDT) (Factor)[f] 0600 0.0 0800 1.0 1830 1.0 1930 0.0

(continued)

Table 22 (continued) - 2

	Static	Dynamic
Aloft Pollutants, day 1	(not applicable)	None
Aloft Pollutants, day 2	(not applicable)	Calculated[g]

[a]LDT = Local daylight time.
[b]Ending time on the static calculations varied. See Table 23.
[c]Inversion height for intermediate times in the dynamic simulation are determined by linear interpolation of tabulated values. Static calculations had no dilution, and thus variable inversion height is not used.
[d]ROG composition for dynamic calculations were derived from total VOC emissions into California air basins on the 1983 ARB emissions inventory, which is given in Tables 13, 15, and 16. These data were converted to species in the mechanism using the emissions assignments given in Section III and the emissions processing software and procedures discussed in a separate report (Carter 1988). The 12.0 millimoles C m^{-3} day^{-1} does not count the CO or methane in the inventory, but their contributions were included in the simulations.
[e]NO_x emissions used in the various dynamic calculations are given in Table 23.
[f]Factors tabulated are relative emissions rates. Absolute emissions rates are determined such that the total amounts of pollutants emitted per day are the amounts tabulated above. Relative rates for intermediate times are obtained by linear interpolation between the values for the times tabulated. No emissions at nighttime.
[g]Concentrations of aloft level pollutants which were entrained into the air mass on day 2 were calculated using separate simulations of the aloft level air mass. These simulations began at 2100 LDT on day 1, using as initial conditions the ground level pollutant concentrations at that time, and then continued until 1500 LDT on day 2, when the inversion height increased, and thus entrainment of aloft pollutants into the ground level, was assumed to end. The aloft level air mass was assumed to be diluted with clean air by a factor of 2 between 0800 and 1500 LDT.

Table 23. Initial Reactant Concentrations in the Static Test Calculations

Calculation Designation	Organic(s)[a]	Initial Organics	Initial NO_x	Simulation Time (hrs)	Day 2 NO_x[b]
		Static Calculations			
TSTHCH1	HCHO	0.5 ppm	0.25 ppm	21	
TSTHCH2	HCHO	1.0	0.25	21	
TSTHCH3	HCHO	0.5	0.5	36	
TSTCCH1	CCHO	0.5	0.25	21	
TSTCCH2	CCHO	1.0	0.25	21	
TSTCCH3	CCHO	0.5	0.5	36	
TSTRCH1	RCHO	0.5	0.25	21	
TSTRCH2	RCHO	1.0	0.25	21	
TSTRCH3	RCHO	0.5	0.5	36	
TSTACE1	ACET	3.0	0.25	21	
TSTACE2	ACET	6.0	0.25	21	
TSTACE3	ACET	3.0	0.5	36	
TSTMEK1	MEK	1.5	0.25	21	
TSTMEK2	MEK	3.0	0.25	21	
TSTMEK3	MEK	1.5	0.5	36	
TSTNIT1	RNO3	4.0	0.25	21	
	HCHO	0.5			
TSTNIT2	RNO3	8.0	0.25	21	
	HCHO	1.0			
TSTNIT3	RNO3	4.0	0.5	36	
	HCHO	0.5			
TSTETH1	ETHE	0.5	0.25	21	
TSTETH2	ETHE	1.0	0.25	21	
TSTETH3	ETHE	0.5	0.5	36	
TSTPRP1	PROPENE	0.25	0.25	21	
TSTPRP2	PROPENE	0.5	0.25	21	
TSTPRP3	PROPENE	0.25	0.5	36	
TSTT2B1	T-2-BUTE	0.2	0.25	21	
TSTT2B2	T-2-BUTE	0.4	0.25	21	
TSTT2B3	T-2-BUTE	0.2	0.5	36	
TSTALK1	C6PLUS	0.5	0.25	21	
	HCHO	0.5			
TSTALK2	C6PLUS	1.0	0.25	21	
	HCHO	1.0			

(continued)

Table 23 (continued) - 2

Calculation Designation	Organic(s)[a]	Initial Organics	Initial NO_x	Simulation Time (hrs)	Day 2 NO_x[b]
TSTALK3	C6PLUS	0.5 ppm	0.5 ppm	36	
	HCHO	0.5			
TSTALK4	C6PLUS	0.5	1.0	36	
	HCHO	0.5			
TSTBEN1	BENZENE	5.0	0.25	21	
TSTBEN2	BENZENE	10.0	0.25	21	
TSTBEN3	BENZENE	5.0	0.5	36	
TSTTOL1	TOLUENE	0.4	0.25	21	
TSTTOL2	TOLUENE	0.8	0.25	21	
TSTTOL3	TOLUENE	0.4	0.5	36	
TSTXYL1	M-XYLENE	0.1	0.25	21	
TSTXYL2	M-XYLENE	0.2	0.25	21	
TSTXYL3	M-XYLENE	0.1	0.5	36	
TSTMES1	135-TMB	0.08	0.25	21	
TSTMES2	135-TMB	0.16	0.25	21	
TSTMES3	135-TMB	0.08	0.5	36	
TSTMXA1	MIX-A[c]	1.0 ppmC	0.5	36	
TSTMXA2	MIX-A	1.0	0.25	36	
TSTMXA3	MIX-A	1.0	0.13	36	0.13 ppm
TSTMXB1	MIX-B	1.0	0.5	36	
TSTMXB2	MIX-B	1.0	0.25	36	
TSTMXB3	MIX-B	1.0	0.13	36	0.13
TSTMXC1	MIX-C	1.0	0.25	36	
TSTMXC2	MIX-C	1.0	0.13	36	
TSTMXC3	MIX-C	1.0	0.08	36	0.08
TSTMXD1	MIX-D	1.0	0.5	36	
TSTMXD2	MIX-D	1.0	0.3	36	
TSTMXD3	MIX-D	1.0	0.16	36	0.16
TSTMXE1	MIX-E	1.0	0.5	36	
TSTMXE2	MIX-E	1.0	0.25	36	
TSTMXE3	MIX-E	1.0	0.13	36	0.13
TSTCAL1	EMISSIONS[d]	1.0[e]	0.5	36	
TSTCAL2	EMISSIONS	1.0	0.25	36	
TSTCAL3	EMISSIONS	1.0	0.14	36	
TSTCAL4	EMISSIONS	1.0	0.08	36	0.08

(continued)

Table 23 (continued) - 3

Calculation Designation	Organic(s)[a]	Initial Organics	Initial NO_x	Simulation Time (hrs)	Day 2 NO_x[b]
		Dynamic Calculations			
MD2CAL1	EMISSIONS	12.0[f]	3.0[g]	(see Table 22)	
MD2CAL2	EMISSIONS	12.0	2.0		
MD2CAL3	EMISSIONS	12.0	1.5		
MD2CAL4	EMISSIONS	12.0	1.2		
MD2CAL5	EMISSIONS	12.0	1.0		
MD2CAL6	EMISSIONS	12.0	0.75		
MD2CAL7	EMISSIONS	12.0	0.60		
MD2CAL8	EMISSIONS	12.0	0.30		

[a]Organics are designated by names used for explicit or detailed model species. See Table 12 for a list and description of these species.
[b]NO_x was added at 0700 LDT on day 2 in some of the static calculations. This column gives the amount added.
[c]The composition of these mixtures are given in Table 24.
[d]Composition of VOC surrogate derived from emissions data as indicated in footnote d of Table 22.
[e]Methane and CO content of emissions not counted in determining ppmC of ROG emissions.
[f]Units of ROG input in the MD2 calculations are millimoles C m^{-2} day^{-1}.
[g]Units of NO_x input in the MD2 calculations are millimoles m^{-2} day^{-1}.

through "E," are simple mixtures of representative alkanes, aromatics, alkenes, and oxygenates, with varying relative levels of each. The compositions of these mixtures are given in Table 24. These mixtures were derived for the calculations to test condensations of the numbers of reactive organic product species. In addition, some of the static, and all of the dynamic, test calculations used a sixth mixture which was derived from the total emissions into California air basins which are on the CARB 1983 emissions inventory. This mixture was used primarily in the calculations to test condensations of the numbers of lumped species used to represent emitted primary organics. The composition of this mixture, given in terms of mass emissions of the SAROAD species used in emissions inventories, is given in Tables 13, 15, and 16 in Section III. The emissions assignments discussed in Section III were used to derive the composition of detailed model species in this mixture. The distribution of detailed model species in this mixture, and those for the test mixtures "A" through "E" listed in Table 24, were then used to derive the concentrations and mechanistic parameters of the lumped species in the mechanisms, using the lumping alternatives given in Table 21 of the previous section.

2. Effects of Condensation of Reactive Organic Products

Selected comparisons of results of the test calculations using the mechanisms with the condensed representations of the reactive organic products with those using the more detailed mechanism are shown in Tables 25 through 27. These tables show comparisons of predictions of ozone, OH radicals, and H_2O_2, each of which reflect performance of different aspects of the mechanism. Predictions of ozone are obviously important, since accurate ozone predictions is one of the major objectives of using airshed models. It also reflects a number of factors in the mechanism, including rates of NO to NO_2 conversions caused by the reactions of the organics, and the rates of removal of NO_x from the system. Predictions of OH radicals are important, since for many organics reaction with OH radicals is their major loss process, and thus the OH radical levels are directly proportional to their loss rates. Predictions of H_2O_2 are of interest in models concerned with prediction of acid deposition, but they are also useful as a means of mechanism comparison because it is extremely sensitive to relatively small differences in the mechanism, since its rate of

Table 24. Compositions of the Mixtures of Organics Used in the Condensation of Reactive Organic Product Species Tests

Detailed Model Species	Composition (ppb Species/ppmC Mixture)				
	Mix A (Standard)	Mix B (High Alkenes)	Mix C (High Alkanes)	Mix D (High Aromatics)	Mix E (High Oxygenates)
C4-C5	41.43	16.57	116.00	16.57	16.57
C6PLUS	23.95	9.58	67.10	9.58	9.58
ETHENE	39.84	111.60	15.94	15.94	15.94
PROPENE	9.70	27.20	3.88	3.88	3.88
T-2-BUTE	9.48	26.50	3.79	3.79	3.79
BENZENE	40.86	16.34	16.34	114.40	16.34
TOLUENE	11.97	4.79	4.79	33.50	4.79
M-XYL	7.32	2.93	2.93	20.50	2.93
135-TMB	7.11	2.84	2.84	19.90	2.84
HCHO	19.41	7.76	7.76	7.76	54.30
CCHO	15.81	6.32	6.32	6.32	44.30

Table 25. Comparison of the Ozone, OH Radical, and H_2O_2 Predictions for the Test Calculations using the "Level C" (Standard) Condensed Mechanism for the Reactive Organic Products with those using the Detailed Mechanism

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
			Ozone			
TSTHCH1	-1	2.242	2.242	0.000	0.00	0.01
TSTHCH2	-1	6.307	6.307	0.000	0.00	0.01
TSTHCH3	-2	4.790	4.789	-0.001	-0.02	0.03
TSTCCH1	-1	5.487	5.493	0.006	0.10	0.98
TSTCCH2	-1	6.087	6.181	0.093	1.54	1.08
TSTCCH3	-1	5.098	5.075	-0.023	-0.45	0.38
TSTRCH1	-1	5.970	6.015	0.045	0.75	5.15
TSTRCH2	-1	6.299	6.267	-0.032	-0.50	5.50
TSTRCH3	-1	6.590	6.203	-0.387	-5.87	11.79
TSTACE1	-1	4.801	4.065	-0.736	-15.33	21.78
TSTACE2	-1	5.774	6.608	0.835	14.46	13.74
TSTACE3	-1	8.536	8.848	0.311	3.65	2.90
TSTMEK1	-1	5.901	6.086	0.185	3.13	2.99
TSTMEK2	-1	6.810	7.137	0.327	4.80	3.86
TSTMEK3	-1	4.586	4.693	0.107	2.33	5.38
TSTNIT1	-1	8.436	7.242	-1.193	-14.15	15.67
TSTNIT2	0	1.544	1.358	-0.186	-12.06	13.03
TSTNIT3	0	1.159	1.091	-0.068	-5.89	13.76
TSTETH1	-1	6.742	6.742	0.000	0.00	0.40
TSTETH2	-1	9.683	9.682	0.000	0.00	0.35
TSTETH3	-1	5.015	5.006	-0.009	-0.19	0.15
TSTPRP1	-1	4.888	4.884	-0.004	-0.08	0.83
TSTPRP2	-1	6.592	6.673	0.081	1.22	0.78
TSTPRP3	-1	3.572	3.516	-0.056	-1.57	1.93
TSTT2B1	-1	5.283	5.292	0.009	0.16	0.72
TSTT2B2	-1	6.254	6.371	0.117	1.88	1.00
TSTT2B3	-1	4.665	4.692	0.027	0.59	0.58
TSTALK1	-1	8.389	8.377	-0.012	-0.14	1.00
TSTALK2	0	1.088	1.068	-0.020	-1.81	1.38
TSTALK3	-1	5.801	5.682	-0.119	-2.05	3.62
TSTALK4	-2	3.744	3.676	-0.067	-1.80	4.09

(continued)

Table 25 (continued) - 2

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
TSTBEN1	-1	3.193	2.867	-0.326	-10.21	10.03
TSTBEN2	-1	4.839	4.587	-0.252	-5.21	6.94
TSTBEN3	-1	3.680	0.228	-3.452	-93.81	85.85
TSTTOL1	-1	3.409	3.474	0.065	1.90	3.01
TSTTOL2	-1	4.229	4.337	0.108	2.55	2.87
TSTTOL3	-2	6.428	5.322	-1.106	-17.21	16.81
TSTXYL1	-1	3.329	3.194	-0.136	-4.07	5.84
TSTXYL2	-1	4.363	4.831	0.468	10.73	9.28
TSTXYL3	-2	7.322	6.265	-1.057	-14.43	20.09
TSTMES1	-1	3.154	3.114	-0.040	-1.28	1.70
TSTMES2	-1	4.720	4.981	0.261	5.54	5.87
TSTMES3	-1	1.069	1.072	0.003	0.25	1.71
TSTMXA1	-2	2.190	2.127	-0.063	-2.89	2.53
TSTMXA2	-1	3.119	3.185	0.066	2.11	2.82
TSTMXA3	-1	3.515	3.584	0.068	1.94	1.76
TSTMXB1	-2	3.789	3.709	-0.080	-2.12	1.86
TSTMXB2	-1	3.013	3.063	0.050	1.67	1.15
TSTMXB3	-1	4.229	4.271	0.042	0.99	1.39
TSTMXC1	-2	4.397	3.942	-0.455	-10.35	8.10
TSTMXC2	-1	2.821	2.979	0.158	5.61	4.82
TSTMXC3	-1	3.717	3.597	-0.119	-3.21	2.14
TSTMXD1	-2	3.355	3.146	-0.209	-6.23	6.29
TSTMXD2	-1	2.367	2.451	0.083	3.52	4.52
TSTMXD3	-1	3.313	3.445	0.132	3.98	3.17
TSTMXE1	-2	1.666	1.650	-0.016	-0.93	0.78
TSTMXE2	-1	1.024	0.990	-0.034	-3.28	2.18
TSTMXE3	-1	2.377	2.368	-0.009	-0.37	1.73
TSTCAL1	-2	1.383	1.309	-0.074	-5.33	4.11
TSTCAL2	-2	9.790	8.477	-1.314	-13.42	12.45
TSTCAL3	-1	2.495	2.494	-0.001	-0.02	4.56
TSTCAL4	-1	4.381	4.299	-0.082	-1.88	1.17
MD2CAL1	-2	3.195	2.959	-0.236	-7.38	6.33
MD2CAL2	-1	1.227	1.137	-0.090	-7.35	7.86
MD2CAL3	-1	2.801	2.782	-0.018	-0.66	2.71

(continued)

Table 25 (continued) - 3

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
MD2CAL4	-1	2.879	2.941	0.061	2.13	1.97
MD2CAL5	-1	2.743	2.799	0.057	2.06	1.14
MD2CAL6	-1	2.495	2.544	0.049	1.95	1.25
MD2CAL7	-1	2.274	2.320	0.046	2.04	1.56
MD2CAL8	-1	1.620	1.650	0.030	1.87	1.67
			OH Radicals			
TSTHCH1	-7	2.207	2.206	-0.001	-0.03	0.05
TSTHCH2	-6	1.140	1.141	0.001	0.13	0.05
TSTHCH3	-7	1.803	1.803	0.000	-0.01	0.07
TSTCCH1	-7	1.397	1.398	0.002	0.13	3.29
TSTCCH2	-8	8.805	8.853	0.048	0.55	7.50
TSTCCH3	-7	6.363	6.884	0.521	8.19	5.87
TSTRCH1	-7	1.256	1.142	-0.115	-9.12	20.86
TSTRCH2	-8	7.019	6.006	-1.013	-14.44	21.39
TSTRCH3	-7	2.580	5.575	2.995	116.09	60.09
TSTACE1	-7	4.877	1.156	-3.721	-76.29	60.87
TSTACE2	-7	4.826	1.592	-3.234	-67.02	50.94
TSTACE3	-7	1.030	1.158	0.127	12.34	12.07
TSTMEK1	-7	1.352	1.542	0.191	14.11	10.99
TSTMEK2	-7	1.268	1.338	0.070	5.56	12.68
TSTMEK3	-8	8.491	9.986	1.495	17.61	12.53
TSTNIT1	-8	5.927	5.249	-0.678	-11.44	11.69
TSTNIT2	-8	6.319	5.489	-0.830	-13.14	11.40
TSTNIT3	-8	6.555	5.779	-0.776	-11.84	10.54
TSTETH1	-7	3.152	3.154	0.003	0.08	0.66
TSTETH2	-7	3.619	3.616	-0.003	-0.07	1.08
TSTETH3	-7	1.841	1.842	0.000	0.02	0.14
TSTPRP1	-7	1.825	1.820	-0.005	-0.27	1.95
TSTPRP2	-7	2.203	2.203	0.000	0.00	6.33
TSTPRP3	-7	1.203	1.174	-0.029	-2.38	1.85
TSTT2B1	-7	2.226	2.308	0.082	3.67	3.41
TSTT2B2	-7	1.100	1.246	0.147	13.32	9.88
TSTT2B3	-7	7.503	7.851	0.348	4.64	3.69

(continued)

Table 25 (continued) - 4

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
TSTALK1	-7	2.366	2.235	-0.132	-5.56	3.98
TSTALK2	-7	1.885	1.831	-0.055	-2.89	3.66
TSTALK3	-7	1.193	1.183	-0.010	-0.85	2.09
TSTALK4	-8	9.989	9.938	-0.051	-0.51	2.87
TSTBEN1	-7	0.969	1.073	0.104	10.76	15.74
TSTBEN2	-7	1.289	1.259	-0.030	-2.32	50.22
TSTBEN3	-7	1.050	0.197	-0.853	-81.24	69.09
TSTTOL1	-7	3.205	3.569	0.363	11.34	21.17
TSTTOL2	-7	2.701	3.650	0.949	35.14	15.97
TSTTOL3	-8	6.714	5.896	-0.818	-12.18	7.86
TSTXYL1	-7	4.991	3.454	-1.538	-30.81	20.73
TSTXYL2	-7	5.331	8.252	2.921	54.78	48.57
TSTXYL3	-7	1.476	1.445	-0.031	-2.10	7.58
TSTMES1	-7	3.739	3.340	-0.399	-10.66	8.50
TSTMES2	-6	1.039	1.321	0.282	27.10	24.05
TSTMES3	-7	2.064	2.107	0.043	2.07	2.88
TSTMXA1	-8	5.757	5.651	-0.106	-1.85	2.17
TSTMXA2	-7	4.185	4.401	0.215	5.14	8.13
TSTMXA3	-5	1.062	1.133	0.072	6.74	5.99
TSTMXB1	-8	5.766	5.713	-0.053	-0.92	0.88
TSTMXB2	-7	3.675	3.902	0.227	6.16	4.54
TSTMXB3	-5	1.211	1.277	0.066	5.47	5.52
TSTMXC1	-8	4.423	4.251	-0.173	-3.90	5.03
TSTMXC2	-7	2.078	2.200	0.122	5.87	8.52
TSTMXC3	-6	6.316	6.715	0.399	6.31	4.79
TSTMXD1	-8	9.952	9.669	-0.283	-2.85	3.45
TSTMXD2	-7	3.332	4.143	0.810	24.31	13.36
TSTMXD3	-5	1.214	1.294	0.079	6.54	7.47
TSTMXE1	-8	6.390	6.350	-0.039	-0.62	0.85
TSTMXE2	-8	9.601	9.553	-0.048	-0.50	2.00
TSTMXE3	-5	1.159	1.208	0.050	4.29	3.93
TSTCAL1	-8	2.563	2.352	-0.211	-8.25	7.13
TSTCAL2	-8	5.187	4.882	-0.304	-5.87	6.49
TSTCAL3	-7	1.317	1.383	0.066	5.01	6.18
TSTCAL4	-6	5.726	6.253	0.526	9.19	6.88

(continued)

Table 25 (continued) - 5

CALC ID	Maximum Concentration[a] EXP	STD.	TEST	DIFF	% CHG	% FIT[b]
MD2CAL1	-8	6.736	6.344	-0.393	-5.83	5.10
MD2CAL2	-7	1.035	0.989	-0.047	-4.53	5.22
MD2CAL3	-7	2.939	2.846	-0.093	-3.16	3.67
MD2CAL4	-7	3.504	3.522	0.017	0.50	2.89
MD2CAL5	-7	3.223	3.235	0.011	0.35	2.23
MD2CAL6	-7	3.701	3.748	0.047	1.28	2.79
MD2CAL7	-7	3.686	3.702	0.016	0.43	2.67
MD2CAL8	-7	2.726	2.716	-0.010	-0.37	2.60
			H_2O_2			
TSTHCH1	-5	4.921	4.924	0.003	0.06	0.07
TSTHCH2	-2	1.562	1.561	-0.001	-0.05	0.03
TSTHCH3	-7	6.709	6.710	0.001	0.01	0.02
TSTCCH1	-2	1.194	1.574	0.380	31.87	24.32
TSTCCH2	-2	5.695	7.000	1.305	22.92	18.21
TSTCCH3	-2	2.994	3.144	0.150	5.02	9.26
TSTRCH1	-2	3.486	4.318	0.832	23.87	18.75
TSTRCH2	-1	1.026	1.194	0.168	16.33	14.17
TSTRCH3	-2	5.494	6.620	1.125	20.48	29.25
TSTACE1	-2	1.677	0.293	-1.384	-82.52	93.32
TSTACE2	-2	6.742	2.841	-3.902	-57.87	68.84
TSTACE3	-1	1.222	1.482	0.260	21.26	27.33
TSTMEK1	-2	1.062	1.455	0.393	37.05	47.37
TSTMEK2	-2	4.126	5.354	1.227	29.74	31.54
TSTMEK3	-2	4.910	5.840	0.930	18.94	20.92
TSTNIT1	-2	0.878	1.097	0.219	24.96	22.86
TSTNIT2	-2	3.072	3.497	0.425	13.82	14.97
TSTNIT3	-2	1.548	0.766	-0.782	-50.52	65.88
TSTETH1	-2	1.557	1.641	0.085	5.43	2.59
TSTETH2	-1	1.216	1.238	0.022	1.79	1.03
TSTETH3	-4	6.106	6.048	-0.058	-0.96	0.72
TSTPRP1	-3	5.060	6.707	1.647	32.55	23.29
TSTPRP2	-2	5.862	6.540	0.678	11.57	9.16
TSTPRP3	-5	5.734	5.197	-0.537	-9.37	9.08

(continued)

Table 25 (continued) - 6

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
TSTT2B1	-3	7.299	9.198	1.899	26.01	18.56
TSTT2B2	-2	5.247	6.181	0.934	17.79	15.18
TSTT2B3	-2	1.134	1.123	-0.011	-0.97	0.85
TSTALK1	-2	1.738	1.937	0.199	11.45	10.68
TSTALK2	-2	5.535	5.959	0.424	7.66	6.65
TSTALK3	-2	1.762	2.003	0.241	13.66	18.61
TSTALK4	-7	2.148	2.095	-0.052	-2.43	2.79
TSTBEN1	-3	6.112	4.003	-2.109	-34.51	27.27
TSTBEN2	-2	4.124	2.532	-1.592	-38.60	36.22
TSTBEN3	-3	3.610	0.000	-3.610	-100.00	99.99
TSTTOL1	-2	1.492	1.419	-0.073	-4.89	4.78
TSTTOL2	-2	5.447	5.863	0.416	7.64	7.87
TSTTOL3	-7	4.123	2.646	-1.477	-35.82	33.74
TSTXYL1	-3	1.327	0.659	-0.668	-50.34	61.95
TSTXYL2	-2	3.594	2.956	-0.637	-17.73	21.42
TSTXYL3	-7	5.081	3.539	-1.542	-30.35	28.49
TSTMES1	-4	3.554	2.704	-0.851	-23.94	28.55
TSTMES2	-2	2.051	1.640	-0.411	-20.02	18.29
TSTMES3	-6	1.387	1.402	0.015	1.09	1.52
TSTMXA1	-8	3.140	2.924	-0.216	-6.87	6.20
TSTMXA2	-3	6.383	5.665	-0.718	-11.25	18.05
TSTMXA3	-3	6.242	6.140	-0.101	-1.63	2.68
TSTMXB1	-7	1.184	1.139	-0.045	-3.78	3.52
TSTMXB2	-2	2.071	2.087	0.016	0.77	1.03
TSTMXB3	-2	1.390	1.435	0.045	3.26	2.61
TSTMXC1	-8	8.287	6.449	-1.838	-22.18	15.65
TSTMXC2	-3	9.322	9.875	0.553	5.93	6.70
TSTMXC3	-3	3.930	3.670	-0.260	-6.62	9.12
TSTMXD1	-7	1.118	1.000	-0.117	-10.50	10.68
TSTMXD2	-2	1.227	1.155	-0.072	-5.88	11.44
TSTMXD3	-2	1.208	1.161	-0.047	-3.90	3.24
TSTMXE1	-8	2.065	2.037	-0.028	-1.35	1.45
TSTMXE2	-6	1.183	1.063	-0.120	-10.15	6.06
TSTMXE3	-4	4.913	5.574	0.661	13.46	12.01

(continued)

Table 25 (continued) - 7

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
TSTCAL1	-9	7.148	5.666	-1.482	-20.73	17.37
TSTCAL2	-7	9.147	6.133	-3.014	-32.95	26.50
TSTCAL3	-2	1.998	2.135	0.137	6.86	6.22
TSTCAL4	-2	1.281	1.265	-0.017	-1.29	6.29
MD2CAL1	-7	2.003	1.666	-0.337	-16.81	15.60
MD2CAL2	-5	1.843	1.418	-0.425	-23.08	22.80
MD2CAL3	-3	2.348	2.008	-0.340	-14.50	14.56
MD2CAL4	-3	8.404	8.436	0.032	0.38	0.88
MD2CAL5	-2	1.090	1.112	0.022	2.02	2.31
MD2CAL6	-2	1.327	1.358	0.031	2.35	1.99
MD2CAL7	-2	1.429	1.467	0.038	2.63	2.29
MD2CAL8	-2	1.478	1.517	0.040	2.68	2.21

[a]Maximum concentrations (in ppm) are expressed as follows: Condensed mechanism: TEST x 10^{EXP}; Detailed mechanism: STD. x 10^{EXP}. DIFF = TEST-STD. % CHG = (TEST-STD)/STD.

[b]See text for definition of this quantity, which measures the differences between the simulations at each hour in the simulation.

Table 26. Comparison of the Ozone, OH Radical, and H_2O_2 Predictions for the Test Calculations Using the "Level B" Condensed Mechanism for the Reactive Organic Products with those using the Detailed Mechanism[a]

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
			Ozone			
TSTBEN1	-1	3.193	3.531	0.338	10.57	14.86
TSTBEN2	-1	4.839	4.404	-0.434	-8.98	8.88
TSTBEN3	-1	3.680	4.562	0.882	23.97	71.91
TSTTOL1	-1	3.409	3.610	0.200	5.87	6.16
TSTTOL2	-1	4.229	4.366	0.137	3.23	3.11
TSTTOL3	-2	6.428	7.383	0.954	14.85	9.60
TSTXYL1	-1	3.329	3.383	0.054	1.63	1.43
TSTXYL2	-1	4.363	4.894	0.531	12.17	10.15
TSTXYL3	-2	7.322	7.441	0.119	1.62	3.00
TSTMES1	-1	3.154	3.113	-0.041	-1.29	1.68
TSTMES2	-1	4.720	4.980	0.260	5.51	5.85
TSTMES3	-1	1.069	1.072	0.002	0.23	1.72
TSTMXA1	-2	2.190	2.197	0.007	0.32	0.25
TSTMXA2	-1	3.119	3.183	0.064	2.06	2.18
TSTMXA3	-1	3.515	3.607	0.091	2.60	1.76
TSTMXB1	-2	3.789	3.778	-0.011	-0.29	0.33
TSTMXB2	-1	3.013	3.050	0.037	1.22	0.65
TSTMXB3	-1	4.229	4.274	0.046	1.08	1.29
TSTMXC1	-2	4.397	4.120	-0.277	-6.31	4.74
TSTMXC2	-1	2.821	2.932	0.112	3.96	2.41
TSTMXC3	-1	3.717	3.635	-0.082	-2.20	0.97
TSTMXD1	-2	3.355	3.502	0.148	4.40	4.00
TSTMXD2	-1	2.367	2.322	-0.045	-1.90	4.30
TSTMXD3	-1	3.313	3.482	0.169	5.10	4.61
TSTMXE1	-2	1.666	1.668	0.003	0.16	0.12
TSTMXE2	-1	1.024	1.033	0.009	0.89	1.11
TSTMXE3	-1	2.377	2.407	0.030	1.28	1.13
TSTCAL1	-2	1.383	1.322	-0.061	-4.39	3.35
TSTCAL2	-2	9.790	8.850	-0.941	-9.61	8.87

(continued)

Table 26 (continued) - 2

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
TSTCAL3	-1	2.495	2.506	0.011	0.42	2.35
TSTCAL4	-1	4.381	4.315	-0.066	-1.51	0.79
MD2CAL1	-2	3.195	3.036	-0.159	-4.96	4.21
MD2CAL2	-1	1.227	1.184	-0.043	-3.50	3.83
MD2CAL3	-1	2.801	2.834	0.033	1.17	0.99
MD2CAL4	-1	2.879	2.947	0.067	2.34	1.33
MD2CAL5	-1	2.743	2.804	0.061	2.23	1.47
MD2CAL6	-1	2.495	2.545	0.050	2.01	1.54
MD2CAL7	-1	2.274	2.321	0.048	2.09	1.69
MD2CAL8	-1	1.620	1.650	0.031	1.90	1.68
			OH Radicals			
TSTBEN1	-7	0.969	1.536	0.567	58.47	43.99
TSTBEN2	-7	1.289	1.617	0.328	25.48	22.06
TSTBEN3	-7	1.050	1.796	0.746	71.01	66.26
TSTTOL1	-7	3.205	4.179	0.974	30.37	17.46
TSTTOL2	-7	2.701	2.717	0.016	0.58	10.41
TSTTOL3	-8	6.714	6.902	0.188	2.80	5.11
TSTXYL1	-7	4.991	4.387	-0.605	-12.12	8.50
TSTXYL2	-7	5.331	8.250	2.919	54.75	46.92
TSTXYL3	-7	1.476	1.520	0.044	3.00	2.37
TSTMES1	-7	3.739	3.338	-0.401	-10.71	8.69
TSTMES2	-6	1.039	1.317	0.277	26.68	23.97
TSTMES3	-7	2.064	2.100	0.036	1.75	2.63
TSTMXA1	-8	5.757	5.752	-0.005	-0.08	0.21
TSTMXA2	-7	4.185	4.411	0.226	5.39	5.23
TSTMXA3	-5	1.062	1.141	0.080	7.51	6.20
TSTMXB1	-8	5.766	5.750	-0.015	-0.27	0.22
TSTMXB2	-7	3.675	3.838	0.163	4.43	3.15
TSTMXB3	-5	1.211	1.278	0.067	5.50	5.11
TSTMXC1	-8	4.423	4.316	-0.107	-2.42	3.11
TSTMXC2	-7	2.078	2.135	0.057	2.74	4.72
TSTMXC3	-6	6.316	6.693	0.377	5.97	4.89

(continued)

Table 26 (continued) - 3

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
TSTMXD1	-7	0.995	1.005	0.010	0.97	2.42
TSTMXD2	-7	3.332	2.831	-0.502	-15.06	6.05
TSTMXD3	-5	1.214	1.341	0.126	10.40	9.99
TSTMXE1	-8	6.390	6.385	-0.004	-0.07	0.13
TSTMXE2	-8	9.601	9.605	0.004	0.04	0.62
TSTMXE3	-5	1.159	1.214	0.055	4.78	4.23
TSTCAL1	-8	2.563	2.390	-0.173	-6.76	5.81
TSTCAL2	-8	5.187	4.959	-0.228	-4.39	4.64
TSTCAL3	-7	1.317	1.389	0.072	5.47	4.94
TSTCAL4	-6	5.726	6.266	0.540	9.43	6.90
MD2CAL1	-8	6.736	6.462	-0.274	-4.07	3.63
MD2CAL2	-7	1.035	1.007	-0.029	-2.77	2.90
MD2CAL3	-7	2.939	2.945	0.006	0.19	1.12
MD2CAL4	-7	3.504	3.523	0.019	0.54	2.28
MD2CAL5	-7	3.223	3.239	0.015	0.47	1.94
MD2CAL6	-7	3.701	3.744	0.043	1.17	2.18
MD2CAL7	-7	3.686	3.732	0.046	1.24	2.31
MD2CAL8	-7	2.726	2.719	-0.007	-0.25	2.27
			H_2O_2			
TSTBEN1	-2	0.611	1.470	0.859	140.52	199.33
TSTBEN2	-2	4.124	5.168	1.044	25.31	27.53
TSTBEN3	-2	0.361	3.656	3.295	912.87	2342.81
TSTTOL1	-2	1.492	1.848	0.356	23.85	30.88
TSTTOL2	-2	5.447	6.430	0.983	18.05	19.08
TSTTOL3	-7	4.123	5.951	1.828	44.34	25.71
TSTXYL1	-3	1.327	0.917	-0.410	-30.89	37.60
TSTXYL2	-2	3.594	3.292	-0.302	-8.40	15.87
TSTXYL3	-7	5.081	5.381	0.300	5.90	6.27
TSTMES1	-4	3.554	2.729	-0.826	-23.23	28.46
TSTMES2	-2	2.051	1.641	-0.410	-20.00	18.27
TSTMES3	-6	1.387	1.401	0.014	0.98	1.43
TSTMXA1	-8	3.140	3.165	0.025	0.80	0.41
TSTMXA2	-3	6.383	7.580	1.197	18.75	22.52
TSTMXA3	-3	6.242	6.780	0.538	8.62	8.00

(continued)

Table 26 (continued) - 4

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
TSTMXB1	-7	1.184	1.178	-0.006	-0.48	0.53
TSTMXB2	-2	2.071	2.125	0.054	2.61	3.05
TSTMXB3	-2	1.390	1.463	0.073	5.25	4.47
TSTMXC1	-8	8.287	7.146	-1.141	-13.77	9.34
TSTMXC2	-2	0.932	1.039	0.107	11.48	9.35
TSTMXC3	-3	3.930	3.976	0.046	1.17	2.46
TSTMXD1	-7	1.118	1.194	0.076	6.80	7.02
TSTMXD2	-2	1.227	1.467	0.240	19.54	24.70
TSTMXD3	-2	1.208	1.339	0.131	10.80	11.53
TSTMXE1	-8	2.065	2.088	0.024	1.15	1.09
TSTMXE2	-6	1.183	1.227	0.044	3.68	3.11
TSTMXE3	-4	4.913	5.979	1.066	21.69	19.95
TSTCAL1	-9	7.148	5.893	-1.255	-17.55	14.37
TSTCAL2	-7	9.147	6.927	-2.220	-24.27	19.28
TSTCAL3	-2	1.998	2.165	0.167	8.37	8.17
TSTCAL4	-2	1.281	1.303	0.022	1.69	2.04
MD2CAL1	-7	2.003	1.778	-0.224	-11.21	10.43
MD2CAL2	-5	1.843	1.660	-0.183	-9.95	10.41
MD2CAL3	-3	2.348	2.344	-0.004	-0.19	0.41
MD2CAL4	-3	8.404	8.743	0.339	4.04	4.42
MD2CAL5	-2	1.090	1.133	0.044	4.00	4.86
MD2CAL6	-2	1.327	1.379	0.051	3.86	4.56
MD2CAL7	-2	1.429	1.485	0.056	3.93	4.33
MD2CAL8	-2	1.478	1.534	0.056	3.80	3.53

[a]Comparisons for TSTHCH1 through TSTALK4 are not shown since the results are the same as for the "Level C" mechanism, as shown in Table 25.

[b]Maximum concentrations (in ppm) are expressed as follows: Condensed mechanism: TEST x 10^{EXP}; Detailed mechanism: STD. x 10^{EXP}.
DIFF = TEST-STD. % CHG = (TEST-STD)/STD.

[c]See text for definition of this quantity, which measures the differences between the simulations at each hour in the simulation.

Table 27. Comparison of the Ozone, OH Radical, and H_2O_2 Predictions for the Test Calculations using the "Level D" Condensed Mechanism for the Reactive Organic Products with those using the Detailed Mechanism[a]

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
			Ozone			
TSTBEN1	-1	3.193	3.091	-0.102	-3.21	2.90
TSTBEN2	-1	4.839	4.455	-0.383	-7.92	6.40
TSTBEN3	-1	3.680	1.232	-2.448	-66.52	56.91
TSTTOL1	-1	3.409	3.728	0.319	9.36	10.62
TSTTOL2	-1	4.229	4.192	-0.037	-0.88	3.66
TSTTOL3	-1	0.643	4.540	3.897	606.31	588.80
TSTXYL1	-1	3.329	4.429	1.100	33.03	31.76
TSTXYL2	-1	4.363	4.846	0.483	11.08	7.15
TSTXYL3	-1	0.732	3.613	2.881	393.43	399.48
TSTMES1	-1	3.154	4.605	1.451	46.01	45.94
TSTMES2	-1	4.720	5.577	0.857	18.16	13.26
TSTMES3	-1	1.069	3.197	2.128	198.95	270.89
TSTMXA1	-2	2.190	3.262	1.071	48.92	44.57
TSTMXA2	-1	3.119	2.722	-0.397	-12.72	37.85
TSTMXA3	-1	3.515	3.815	0.300	8.53	8.69
TSTMXB1	-2	3.789	4.620	0.831	21.94	20.16
TSTMXB2	-1	3.013	3.062	0.049	1.61	12.64
TSTMXB3	-1	4.229	4.328	0.099	2.34	1.90
TSTMXC1	-2	4.397	6.984	2.587	58.83	51.74
TSTMXC2	-1	2.821	2.555	-0.266	-9.41	22.79
TSTMXC3	-1	3.717	3.866	0.149	4.02	8.47
TSTMXD1	-1	0.335	1.805	1.470	438.07	431.62
TSTMXD2	-1	2.367	3.679	1.312	55.41	93.27
TSTMXD3	-1	3.313	3.824	0.512	15.45	17.24
TSTMXE1	-2	1.666	1.877	0.211	12.69	11.69
TSTMXE2	-1	1.024	1.503	0.480	46.86	38.05
TSTMXE3	-1	2.377	2.745	0.369	15.50	16.13
TSTCAL1	-2	1.383	1.561	0.178	12.86	9.25
TSTCAL2	-1	0.979	1.586	0.607	61.96	56.89

(continued)

Table 27 (continued) - 2

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
TSTCAL3	-1	2.495	2.761	0.266	10.66	20.20
TSTCAL4	-1	4.381	4.432	0.051	1.16	4.10
MD2CAL1	-2	3.195	4.173	0.978	30.62	26.56
MD2CAL2	-1	1.227	1.773	0.546	44.53	40.76
MD2CAL3	-1	2.801	3.091	0.291	10.37	19.01
MD2CAL4	-1	2.879	2.987	0.108	3.75	11.57
MD2CAL5	-1	2.743	2.837	0.094	3.42	7.47
MD2CAL6	-1	2.495	2.558	0.063	2.51	3.25
MD2CAL7	-1	2.274	2.325	0.051	2.25	2.44
MD2CAL8	-1	1.620	1.643	0.023	1.45	1.27
			OH Radicals			
TSTBEN1	-7	0.969	1.174	0.205	21.11	13.85
TSTBEN2	-7	1.289	1.665	0.376	29.20	25.36
TSTBEN3	-7	1.050	0.439	-0.611	-58.23	36.96
TSTTOL1	-7	3.205	2.882	-0.323	-10.08	23.06
TSTTOL2	-7	2.701	3.135	0.434	16.05	15.64
TSTTOL3	-7	0.671	3.230	2.558	381.06	212.97
TSTXYL1	-7	4.991	7.393	2.402	48.12	44.49
TSTXYL2	-7	5.331	3.767	-1.564	-29.34	31.92
TSTXYL3	-6	0.148	1.037	0.890	602.83	738.64
TSTMES1	-6	0.374	1.217	0.844	225.61	140.15
TSTMES2	-6	1.039	0.762	-0.277	-26.69	32.54
TSTMES3	-7	2.064	9.746	7.682	372.15	688.01
TSTMXA1	-8	5.757	7.237	1.480	25.70	21.11
TSTMXA2	-7	4.185	2.730	-1.455	-34.76	27.28
TSTMXA3	-5	1.062	1.175	0.113	10.68	12.60
TSTMXB1	-8	5.766	6.299	0.533	9.25	7.24
TSTMXB2	-7	3.675	3.884	0.209	5.69	7.05
TSTMXB3	-5	1.211	1.288	0.077	6.38	5.38
TSTMXC1	-8	4.423	5.276	0.853	19.28	20.69
TSTMXC2	-7	2.078	1.436	-0.642	-30.88	19.25
TSTMXC3	-6	6.316	6.685	0.369	5.85	8.95

(continued)

Table 27 (continued) - 3

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
TSTMXD1	-7	0.995	1.273	0.278	27.91	100.32
TSTMXD2	-7	3.332	3.471	0.138	4.15	43.63
TSTMXD3	-5	1.214	1.469	0.254	20.94	22.61
TSTMXE1	-8	6.390	6.898	0.509	7.96	8.11
TSTMXE2	-7	0.960	1.125	0.165	17.14	35.94
TSTMXE3	-5	1.159	1.240	0.081	7.01	9.55
TSTCAL1	-8	2.563	2.870	0.307	11.98	13.39
TSTCAL2	-8	5.187	6.759	1.572	30.31	24.90
TSTCAL3	-7	1.317	1.511	0.194	14.71	16.13
TSTCAL4	-6	5.726	6.441	0.715	12.48	10.39
MD2CAL1	-8	6.736	7.336	0.600	8.91	12.65
MD2CAL2	-7	1.035	1.422	0.387	37.35	23.09
MD2CAL3	-7	2.939	3.494	0.555	18.90	17.82
MD2CAL4	-7	3.504	3.416	-0.088	-2.52	9.28
MD2CAL5	-7	3.223	3.277	0.054	1.67	5.56
MD2CAL6	-7	3.701	3.743	0.042	1.14	3.07
MD2CAL7	-7	3.686	3.650	-0.036	-0.96	2.46
MD2CAL8	-7	2.726	2.671	-0.055	-2.01	2.62
			H_2O_2			
TSTBEN1	-3	6.112	6.455	0.343	5.61	20.81
TSTBEN2	-2	4.124	3.223	-0.901	-21.85	19.40
TSTBEN3	-3	3.610	0.007	-3.603	-99.82	99.73
TSTTOL1	-2	1.492	3.438	1.946	130.41	147.25
TSTTOL2	-1	0.545	1.013	0.468	85.92	80.62
TSTTOL3	-2	0.000	4.474	4.474	*******	********
TSTXYL1	-2	0.133	1.121	0.988	744.80	1006.93
TSTXYL2	-2	3.594	8.651	5.057	140.74	135.87
TSTXYL3	-3	0.001	6.127	6.126	*******	********
TSTMES1	-3	0.355	6.901	6.546	1841.61	2856.91
TSTMES2	-2	2.051	7.202	5.151	251.15	236.08
TSTMES3	-3	0.001	3.411	3.410	*******	********
TSTMXA1	-8	3.140	7.820	4.681	149.06	136.97
TSTMXA2	-2	0.638	1.645	1.006	157.66	333.33
TSTMXA3	-2	0.624	1.117	0.492	78.90	85.02

(continued)

Table 27 (continued) - 4

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
TSTMXB1	-7	1.184	1.791	0.607	51.30	44.89
TSTMXB2	-2	2.071	2.214	0.143	6.90	12.87
TSTMXB3	-2	1.390	1.658	0.268	19.31	19.61
TSTMXC1	-7	0.829	2.454	1.625	196.09	137.10
TSTMXC2	-2	0.932	1.281	0.348	37.37	64.79
TSTMXC3	-3	3.930	6.126	2.196	55.87	100.22
TSTMXD1	-6	0.112	6.577	6.465	5784.84	2449.49
TSTMXD2	-2	1.227	1.962	0.735	59.88	121.16
TSTMXD3	-2	1.208	2.267	1.058	87.61	93.02
TSTMXE1	-8	2.065	2.780	0.715	34.65	33.77
TSTMXE2	-6	1.183	6.465	5.282	446.45	236.50
TSTMXE3	-3	0.491	1.082	0.590	120.18	146.40
TSTCAL1	-8	0.715	1.941	1.226	171.57	158.33
TSTCAL2	-6	0.915	4.251	3.336	364.73	236.85
TSTCAL3	-2	1.998	2.464	0.467	23.37	31.80
TSTCAL4	-2	1.281	1.593	0.312	24.33	46.47
MD2CAL1	-7	2.003	4.048	2.045	102.09	71.30
MD2CAL2	-5	1.843	9.303	7.460	404.77	406.12
MD2CAL3	-3	2.348	5.471	3.123	133.03	148.82
MD2CAL4	-2	0.840	1.059	0.219	26.06	36.34
MD2CAL5	-2	1.090	1.276	0.187	17.12	30.10
MD2CAL6	-2	1.327	1.510	0.183	13.77	20.71
MD2CAL7	-2	1.429	1.614	0.184	12.89	16.60
MD2CAL8	-2	1.478	1.663	0.186	12.57	13.00

[a]Comparisons for TSTHCH1 through TSTALK4 are not shown since the results are the same as for the "Level C" mechanism, as shown in Table 25.

[b]Maximum concentrations (in ppm) are expressed as follows: Condensed mechanism: TEST x 10^{EXP}; Detailed mechanism: STD. x 10^{EXP}. DIFF = TEST-STD. % CHG = (TEST-STD)/STD.

[c]See text for definition of this quantity, which measures the differences between the simulations at each hour in the simulation.

formation is determined by the square of the HO_2 concentration, and HO_2 is a key intermediate species involved in the overall photochemical smog formation process.

The ability of the condensed mechanisms to simulate the results of the detailed calculation are measured both by the percent differences of the maximum concentrations of these species, and by a measure we call the "percent fit." This latter quantity can be thought of as the ratio of the absolute area of the differences between the calculated concentration time profiles for the compound of interest, to the area under the concentration-time curve predicted by the detailed mechanism. It is defined as follows:

$$\% \text{ Fit} = 100\% \times \frac{\sum_i \left| C_i - D_i \right|}{\sum_i D_i}$$

where C_i and D_i are the concentrations of the species of interest calculated using the condensed and the detailed mechanism, respectively, at hour i, and the summations are over all the hours of the simulation. This quantity is perhaps a better measure of fit between the mechanisms being compared, than just the maximum concentrations, since it reflects the differences between the predictions of the mechanisms at all times during the simulation.

The results shown in Tables 25 show that in simulations involving mixtures of organics, the "Level C," or standard, condensed mechanism in most cases gives fair agreements with the predictions of the more detailed mechanism. In calculations involving mixtures, the condensed mechanism can fit ozone and OH radical profiles to within 13%, and can fit H_2O_2 profiles to within 25%, with the fits in most cases being within 5% for ozone, 7% for OH radicals, and 10% for H_2O_2. There appears to be no systematic difference between the quality of fits in the dynamic compared to the static test calculations. As expected, the fits in the test calculations employing single organics are more variable. The fits are the best in the test calculations employing only formaldehyde,

acetaldehyde, or the simple alkenes, as is expected since the major aspects of the mechanisms for those species were not condensed. The fits are the worst in the simulations of the individual products which are affected by the condensations, and also for the simulations of the individual aromatics. The differences in the cases of the aromatics may be due in part to the removal of phenol, nitrophenols and (probably to a lesser extent) benzaldehyde, and in part to the fact that the yields of the uncharacterized aromatic ring opening products were re-optimized for the condensed mechanisms.

A comparison of the results shown in Table 26 with those in Table 25 show that the "Level B" and "Level C" condensed mechanisms give essentially the same degree of fit to the more detailed mechanism in predictions of the three representative species. A more direct comparison between these two condensed mechanisms is shown in Table 28, which gives the fits of the standard, "Level C" mechanism to the more detailed "Level B" version. (Comparisons of calculations for single compounds where the two mechanisms are exactly the same are not shown.) As expected, the greatest discrepancy between the two are in the simulations employing benzene by itself; this is attributed to the fact that the difference between these two mechanisms concerns the two products (glyoxal and "AFG1") which are much more important in the benzene system than in any of the others. The differences for the other aromatics are less, though the fits are not very good for the TSTTOL3 and TSTXYL3 simulations. The larger discrepancies observed in the TSTxxx3 simulations compared to the others is due in large part to the fact that these are full two-day simulations, while the others are one day and one night. If the fits are not good on day 1, the discrepancies can become magnified on day 2, due to differences in starting conditions. However, except for the simulations employing the high-aromatics mix "D," the simulations employing mixtures agree to within 4% for ozone and OH radicals, and to within 10% (in all but two cases) for H_2O_2. In view of the similarities between these two mechanisms, we see relatively little advantage to using the more detailed "Level B" mechanism compared to using "Level C," except perhaps for problems involving significant emissions of benzene.

On the other hand, as shown in Table 27, the "Level D" mechanism performs significantly worse in duplicating the predictions of the detailed mechanism than do the other two condensed mechanisms. This is true not

Table 28. Comparison of the Ozone, OH Radical, and H_2O_2 Predictions for the Test Calculations using the "Level C" (Standard) Condensed Mechanism for the Reactive Organic Products with those using the "Level B" Condensed Mechanism[a]

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
			Ozone			
TSTBEN1	-1	3.531	2.867	-0.664	-18.79	21.15
TSTBEN2	-1	4.404	4.587	0.182	4.14	9.79
TSTBEN3	-1	4.562	0.228	-4.335	-95.01	91.76
TSTTOL1	-1	3.610	3.474	-0.135	-3.75	6.14
TSTTOL2	-1	4.366	4.337	-0.029	-0.66	1.54
TSTTOL3	-2	7.383	5.322	-2.061	-27.91	24.05
TSTXYL1	-1	3.383	3.194	-0.190	-5.61	7.17
TSTXYL2	-1	4.894	4.831	-0.063	-1.28	1.90
TSTXYL3	-2	7.441	6.265	-1.176	-15.80	22.20
TSTMES1	-1	3.113	3.114	0.000	0.01	0.04
TSTMES2	-1	4.980	4.981	0.001	0.02	0.04
TSTMES3	-1	1.072	1.072	0.000	0.02	0.04
TSTMXA1	-2	2.197	2.127	-0.070	-3.20	2.76
TSTMXA2	-1	3.183	3.185	0.002	0.05	4.01
TSTMXA3	-1	3.607	3.584	-0.023	-0.64	1.18
TSTMXB1	-2	3.778	3.709	-0.069	-1.83	1.54
TSTMXB2	-1	3.050	3.063	0.014	0.45	1.04
TSTMXB3	-1	4.274	4.271	-0.004	-0.08	0.25
TSTMXC1	-2	4.120	3.942	-0.178	-4.31	3.52
TSTMXC2	-1	2.932	2.979	0.047	1.59	2.43
TSTMXC3	-1	3.635	3.597	-0.037	-1.03	1.28
TSTMXD1	-2	3.502	3.146	-0.357	-10.18	9.90
TSTMXD2	-1	2.322	2.451	0.128	5.52	8.47
TSTMXD3	-1	3.482	3.445	-0.037	-1.06	2.10
TSTMXE1	-2	1.668	1.650	-0.018	-1.10	0.90
TSTMXE2	-1	1.033	0.990	-0.043	-4.13	3.25
TSTMXE3	-1	2.407	2.368	-0.039	-1.62	1.97
TSTCAL1	-2	1.322	1.309	-0.013	-0.98	0.79
TSTCAL2	-2	8.850	8.477	-0.373	-4.22	3.92

(continued)

Table 28 (continued) - 2

CALC ID	Maximum Concentration[b] EXP	STD.	TEST	DIFF	% CHG	% FIT[c]
TSTCAL3	-1	2.506	2.494	-0.011	-0.44	2.36
TSTCAL4	-1	4.315	4.299	-0.016	-0.37	0.88
MD2CAL1	-2	3.036	2.959	-0.077	-2.55	2.21
MD2CAL2	-1	1.184	1.137	-0.047	-4.00	4.19
MD2CAL3	-1	2.834	2.782	-0.051	-1.80	2.65
MD2CAL4	-1	2.947	2.941	-0.006	-0.20	1.57
MD2CAL5	-1	2.804	2.799	-0.005	-0.16	1.16
MD2CAL6	-1	2.545	2.544	-0.002	-0.06	0.45
MD2CAL7	-1	2.321	2.320	-0.001	-0.05	0.25
MD2CAL8	-1	1.650	1.650	0.000	-0.03	0.08
			OH Radicals			
TSTBEN1	-7	1.536	1.073	-0.462	-30.10	50.78
TSTBEN2	-7	1.617	1.259	-0.358	-22.16	44.02
TSTBEN3	-7	1.796	0.197	-1.599	-89.03	73.75
TSTTOL1	-7	4.179	3.569	-0.610	-14.60	30.12
TSTTOL2	-7	2.717	3.650	0.933	34.36	18.81
TSTTOL3	-8	6.902	5.896	-1.006	-14.58	11.97
TSTXYL1	-7	4.387	3.454	-0.933	-21.27	16.84
TSTXYL2	-7	8.250	8.252	0.002	0.02	2.39
TSTXYL3	-7	1.520	1.445	-0.075	-4.95	7.04
TSTMES1	-7	3.338	3.340	0.002	0.06	0.25
TSTMES2	-6	1.317	1.321	0.004	0.33	0.10
TSTMES3	-7	2.100	2.107	0.007	0.32	0.31
TSTMXA1	-8	5.752	5.651	-0.102	-1.77	2.25
TSTMXA2	-7	4.411	4.401	-0.011	-0.24	9.73
TSTMXA3	-5	1.141	1.133	-0.008	-0.72	1.41
TSTMXB1	-8	5.750	5.713	-0.037	-0.65	0.76
TSTMXB2	-7	3.838	3.902	0.064	1.66	1.51
TSTMXB3	-5	1.278	1.277	0.000	-0.03	0.54
TSTMXC1	-8	4.316	4.251	-0.065	-1.52	1.97
TSTMXC2	-7	2.135	2.200	0.065	3.05	3.70
TSTMXC3	-6	6.693	6.715	0.021	0.32	0.91

(continued)

Table 28 (continued) - 3

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
TSTMXD1	-7	1.005	0.967	-0.038	-3.78	5.73
TSTMXD2	-7	2.831	4.143	1.312	46.35	18.30
TSTMXD3	-5	1.341	1.294	-0.047	-3.49	4.32
TSTMXE1	-8	6.385	6.350	-0.035	-0.55	0.87
TSTMXE2	-8	9.605	9.553	-0.052	-0.54	2.60
TSTMXE3	-5	1.214	1.208	-0.006	-0.47	0.80
TSTCAL1	-8	2.390	2.352	-0.038	-1.60	1.40
TSTCAL2	-8	4.959	4.882	-0.077	-1.55	1.94
TSTCAL3	-7	1.389	1.383	-0.006	-0.44	1.52
TSTCAL4	-6	6.266	6.253	-0.014	-0.22	0.58
MD2CAL1	-8	6.462	6.344	-0.118	-1.83	1.55
MD2CAL2	-7	1.007	0.989	-0.018	-1.81	2.52
MD2CAL3	-7	2.945	2.846	-0.099	-3.35	2.96
MD2CAL4	-7	3.523	3.522	-0.001	-0.04	1.75
MD2CAL5	-7	3.239	3.235	-0.004	-0.12	1.31
MD2CAL6	-7	3.744	3.748	0.004	0.11	0.90
MD2CAL7	-7	3.732	3.702	-0.030	-0.80	0.66
MD2CAL8	-7	2.719	2.716	-0.003	-0.12	0.47
			H_2O_2			
TSTBEN1	-2	1.470	0.400	-1.070	-72.77	75.38
TSTBEN2	-2	5.168	2.532	-2.636	-51.00	48.11
TSTBEN3	-2	3.656	0.000	-3.656	-100.00	100.00
TSTTOL1	-2	1.848	1.419	-0.429	-23.20	27.24
TSTTOL2	-2	6.430	5.863	-0.567	-8.82	9.92
TSTTOL3	-7	5.951	2.646	-3.305	-55.53	47.28
TSTXYL1	-4	9.171	6.590	-2.581	-28.14	39.21
TSTXYL2	-2	3.292	2.956	-0.335	-10.19	10.18
TSTXYL3	-7	5.381	3.539	-1.842	-34.23	32.69
TSTMES1	-4	2.729	2.704	-0.025	-0.93	0.36
TSTMES2	-2	1.641	1.640	0.000	-0.03	0.02
TSTMES3	-6	1.401	1.402	0.002	0.11	0.11
TSTMXA1	-8	3.165	2.924	-0.241	-7.61	6.50
TSTMXA2	-3	7.580	5.665	-1.915	-25.27	33.11
TSTMXA3	-3	6.780	6.140	-0.640	-9.44	9.89

(continued)

Table 28 (continued) - 4

CALC ID	Maximum Concentration[b]					% FIT[c]
	EXP	STD.	TEST	DIFF	% CHG	
TSTMXB1	-7	1.178	1.139	-0.039	-3.31	3.00
TSTMXB2	-2	2.125	2.087	-0.038	-1.80	1.98
TSTMXB3	-2	1.463	1.435	-0.028	-1.89	1.94
TSTMXC1	-8	7.146	6.449	-0.697	-9.75	6.97
TSTMXC2	-2	1.039	0.987	-0.052	-4.97	7.72
TSTMXC3	-3	3.976	3.670	-0.306	-7.70	9.99
TSTMXD1	-7	1.194	1.000	-0.193	-16.20	16.54
TSTMXD2	-2	1.467	1.155	-0.312	-21.26	28.98
TSTMXD3	-2	1.339	1.161	-0.178	-13.27	13.25
TSTMXE1	-8	2.088	2.037	-0.052	-2.47	2.51
TSTMXE2	-6	1.227	1.063	-0.164	-13.34	8.89
TSTMXE3	-4	5.979	5.574	-0.404	-6.76	8.09
TSTCAL1	-9	5.893	5.666	-0.227	-3.86	3.51
TSTCAL2	-7	6.927	6.133	-0.794	-11.46	8.94
TSTCAL3	-2	2.165	2.135	-0.030	-1.39	2.05
TSTCAL4	-2	1.303	1.265	-0.038	-2.93	6.29
MD2CAL1	-7	1.778	1.666	-0.112	-6.30	5.82
MD2CAL2	-5	1.660	1.418	-0.242	-14.58	13.82
MD2CAL3	-3	2.344	2.008	-0.336	-14.34	14.54
MD2CAL4	-3	8.743	8.436	-0.307	-3.51	4.62
MD2CAL5	-2	1.133	1.112	-0.021	-1.90	3.47
MD2CAL6	-2	1.379	1.358	-0.020	-1.46	2.81
MD2CAL7	-2	1.485	1.467	-0.019	-1.25	2.05
MD2CAL8	-2	1.534	1.517	-0.016	-1.07	1.35

[a]Comparisons for TSTHCH1 through TSTALK4 are not shown since these two mechanisms are the same for the species present in these test calculations.

[b]Maximum concentrations (in ppm) are expressed as follows: Level C mechanism: TEST x 10^{EXP}; Level B mechanism: STD. x 10^{EXP}. DIFF = TEST-STD. % CHG = (TEST-STD)/STD.

[c]See text for definition of this quantity, which measures the differences between the simulations at each hour in the simulation.

only for the simulations of the single aromatics, where especially poor fits are observed in the two-day cases, but also in the simulations of the mixtures as well. The main difference between this and the other condensed mechanisms is the fact that only one species is used to represent the reactive aromatic ring fragmentation products. Based on these results, it is apparent that using mechanisms employing a single product to represent these species will result in different predictions than using those which use more than one. This is despite the fact that the yields of these products in both mechanisms were adjusted to fit the same set of chamber data, and the quality of fits of these mechanisms to those data were similar. Since we are using the detailed mechanism for the aromatics as the standard, we conclude that the "Level D" condensation should not be employed. However, in view of the significant uncertainties in yields, identities, and reactions of the aromatic ring opening products, and the fact that the detailed mechanism itself is largely arbitrary and empirical in this regard, the possibility that the predictions of the "Level D" mechanism may actually turn out to be more accurate than the current "detailed" mechanism cannot be totally ruled out.

3. Effects of Alternative Lumpings of Primary Emitted Organics

A number of test calculations were carried out to determine the effects of alternative degrees of lumping of the primary emitted organics. Since lumping of primary emissions is of concern primarily in model simulations employing complex mixtures of organics, the test calculations employing the processed California emissions data to represent the organics were used for this purpose. All these calculations employed the more detailed mechanism for the reactive organic products, but the numbers of species employed to represent alkanes (and compounds lumped with them), the aromatics, and the non-ethene alkenes were varied. The most detailed mechanism in this regard employed six lumped alkenes, three lumped aromatics, and two lumped higher alkenes. This mechanism was used as a standard against which the performance of the more condensed mechanisms were evaluated. A comparison of the ozone predictions in the individual test calculations for the more condensed mechanisms and the standard "(6,3,2)" mechanism is given in Table 29, and the averages in the "% Fit" quantities for ozone, OH radicals, H_2O_2, PAN, and formaldehyde are shown in Table 30.

Table 29. Comparison of Ozone Predictions for Mechanisms using Various Numbers of Lumped Alkane, Aromatic, and Non-Ethene Species, to Predictions of a Mechanism using Six Lumped Alkanes, Three Lumped Aromatics, and Two Lumped Non-Ethene Alkenes

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
		Test Mechanism = (3,3,2)				
TSTCAL1	-2	1.392	1.396	0.004	0.28	0.22
TSTCAL2	-1	0.984	1.002	0.018	1.80	1.28
TSTCAL3	-1	2.515	2.526	0.011	0.44	0.74
TSTCAL4	-1	4.389	4.408	0.019	0.43	0.48
MD2CAL1	-2	3.233	3.257	0.024	0.74	0.58
MD2CAL2	-1	1.236	1.254	0.018	1.43	1.23
MD2CAL3	-1	2.808	2.829	0.021	0.76	0.95
MD2CAL4	-1	2.891	2.895	0.004	0.13	0.55
MD2CAL5	-1	2.754	2.762	0.008	0.29	0.44
MD2CAL6	-1	2.508	2.511	0.004	0.14	0.24
MD2CAL7	-1	2.285	2.287	0.002	0.11	0.15
MD2CAL8	-1	1.624	1.626	0.002	0.12	0.14
AVERAGE					0.56	0.58
		Test Mechanism = (3,2,2)				
TSTCAL1	-2	1.392	1.404	0.012	0.88	0.63
TSTCAL2	-1	0.984	1.029	0.044	4.52	3.71
TSTCAL3	-1	2.515	2.543	0.028	1.11	2.17
TSTCAL4	-1	4.389	4.409	0.020	0.46	0.76
MD2CAL1	-2	3.233	3.307	0.074	2.29	1.91
MD2CAL2	-1	1.236	1.278	0.042	3.41	3.41
MD2CAL3	-1	2.808	2.845	0.037	1.32	2.12
MD2CAL4	-1	2.891	2.899	0.008	0.27	1.31
MD2CAL5	-1	2.754	2.764	0.010	0.36	0.93
MD2CAL6	-1	2.508	2.511	0.003	0.13	0.40
MD2CAL7	-1	2.285	2.288	0.003	0.11	0.25
MD2CAL8	-1	1.624	1.625	0.000	0.02	0.15
AVERAGE					1.24	1.48

(continued)

Table 29 (continued) - 2

CALC ID	Maximum Concentration[a] EXP	STD.	TEST	DIFF	% CHG	% FIT[b]
		Test Mechanism = (2,2,2)				
TSTCAL1	-2	1.392	1.403	0.010	0.75	0.53
TSTCAL2	-1	0.984	1.018	0.033	3.38	2.95
TSTCAL3	-1	2.515	2.534	0.018	0.73	1.76
TSTCAL4	-1	4.389	4.400	0.011	0.25	0.48
MD2CAL1	-2	3.233	3.285	0.052	1.61	1.44
MD2CAL2	-1	1.236	1.265	0.029	2.36	2.62
MD2CAL3	-1	2.808	2.828	0.020	0.72	1.50
MD2CAL4	-1	2.891	2.891	-0.001	-0.03	0.84
MD2CAL5	-1	2.754	2.756	0.002	0.07	0.59
MD2CAL6	-1	2.508	2.505	-0.003	-0.13	0.22
MD2CAL7	-1	2.285	2.283	-0.002	-0.10	0.13
MD2CAL8	-1	1.624	1.622	-0.002	-0.14	0.10
AVERAGE					0.79	1.10
		Test Mechanism = (1,2,2)				
TSTCAL1	-2	1.392	1.399	0.007	0.50	0.37
TSTCAL2	-1	0.984	1.006	0.021	2.16	2.28
TSTCAL3	-1	2.515	2.518	0.003	0.11	1.35
TSTCAL4	-1	4.389	4.386	-0.003	-0.06	0.28
MD2CAL1	-2	3.233	3.271	0.037	1.15	1.19
MD2CAL2	-1	1.236	1.249	0.013	1.08	1.80
MD2CAL3	-1	2.808	2.792	-0.016	-0.56	0.98
MD2CAL4	-1	2.891	2.867	-0.024	-0.84	0.86
MD2CAL5	-1	2.754	2.736	-0.018	-0.66	0.51
MD2CAL6	-1	2.508	2.488	-0.019	-0.78	0.49
MD2CAL7	-1	2.285	2.269	-0.016	-0.69	0.51
MD2CAL8	-1	1.624	1.615	-0.009	-0.58	0.40
AVERAGE					0.07	0.92
		Test Mechanism = (2,1,2)				
TSTCAL1	-2	1.392	1.380	-0.013	-0.91	1.00
TSTCAL2	-2	9.843	9.761	-0.082	-0.84	2.02
TSTCAL3	-1	2.515	2.554	0.038	1.53	1.48
TSTCAL4	-1	4.389	4.395	0.006	0.14	0.23

(continued)

Table 29 (continued) - 3

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
MD2CAL1	-2	3.233	3.188	-0.046	-1.42	1.73
MD2CAL2	-1	1.236	1.214	-0.022	-1.81	2.05
MD2CAL3	-1	2.808	2.771	-0.036	-1.29	1.46
MD2CAL4	-1	2.891	2.903	0.012	0.42	0.95
MD2CAL5	-1	2.754	2.771	0.017	0.63	0.91
MD2CAL6	-1	2.508	2.526	0.019	0.74	0.41
MD2CAL7	-1	2.285	2.304	0.019	0.85	0.32
MD2CAL8	-1	1.624	1.636	0.011	0.69	0.32
AVERAGE					-0.10	1.07
	Test Mechanism = (1,1,2)					
TSTCAL1	-2	1.392	1.378	-0.015	-1.05	1.10
TSTCAL2	-2	9.843	9.657	-0.186	-1.89	2.65
TSTCAL3	-1	2.515	2.539	0.023	0.93	1.52
TSTCAL4	-1	4.389	4.381	-0.008	-0.17	0.46
MD2CAL1	-2	3.233	3.173	-0.060	-1.87	1.95
MD2CAL2	-1	1.236	1.197	-0.039	-3.13	2.92
MD2CAL3	-1	2.808	2.734	-0.073	-2.61	2.37
MD2CAL4	-1	2.891	2.878	-0.013	-0.46	1.38
MD2CAL5	-1	2.754	2.750	-0.004	-0.14	1.22
MD2CAL6	-1	2.508	2.510	0.002	0.09	0.55
MD2CAL7	-1	2.285	2.290	0.005	0.22	0.38
MD2CAL8	-1	1.624	1.628	0.004	0.24	0.20
AVERAGE					-0.82	1.39
	Test Mechanism = (3,2,1)					
TSTCAL1	-2	1.392	1.451	0.059	4.24	3.02
TSTCAL2	-1	0.984	1.081	0.097	9.84	11.01
TSTCAL3	-1	2.515	2.574	0.059	2.35	5.09
TSTCAL4	-1	4.389	4.401	0.012	0.27	0.94
MD2CAL1	-2	3.233	3.460	0.226	7.00	5.95
MD2CAL2	-1	1.236	1.326	0.090	7.25	8.29
MD2CAL3	-1	2.808	2.851	0.044	1.56	3.95
MD2CAL4	-1	2.891	2.883	-0.008	-0.28	2.40
MD2CAL5	-1	2.754	2.750	-0.004	-0.14	1.44
MD2CAL6	-1	2.508	2.495	-0.013	-0.52	0.54

(continued)

Table 29 (continued) - 4

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
MD2CAL7	-1	2.285	2.270	-0.015	-0.67	0.41
MD2CAL8	-1	1.624	1.607	-0.017	-1.07	0.74
AVERAGE					2.49	3.65
		Test Mechanism = (2,2,1)				
TSTCAL1	-2	1.392	1.448	0.056	4.01	2.87
TSTCAL2	-1	0.984	1.072	0.088	8.92	10.28
TSTCAL3	-1	2.515	2.564	0.048	1.93	4.62
TSTCAL4	-1	4.389	4.394	0.005	0.12	0.73
MD2CAL1	-2	3.233	3.446	0.212	6.57	5.56
MD2CAL2	-1	1.236	1.313	0.077	6.21	7.50
MD2CAL3	-1	2.808	2.834	0.027	0.96	3.34
MD2CAL4	-1	2.891	2.876	-0.015	-0.51	2.11
MD2CAL5	-1	2.754	2.742	-0.012	-0.45	1.29
MD2CAL6	-1	2.508	2.488	-0.019	-0.77	0.52
MD2CAL7	-1	2.285	2.265	-0.020	-0.89	0.58
MD2CAL8	-1	1.624	1.604	-0.020	-1.24	0.86
AVERAGE					2.07	3.36
		Test Mechanism = (1,2,1)				
TSTCAL1	-2	1.392	1.445	0.053	3.83	2.74
TSTCAL2	-1	0.984	1.058	0.073	7.47	9.49
TSTCAL3	-1	2.515	2.546	0.030	1.21	4.19
TSTCAL4	-1	4.389	4.379	-0.010	-0.23	0.59
MD2CAL1	-2	3.233	3.423	0.189	5.85	5.20
MD2CAL2	-1	1.236	1.296	0.060	4.82	6.60
MD2CAL3	-1	2.808	2.798	-0.010	-0.36	2.53
MD2CAL4	-1	2.891	2.851	-0.040	-1.39	2.12
MD2CAL5	-1	2.754	2.721	-0.033	-1.20	1.25
MD2CAL6	-1	2.508	2.472	-0.036	-1.44	0.85
MD2CAL7	-1	2.285	2.251	-0.034	-1.48	1.03
MD2CAL8	-1	1.624	1.597	-0.027	-1.66	1.18
AVERAGE					1.29	3.15

(continued)

Table 29 (continued) - 5

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
			Test Mechanism = (2,1,1)			
TSTCAL1	-2	1.392	1.426	0.034	2.42	1.47
TSTCAL2	-1	0.984	1.026	0.041	4.20	4.81
TSTCAL3	-1	2.515	2.585	0.070	2.78	1.94
TSTCAL4	-1	4.389	4.391	0.002	0.05	0.21
MD2CAL1	-2	3.233	3.341	0.108	3.33	2.36
MD2CAL2	-1	1.236	1.259	0.023	1.88	2.72
MD2CAL3	-1	2.808	2.783	-0.024	-0.86	1.16
MD2CAL4	-1	2.891	2.887	-0.005	-0.16	0.52
MD2CAL5	-1	2.754	2.760	0.006	0.22	0.22
MD2CAL6	-1	2.508	2.511	0.003	0.12	0.23
MD2CAL7	-1	2.285	2.288	0.003	0.15	0.23
MD2CAL8	-1	1.624	1.617	-0.007	-0.43	0.53
AVERAGE					1.14	1.37
			Test Mechanism = (1,1,1)			
TSTCAL1	-2	1.392	1.422	0.030	2.15	1.32
TSTCAL2	-1	0.984	1.016	0.032	3.23	4.18
TSTCAL3	-1	2.515	2.566	0.051	2.01	1.53
TSTCAL4	-1	4.389	4.378	-0.011	-0.25	0.31
MD2CAL1	-2	3.233	3.323	0.090	2.78	2.07
MD2CAL2	-1	1.236	1.242	0.006	0.46	1.81
MD2CAL3	-1	2.808	2.745	-0.063	-2.23	1.63
MD2CAL4	-1	2.891	2.863	-0.029	-0.99	0.69
MD2CAL5	-1	2.754	2.737	-0.016	-0.59	0.77
MD2CAL6	-1	2.508	2.494	-0.014	-0.55	0.70
MD2CAL7	-1	2.285	2.273	-0.012	-0.52	0.67
MD2CAL8	-1	1.624	1.611	-0.013	-0.83	0.77
AVERAGE					0.39	1.37

[a]Maximum concentrations (in ppm) are expressed as follows: Test mechanism: TEST x 10^{EXP}; (6,3,2) mechanism: STD. x 10^{EXP}. DIFF = TEST-STD. % CHG = (TEST-STD)/STD.

[b]See text for definition of this quantity, which measures the differences between the simulations at each hour in the simulation.

Table 30. Averages of Percent Fits to Predictions of Ozone, OH Radicals, H_2O_2, PAN, and Formaldehyde for Mechanisms using Various Numbers of Lumped Alkane, Aromatic, and Non-Ethene Species, to Predictions of a Mechanism Using Six Lumped Alkanes, Three Lumped Aromatics, and Two Lumped Non-Ethene Alkenes

	Average Percent Fits[a]					
No. Lumped Aromatics:	3	2			1	
No. Lumped Alkanes:	3	3	2	1	2	1
2 Lumped Higher Alkenes						
Ozone	0.6	1.5	1.1	0.9	1.1	1.4
OH Radicals	0.5	1.1	1.0	1.3	1.6	1.8
H2O2	1.1	2.8	1.7	1.1	4.9	6.8
PAN	1.3	2.8	1.9	2.0	2.0	2.8
Formaldehyde	0.3	0.6	0.5	0.8	0.8	1.0
1 Lumped Higher Alkene						
Ozone		3.7	3.4	3.2	1.4	1.4
OH Radicals		3.7	3.8	4.2	2.9	3.3
H2O2		5.8	4.6	3.1	2.3	4.3
PAN		8.0	6.9	6.6	4.0	3.7
Formaldehyde		3.2	3.4	3.8	3.0	3.4

[a]See text for the definition of this quantity, which measures the differences between the simulations at each hour in the simulations.

It is interesting to note that condensation, even to relatively extreme levels, of the numbers of species used to represent primary emitted organics have relatively small effects on the predictions of the mechanism for these test calculations. There is essentially no difference between the simulations using the (6,3,2) and the next more condensed (3,3,2) mechanism, suggesting that using an even more detailed mechanism than the (6,3,2) mechanism as the standard would not significantly affect the results. Even the highly condensed (1,1,1) mechanism, which has only one species each for lumped alkanes, aromatics, and higher alkenes, fits the ozone predictions of the (6,3,2) mechanism to better than 2% in all but two cases (where the fits are 2.1% and 4.2%), and even fits H_2O_2, generally among the most sensitive of the model species to mechanism differences, to better than 5% in all but two cases (where the fits are 7.0% and 10.7%). However, the fits of the most condensed mechanism for the organic products is not quite as good as it is for ozone and H_2O_2 (see Table 30), though the differences are still relatively small.

The summary of the fits in Table 30 suggest that there do not appear to be any consistent differences between mechanisms employing only one or two lumped alkane species compared to those using three or more. For the aromatics, it appears that there are slight differences in going from three to one lumped aromatic, and that probably use of two species for this purpose would be appropriate. The lumping of the higher alkenes appear to have the greatest effect; Table 30 indicates that the fits for most species are consistently worse when only one lumped species is used for higher alkenes. These results suggest that, at least for single-cell airshed model calculations of the type represented by these test calculations, use of only one lumped species for the alkanes, and two each for the aromatics and the alkenes, might be appropriate.

4. Effects of Neglecting Reactions of Hydroperoxides

As discussed above, an additional option with regard to mechanism condensation concerns whether to include the reactions of H_2O_2 and lumped organic hydroperoxides ("-OOH") in the mechanism. These must be included in models were predictions of acid deposition is of concern, but Lurmann et al. (1987a) indicated that they can be removed in models where predictions of ozone is the major objective. To evaluate this, we carried out the test calculations for the "Level C" condensed model without including

the H_2O_2 and -OOH reactions. The results are compared with the condensed model calculations where these reactions are included in Table 31. It can be seen that the effects on predictions of ozone and OH radicals are indeed quite small for essentially all simulations, particularly those employing mixtures. On the other hand, as expected, removing the reactions of these species results in overpredictions of H_2O_2 by typically 20%.

Table 31. Comparison of the Ozone, OH Radical, and H_2O_2 Predictions for the Test Calculations using the "Level C" (Standard) Condensed Mechanism Both with and without Reactions of H_2O_2 and Lumped Organic Hydroperoxides

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
			Ozone			
TSTHCH1	-1	2.242	2.242	0.000	0.00	0.01
TSTHCH2	-1	6.307	6.299	-0.008	-0.13	0.08
TSTHCH3	-2	4.789	4.790	0.001	0.02	0.02
TSTCCH1	-1	5.493	5.492	0.000	0.00	0.04
TSTCCH2	-1	6.181	6.183	0.002	0.03	0.03
TSTCCH3	-1	5.075	4.936	-0.139	-2.74	0.93
TSTRCH1	-1	6.015	6.009	-0.006	-0.09	0.08
TSTRCH2	-1	6.267	6.291	0.024	0.38	0.31
TSTRCH3	-1	6.203	5.992	-0.212	-3.41	0.85
TSTACE1	-1	4.065	4.064	-0.001	-0.02	0.02
TSTACE2	-1	6.608	6.603	-0.006	-0.09	0.06
TSTACE3	-1	8.848	8.846	-0.002	-0.02	0.05
TSTMEK1	-1	6.086	6.084	-0.002	-0.03	0.02
TSTMEK2	-1	7.137	7.129	-0.008	-0.12	0.08
TSTMEK3	-1	4.693	4.670	-0.023	-0.49	0.16
TSTNIT1	-1	7.242	7.244	0.001	0.02	0.02
TSTNIT2	0	1.358	1.357	0.000	-0.03	0.02
TSTNIT3	0	1.091	1.089	-0.002	-0.16	0.09
TSTETH1	-1	6.742	6.732	-0.009	-0.14	0.15
TSTETH2	-1	9.682	9.662	-0.021	-0.21	0.35
TSTETH3	-1	5.006	5.010	0.005	0.09	0.08
TSTPRP1	-1	4.884	4.884	0.000	-0.01	0.02
TSTPRP2	-1	6.673	6.643	-0.030	-0.45	0.36
TSTPRP3	-1	3.516	3.513	-0.003	-0.08	0.07
TSTT2B1	-1	5.292	5.290	-0.002	-0.03	0.03
TSTT2B2	-1	6.371	6.339	-0.032	-0.51	0.36
TSTT2B3	-1	4.692	4.640	-0.053	-1.12	0.39
TSTALK1	-1	8.377	8.365	-0.012	-0.14	0.12
TSTALK2	0	1.068	1.067	-0.001	-0.09	0.20

(continued)

Table 31 (continued) - 2

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
TSTALK3	-1	5.682	5.682	0.000	0.00	0.10
TSTALK4	-2	3.677	3.677	0.000	0.00	0.01
TSTBEN1	-1	2.867	2.861	-0.007	-0.23	0.24
TSTBEN2	-1	4.587	4.582	-0.004	-0.10	0.15
TSTBEN3	-2	2.277	2.279	0.002	0.11	0.13
TSTTOL1	-1	3.474	3.472	-0.002	-0.07	0.08
TSTTOL2	-1	4.337	4.320	-0.017	-0.39	0.34
TSTTOL3	-2	5.322	5.345	0.023	0.43	0.59
TSTXYL1	-1	3.194	3.193	-0.001	-0.03	0.04
TSTXYL2	-1	4.831	4.678	-0.153	-3.16	2.57
TSTXYL3	-2	6.265	6.260	-0.005	-0.08	0.08
TSTMES1	-1	3.114	3.113	-0.001	-0.03	0.05
TSTMES2	-1	4.981	4.850	-0.132	-2.64	2.34
TSTMES3	-1	1.072	1.073	0.001	0.08	0.14
TSTMXA1	-2	2.127	2.127	0.000	0.00	0.02
TSTMXA2	-1	3.185	3.175	-0.009	-0.30	0.10
TSTMXA3	-1	3.584	3.578	-0.006	-0.16	0.70
TSTMXB1	-2	3.709	3.706	-0.003	-0.08	0.05
TSTMXB2	-1	3.063	3.011	-0.052	-1.70	0.50
TSTMXB3	-1	4.271	4.257	-0.014	-0.32	1.25
TSTMXC1	-2	3.942	3.940	-0.002	-0.05	0.03
TSTMXC2	-1	2.979	2.965	-0.014	-0.47	0.14
TSTMXC3	-1	3.597	3.553	-0.044	-1.24	0.55
TSTMXD1	-2	3.146	3.146	0.000	0.00	0.02
TSTMXD2	-1	2.451	2.430	-0.021	-0.86	0.23
TSTMXD3	-1	3.445	3.426	-0.019	-0.54	1.11
TSTMXE1	-2	1.650	1.650	0.000	0.00	0.02
TSTMXE2	-2	9.900	9.899	0.000	0.00	0.04
TSTMXE3	-1	2.368	2.368	0.000	-0.02	0.13
TSTCAL1	-2	1.309	1.309	0.000	0.00	0.03
TSTCAL2	-2	8.477	8.466	-0.011	-0.13	0.07
TSTCAL3	-1	2.494	2.480	-0.015	-0.59	0.18
TSTCAL4	-1	4.299	4.249	-0.049	-1.15	0.52

(continued)

Table 31 (continued) - 3

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
MD2CAL1	-2	2.959	2.959	0.000	0.01	0.02
MD2CAL2	-1	1.137	1.136	-0.001	-0.05	0.08
MD2CAL3	-1	2.782	2.772	-0.010	-0.37	0.18
MD2CAL4	-1	2.941	2.918	-0.022	-0.76	0.31
MD2CAL5	-1	2.799	2.772	-0.028	-0.98	0.42
MD2CAL6	-1	2.544	2.518	-0.026	-1.02	0.54
MD2CAL7	-1	2.320	2.295	-0.025	-1.06	0.68
MD2CAL8	-1	1.650	1.635	-0.014	-0.87	0.69
			OH Radicals			
TSTHCH1	-7	2.206	2.207	0.001	0.04	0.05
TSTHCH2	-6	1.141	1.151	0.010	0.83	1.51
TSTHCH3	-7	1.803	1.803	0.000	0.01	0.05
TSTCCH1	-7	1.398	1.397	-0.001	-0.10	0.90
TSTCCH2	-8	8.853	8.852	-0.001	-0.01	1.78
TSTCCH3	-7	6.884	7.481	0.597	8.68	3.74
TSTRCH1	-7	1.142	1.146	0.005	0.42	1.25
TSTRCH2	-8	6.006	5.998	-0.008	-0.14	2.94
TSTRCH3	-7	5.575	6.415	0.840	15.07	6.69
TSTACE1	-7	1.156	1.157	0.000	0.02	0.08
TSTACE2	-7	1.592	1.590	-0.002	-0.12	0.49
TSTACE3	-7	1.158	1.157	0.000	-0.01	3.03
TSTMEK1	-7	1.542	1.542	0.000	0.01	0.43
TSTMEK2	-7	1.338	1.338	0.000	-0.02	0.96
TSTMEK3	-8	9.986	9.713	-0.273	-2.74	1.64
TSTNIT1	-8	5.249	5.249	0.000	0.00	0.02
TSTNIT2	-8	5.489	5.488	0.000	-0.01	0.10
TSTNIT3	-8	5.779	5.758	-0.021	-0.37	0.18
TSTETH1	-7	3.154	3.153	-0.001	-0.05	0.25
TSTETH2	-7	3.616	3.614	-0.002	-0.06	1.46
TSTETH3	-7	1.842	1.838	-0.003	-0.18	0.09
TSTPRP1	-7	1.820	1.819	-0.001	-0.06	0.40
TSTPRP2	-7	2.203	2.197	-0.006	-0.28	2.11
TSTPRP3	-7	1.174	1.173	-0.001	-0.12	0.11

(continued)

Table 31 (continued) - 4

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
TSTT2B1	-7	2.308	2.250	-0.058	-2.52	1.13
TSTT2B2	-7	1.246	1.225	-0.022	-1.75	2.46
TSTT2B3	-7	7.851	8.072	0.221	2.82	1.29
TSTALK1	-7	2.236	2.231	-0.005	-0.21	0.56
TSTALK2	-7	1.831	1.830	-0.001	-0.06	1.83
TSTALK3	-7	1.184	1.183	-0.001	-0.06	1.05
TSTALK4	-8	9.938	9.938	0.000	0.00	0.01
TSTBEN1	-7	1.073	1.085	0.012	1.13	0.68
TSTBEN2	-7	1.259	1.269	0.010	0.82	1.89
TSTBEN3	-8	1.970	1.971	0.001	0.05	0.11
TSTTOL1	-7	3.569	3.534	-0.035	-0.98	0.59
TSTTOL2	-7	3.650	3.646	-0.004	-0.12	1.80
TSTTOL3	-8	5.896	5.916	0.020	0.34	0.39
TSTXYL1	-7	3.454	3.453	-0.001	-0.02	0.22
TSTXYL2	-7	8.252	9.973	1.722	20.86	11.27
TSTXYL3	-7	1.445	1.442	-0.003	-0.20	0.22
TSTMES1	-7	3.340	3.338	-0.003	-0.08	0.31
TSTMES2	-6	1.321	1.409	0.088	6.67	6.04
TSTMES3	-7	2.107	2.090	-0.017	-0.82	0.91
TSTMXA1	-8	5.651	5.656	0.005	0.10	0.06
TSTMXA2	-7	4.401	4.393	-0.008	-0.18	0.22
TSTMXA3	-5	1.133	1.150	0.016	1.46	1.95
TSTMXB1	-8	5.713	5.713	0.000	0.01	0.02
TSTMXB2	-7	3.902	4.019	0.117	3.01	1.37
TSTMXB3	-5	1.277	1.317	0.039	3.08	4.54
TSTMXC1	-8	4.251	4.248	-0.003	-0.07	0.03
TSTMXC2	-7	2.200	2.191	-0.009	-0.39	0.31
TSTMXC3	-6	6.715	6.733	0.018	0.27	1.00
TSTMXD1	-8	9.669	9.669	0.001	0.01	0.02
TSTMXD2	-7	4.143	4.143	0.001	0.02	1.27
TSTMXD3	-5	1.294	1.326	0.032	2.48	2.78
TSTMXE1	-8	6.350	6.353	0.003	0.05	0.08
TSTMXE2	-8	9.553	9.555	0.002	0.02	0.05
TSTMXE3	-5	1.208	1.210	0.002	0.14	0.19

(continued)

Table 31 (continued) - 5

CALC ID	Maximum Concentration[a] EXP	STD.	TEST	DIFF	% CHG	% FIT[b]
TSTCAL1	-8	2.352	2.352	0.000	0.00	0.03
TSTCAL2	-8	4.882	4.881	-0.002	-0.03	0.03
TSTCAL3	-7	1.383	1.355	-0.028	-2.03	1.59
TSTCAL4	-6	6.253	6.279	0.027	0.42	1.03
MD2CAL1	-8	6.344	6.348	0.004	0.06	0.03
MD2CAL2	-8	9.885	9.881	-0.004	-0.04	0.09
MD2CAL3	-7	2.846	2.831	-0.015	-0.52	0.30
MD2CAL4	-7	3.522	3.505	-0.017	-0.48	0.42
MD2CAL5	-7	3.235	3.217	-0.018	-0.56	0.67
MD2CAL6	-7	3.748	3.731	-0.017	-0.46	0.78
MD2CAL7	-7	3.702	3.685	-0.017	-0.46	0.88
MD2CAL8	-7	2.716	2.715	-0.001	-0.04	1.15
			H_2O_2			
TSTHCH1	-5	4.924	6.379	1.455	29.54	25.69
TSTHCH2	-2	1.561	2.519	0.958	61.34	55.23
TSTHCH3	-7	6.710	8.149	1.439	21.44	29.67
TSTCCH1	-2	1.574	1.639	0.065	4.13	3.68
TSTCCH2	-2	7.000	7.302	0.302	4.31	3.50
TSTCCH3	-2	3.144	4.497	1.353	43.03	26.44
TSTRCH1	-2	4.318	4.523	0.204	4.74	3.91
TSTRCH2	-1	1.194	1.235	0.041	3.42	2.74
TSTRCH3	-2	6.620	9.213	2.593	39.17	21.49
TSTACE1	-3	2.932	2.960	0.028	0.96	1.14
TSTACE2	-2	2.841	2.955	0.114	4.02	3.63
TSTACE3	-1	1.482	1.664	0.182	12.29	7.63
TSTMEK1	-2	1.455	1.494	0.039	2.70	2.40
TSTMEK2	-2	5.354	5.595	0.242	4.52	3.96
TSTMEK3	-2	5.840	6.398	0.558	9.55	6.83
TSTNIT1	-2	1.097	1.103	0.006	0.57	0.78
TSTNIT2	-2	3.497	3.548	0.051	1.45	2.18
TSTNIT3	-3	7.660	8.282	0.622	8.12	7.73
TSTETH1	-2	1.641	1.749	0.107	6.53	6.11
TSTETH2	-1	1.238	1.418	0.180	14.57	12.04
TSTETH3	-4	6.048	6.504	0.456	7.53	7.22

(continued)

Table 31 (continued) - 6

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
TSTPRP1	-3	6.707	6.952	0.245	3.65	3.84
TSTPRP2	-2	6.540	7.384	0.845	12.92	10.38
TSTPRP3	-5	5.197	5.929	0.732	14.09	10.54
TSTT2B1	-3	9.198	9.768	0.570	6.20	5.50
TSTT2B2	-2	6.181	6.809	0.628	10.17	8.20
TSTT2B3	-2	1.123	1.682	0.558	49.71	31.78
TSTALK1	-2	1.936	2.149	0.213	11.00	9.98
TSTALK2	-2	5.959	6.974	1.015	17.03	14.31
TSTALK3	-2	2.004	2.246	0.242	12.09	7.97
TSTALK4	-7	2.094	2.634	0.540	25.78	24.17
TSTBEN1	-3	4.003	4.039	0.037	0.91	0.77
TSTBEN2	-2	2.532	2.625	0.093	3.66	3.20
TSTBEN3	-8	3.686	4.116	0.430	11.67	8.86
TSTTOL1	-2	1.419	1.483	0.063	4.46	3.62
TSTTOL2	-2	5.863	6.250	0.386	6.59	5.60
TSTTOL3	-7	2.646	2.999	0.353	13.34	11.29
TSTXYL1	-4	6.590	7.114	0.524	7.95	10.45
TSTXYL2	-2	2.956	4.332	1.376	46.54	48.43
TSTXYL3	-7	3.539	4.644	1.105	31.23	15.98
TSTMES1	-4	2.704	3.059	0.355	13.14	18.40
TSTMES2	-2	1.640	3.177	1.537	93.68	88.10
TSTMES3	-6	1.402	1.687	0.285	20.32	20.94
TSTMXA1	-8	2.924	3.954	1.030	35.21	18.92
TSTMXA2	-3	5.665	6.280	0.616	10.87	8.94
TSTMXA3	-3	6.140	6.710	0.570	9.28	18.83
TSTMXB1	-7	1.139	1.427	0.288	25.32	15.90
TSTMXB2	-2	2.087	2.800	0.713	34.18	20.99
TSTMXB3	-2	1.435	1.637	0.202	14.05	24.90
TSTMXC1	-8	6.449	7.798	1.349	20.92	14.59
TSTMXC2	-2	0.987	1.088	0.101	10.20	8.05
TSTMXC3	-3	3.670	4.875	1.205	32.82	15.94
TSTMXD1	-7	1.000	1.294	0.293	29.32	19.80
TSTMXD2	-2	1.155	1.393	0.238	20.57	15.34
TSTMXD3	-2	1.161	1.357	0.196	16.88	23.81

(continued)

Table 31 (continued) - 7

CALC ID	Maximum Concentration[a]					% FIT[b]
	EXP	STD.	TEST	DIFF	% CHG	
TSTMXE1	-8	2.037	2.666	0.629	30.89	20.97
TSTMXE2	-6	1.063	1.372	0.309	29.11	17.06
TSTMXE3	-4	5.574	5.730	0.156	2.80	14.39
TSTCAL1	-9	5.666	6.985	1.319	23.28	13.81
TSTCAL2	-7	6.133	6.936	0.803	13.09	11.47
TSTCAL3	-2	2.135	2.395	0.261	12.21	8.64
TSTCAL4	-2	1.265	1.623	0.358	28.33	15.18
MD2CAL1	-7	1.666	1.147	-0.520	-31.18	28.59
MD2CAL2	-5	1.418	1.131	-0.286	-20.19	29.90
MD2CAL3	-3	2.008	1.647	-0.360	-17.93	27.05
MD2CAL4	-3	8.436	7.969	-0.466	-5.53	12.92
MD2CAL5	-2	1.112	1.050	-0.061	-5.51	12.91
MD2CAL6	-2	1.358	1.245	-0.114	-8.38	14.88
MD2CAL7	-2	1.467	1.316	-0.151	-10.27	16.27
MD2CAL8	-2	1.517	1.283	-0.234	-15.45	18.39

[a]Maximum concentrations (in ppm) are expressed as follows: Condensed mechanism: TEST x 10^{EXP}; Detailed mechanism: STD. x 10^{EXP}. DIFF = TEST-STD. % CHG = (TEST-STD)/STD.

[b]See text for definition of this quantity, which measures the differences between the simulations at each hour in the simulation.

V. CONCLUSIONS

We believe that the gas-phase photochemical reaction mechanism documented in this report represents the current state of the art in our knowledge of atmospheric chemistry. It builds upon the previous mechanisms which have been developed at our laboratories and in conjunction with researchers at ERT, which was updated based on a very recent and comprehensive review of our current knowledge of atmospheric chemistry (Atkinson 1988), and was expanded to include the ability to explicitly represent the reactions of over 100 different types of organic compounds. Techniques for condensing this highly detailed mechanism so it can be used in complex airshed models were also developed. These techniques, employing software which was developed in conjunction with the development of this mechanism (Carter 1988), allows airshed models to incorporate condensed mechanisms with relatively few species, while still incorporating, to the maximum extent possible, the detailed chemical information contained in emissions profiles, and our knowledge or estimates of the atmospheric reactions of the many different types of species which are emitted.

However, it should be recognized that despite continuing laboratory studies of the kinetics and mechanisms of the atmospheric reactions of emitted organics, there continues to be significant uncertainties in all chemical mechanisms used in airshed models. For example, we still know very little of the chemical processes accounting for much of the ring fragmentation routes for the aromatic hydrocarbons, and recent laboratory studies tend to indicate that we know even less about these processes than we once thought we did. Likewise, the significant uncertainties remain in the photooxidation mechanisms of the higher alkanes (and their reaction products), the extent of radical formation in ozone - alkene reactions, the photolysis reactions of many of the oxygenated products. The representations of these processes in the photochemical mechanism continue to be largely speculative or based on empirical models derived based on fits to environmental chamber data.

A major characteristic of the mechanism developed in this program is its capability to explicitly represent the kinetics and reaction mechanisms of over 100 detailed model species representing a wide variety of

emitted organic compounds. However, although the initial rates of reaction for most of these species are reasonably well established, either by direct measurement or by experimentally validated estimation techniques, this cannot be said for the product yields and mechanisms assumed for most of these compounds. For most compounds, these had to be estimated based on our knowledge of analogous, but generally lower molecular weight, compounds, whose mechanisms themselves (as indicated above) may be uncertain. Only for a minority of these detailed model species are environmental chamber data available to evaluate the assumptions or estimations made for their mechanistic or product yield parameters. The parameters assumed for the higher molecular weight compounds, which constitute a non-negligible fraction of the emissions, are particularly uncertain.

However, despite these uncertainties, we believe that using these estimates for the detailed model is preferable to the alternative of ignoring our best estimates for the mechanisms of the many emitted species entirely, and just representing their reactions by the much smaller number of surrogate species (or lumped structure groups) for which mechanisms have already been developed and evaluated. As more data become available concerning the kinetics and reaction mechanisms of the many classes of emitted organic compounds, and chamber data available to test their reaction mechanisms, our representation of the detailed model species will become increasingly accurate. The procedures developed in this program (Carter 1988) for incorporating parameters assigned for the detailed species into lumped models provides a framework for this new knowledge to become readily incorporated into the airshed models, without the need to develop and re-evaluate new lumped mechanisms.

An additional area where more work is needed is the classification system used for the chemical compositions of emissions profiles. Ideally, each chemical class used in emissions profiles should refer to an individual chemical, or, at worst, a group of isomeric species which can reasonably be assumed to have similar reactivity. However, this is presently not the case for the SAROAD classification scheme as currently used in the ARB or the EPA data bases. Many categories refer to mixtures of compounds of different reactivity, with no indication of the overall reactivity of the mixtures, and some categories, such as "NAPHTHA," refer to complex

mixtures whose chemical compositions are poorly characterized. Emissions data for many California airsheds include major fractions of emissions of SAROAD categories which refer to lumped structural groups using the Carbon Bond mechanism, making these profiles almost useless for input into airshed models using the current generation of chemically detailed mechanisms. In addition, particularly in the EPA/NAPAP data set, there are cases where more than one SAROAD category is used to represent the same chemical or group of chemicals. Even worse, there are approximately 30 SAROAD classes, some with non-negligible emissions, which refer to different groups of chemicals in the ARB data sets than they do in the EPA/NAPAP data base. These problems have made the already difficult task of assigning of detailed model species to the SAROAD classes even more difficult than it would otherwise be, and we believe in many cases has introduced unnecessary uncertainties in the chemical accuracy of the emissions assignments.

The fully detailed mechanism developed in this program is clearly too large to use in airshed models, and the users of such models are presented with a number of options concerning the extent to which it can be condensed. The test calculations described in this report indicate that the numbers of species used to represent reactive organic products can be reduced from eighteen to eight without having major impacts on the model predictions in model simulations employing complex mixtures. However, the impacts of this condensation is non-negligible in simulations of NO_x-air irradiations of some individual compounds, and use of the full set of eighteen intermediates is recommended in single cell or trajectory models where use of highly condensed mechanisms are not required. The full set of intermediates should also be used in model calculations carried out for the purpose of assessing relative reactivities of individual organics, since chemical accuracy is particularly critical in such applications.

The test calculations which were carried out to test the condensation of reactive organic product species concerned primarily the effects of condensing the numbers of species used to represent aromatic ring opening products. The results indicated that if the representation used in the detailed mechanism is taken as the standard, then the use of a minimum of two species is required. However, these are not the only significant areas of condensation in going from the eighteen organic product species

in the detailed mechanisms to the eight in the condensed version. Calculations similar to those reported here on effects of condensation of aromatic ring fragmentation species should be carried out to assess the effects of the other approximations which are employed in the condensed mechanism. It may be that a mechanism employing only slightly more than the eight organic product species in the current condensed mechanism may give much closer simulations of calculations employing the full set of eighteen in the detailed mechanism. We were unable to carry out a comprehensive study of this within the scope of this program, and further work in this area is required.

The most important way in which the detailed mechanism can be condensed concerns the numbers of species used to represent the many types of primary organic pollutants. In contrast to the test calculations examining condensation of organic products, we found models with extremely condensed representations of the primary organics gave very close simulations of calculations employing much larger numbers of such species. Even models employing only four species to represent primary organics (one lumped alkane, one lumped aromatic, ethene, and one lumped higher alkene) duplicated surprisingly well the more detailed simulations. The correspondence is even better if two species are used to represent the higher alkenes and (somewhat less importantly) if two species are used to represent the aromatics. Employing more species to represent the alkanes (and compounds, such as alcohols and ethers, which are lumped with them) does not appear to have as much of an effect on model simulations, despite the large amounts of such species which are emitted.

One reason for the perhaps surprisingly good performance of the highly condensed mechanisms in simulating the results of the most detailed one may be the use of "reactivity weighing" in determining the contributions of the detailed species which are lumped into the least reactive of the groups. (See Carter 1988 for a full discussion of this approach). In this method, the contribution of the emitted species to the lumped group is determined by the estimated amount of the species which reacts during the model scenario, and not by the amount emitted (Carter 1988). This is used for the least reactive alkane and aromatic lumped groups because those are the groups which necessarily have the widest range in magnitudes of reaction rates. Although the method used to estimate amount

reacted is highly approximate, the results of the test calculations indicate that extreme accuracy in this regard is not necessary. Thus, the use of reactivity weighing in representing the more slowly reacting species appears to be a useful method for achieving a high degree of condensation in mechanisms used in airshed models, with relatively little impact on airshed model predictions.

However, it should be pointed out that all the test calculations employed to evaluate the condensation methods were based on single cell scenarios, and thus do not indicate the effects of extreme lumping of emitted organics on predictions of grid-model calculations where emissions inputs vary in composition with time and location in the modeling region. Since the mechanistic parameters for the lumped species in this mechanism must be constant within a given model simulation, they can thus represent the composition of only a single "representative" emissions profile (Carter 1988). This presents no problem in these test calculations, since only a single profile is input. However, if the profiles input into a more complex model differ significantly in composition of species which are lumped together, then inaccuracies in the representation of the emitted species are introduced. The only way to get around this problem is to utilize more species in the lumped mechanism, where either the differences in the species represented by each lumped species are minimized, or different sets of species are used to represent different types of profiles. Test calculations using multi-celled models are required to evaluate these effects, but such calculations are expensive and are beyond the scope of this program. However, it is important to recognize that this is a problem for all condensed mechanisms, and not just this one. The only difference is that in this case the potential of the mechanism for extreme accuracy (relative to the detailed mechanisms) in simulations with single emissions profiles cannot be realized if the profiles differ significantly in composition within the modeling region. Mechanisms with invariant parameters for lumped species are potentially equally inaccurate in both types of simulations.

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APPENDIX A

PERFORMANCE OF THE MECHANISM IN SIMULATING THE RESULTS OF INDIVIDUAL CHAMBER RUNS

This Appendix contains the tabulations of the results for selected species in the simulations of the over 500 chamber experiments used to evaluate the detailed mechanism. The evaluation of this mechanism against these chamber runs are discussed in Section II.B. The order of the tabulations given in this appendix are shown below. These tabulations are given in the same format and order as the tabulations of the performance of the previous mechanism given in the report of Lurmann et al. (1987a). In addition to the runs tabulated by Lurmann et al. (1987a), we also show the performance of the mechanism in simulating the synthetic jet fuel and synthetic jet exhaust runs, where they can be compared with the tabulations given by Carter et al. (1987) for the previous mechanism.

Table No.	Description of Runs
1	Background Air Runs
2	NO_x-Air and NO_x-CO-Air Irradiations
3	Formaldehyde-Air Runs
4	Acetaldehyde-Air Runs
5	Formaldehyde-NO_x-Air Runs
6	Aldehyde or Ketone-NO_x-Air Runs
7	N-Butane - NO_x-Air Runs
8	Branched Alkane - NO_x-Air Runs
9	Pentane and Higher N-Alkanes - NO_x-Air Runs
10	Ethene-NO_x-Air Runs
11	Propene-NO_x-Air Runs
12	Butene-NO_x-Air Runs
13	Benzene-NO_x-Air Runs
14	Toluene-NO_x-Air Runs
15	Xylene-NO_x-Air Runs
16	1,3,5-Trimethylbenzene-NO_x-Air Runs
17	Mixtures of Like Compounds
18	Miscellaneous Simple (Non-Surrogate) Mixtures
19	Minimum Surrogate Mixtures
20	Full Surrogate Mixtures
21	UNC Auto Exhaust Runs
22	Synthetic Jet Fuel and Jet Exhaust Runs

Table A-1. Background Air Runs

Experiment	Maximum Concentration OZONE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. UNC CHAMBER - PURE AIR				
JN0682R	0.203	0.225	0.023	0.11
OC0684R	0.097	0.108	0.010	0.11
OC0684B	0.119	0.121	0.002	0.02
Group Average	0.139	0.151	0.012	0.08
S. Dev.	0.056	0.064	0.010	0.05
Avg. Abs. Value			0.012	0.08
S. Dev.			0.010	0.05
2. SAPRC ITC - PURE AIR				
ITC940	0.072	0.074	0.002	0.02
ITC955	0.064	0.074	0.010	0.15
ITC1008	0.088	0.074	-0.014	-0.15
Group Average	0.075	0.074	-0.001	0.01
S. Dev.	0.012	0.000	0.012	0.15
Avg. Abs. Value			0.008	0.11
S. Dev.			0.006	0.08

Table A-2. NO_x-Air and NO_x-CO-Air Irradiations

Experiment	Initial Concentrations			Final - Init NO			Final - Init NO_2-UNC			Final - Init PROPENE		
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)
1. SAPRC EC - NO_x-AIR												
EC436	1.79	0.0	0.0	-0.098	-0.048	0.050	-0.071	-0.062	0.010	-0.004	-0.005	-0.001
EC440	0.76	0.0	0.0	-0.063	-0.049	0.015	0.024	0.013	-0.011	-0.005	-0.005	0.000
EC442	0.58	0.0	0.1	0.069	0.093	0.024	-0.172	-0.160	0.012	-0.006	-0.005	0.001
EC457	0.50	0.0	0.1	-0.066	-0.043	0.023	0.008	-0.008	-0.016	-0.007	-0.008	-0.001
EC464	0.19	0.0	0.2	-0.019	-0.004	0.014	-0.002	-0.010	-0.008	-0.006	-0.007	-0.001
EC597	0.56	0.0	0.1	-0.061	-0.032	0.029	0.041	0.005	-0.036	-0.007	-0.007	0.000
EC599	3.40	0.0	0.0	2.276	1.914	-0.362	-2.685	-2.561	0.124	-0.007	-0.008	0.000
Group Average	1.11	0.0	0.1	0.291	0.262	-0.029	-0.408	-0.398	0.011	-0.006	-0.007	0.000
S. Dev.	1.13	0.0	0.1	0.877	0.730	0.147	1.007	0.956	0.052	0.001	0.001	0.001
Avg. Abs. Value				0.379	0.312	0.074	0.429	0.403	0.031	0.006	0.007	0.001
S. Dev.				0.837	0.707	0.128	0.996	0.953	0.042	0.001	0.001	0.000
2. SAPRC ITC - NO_x-AIR												
ITC695	0.50	0.0	0.1	-0.021	-0.008	0.014	0.011	0.001	-0.010	-0.003	-0.002	0.001
ITC826	0.90	0.8	0.9	-0.349	-0.353	-0.004	0.263	0.238	-0.025	-0.005		
ITC882	0.70	0.0	0.0	-0.001	-0.027	-0.026	-0.010	-0.014	-0.004	-0.001	-0.002	0.000
Group Average	0.70	0.3	0.3	-0.124	-0.129	-0.005	0.088	0.075	-0.013	-0.003	-0.002	0.000
S. Dev.	0.20	0.5	0.5	0.195	0.194	0.020	0.152	0.142	0.011	0.002	0.000	0.001
Avg. Abs. Value				0.124	0.129	0.014	0.095	0.084	0.013	0.003	0.002	0.001
S. Dev.				0.195	0.194	0.011	0.146	0.134	0.011	0.002	0.000	0.000

Table A-2 (continued) - 2

Experiment	Initial Concentrations			Final - Init NO			Final - Init NO_2-UNC			Final - Init PROPENE		
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)
3. SAPRC OTC - NO_x-AIR												
OTC185	0.28	0.0	0.1	-0.002	-0.004	-0.002	-0.003	-0.001	0.002	-0.001	-0.002	-0.002
Group Average	0.28	0.0	0.1	-0.002	-0.004	-0.002	-0.003	-0.001	0.002	-0.001	-0.002	-0.002
S. Dev.												
Avg. Abs. Value				0.002	0.004	0.002	0.003	0.001	0.002	0.001	0.002	0.002
S. Dev.												
4. UNC CHAMBER - NO_x-AIR												
JN1782R	0.42	0.0	0.0	-0.061	-0.046	0.015	0.004	0.016	0.011			
JN1782B	0.42	0.0	0.0	-0.044	-0.042	0.003	0.003	0.012	0.009			
JN2782B	0.44	0.0	0.0	-0.113	-0.085	0.028	0.050	0.048	-0.002			
AU0282R	0.39	0.0	0.0	0.035	0.048	0.013	-0.129	-0.093	0.036			
AU2082R	0.41	0.0	0.0	-0.011	0.000	0.012	-0.049	-0.037	0.012			
AU2282R	0.46	0.0	0.0	0.000	0.032	0.032	-0.147	-0.093	0.055			
AU2382R	0.43	0.0	0.0	0.056	0.064	0.008	-0.144	-0.102	0.042			
OC0882R	0.30	0.0	0.0	-0.024	-0.035	-0.011	0.005	0.032	0.026			
OC0882B	0.30	0.0	0.0	-0.017	-0.034	-0.017	0.009	0.032	0.023			
ST0582R	0.50	0.0	0.0	0.070	0.079	0.009	-0.171	-0.133	0.038			
JL2483R	0.31	0.0	0.0	-0.047	-0.033	0.015	0.011	0.007	-0.005			
JL2483B	0.48	0.0	0.0	-0.071	-0.047	0.025	0.014	0.007	-0.007			
JL2783B	0.43	0.0	0.0	-0.090	-0.057	0.033	0.036	0.021	-0.015			
AU0683B	0.37	0.0	0.0	0.001	0.015	0.015	-0.090	-0.048	0.041			
Group Average	0.40	0.0	0.0	-0.023	-0.010	0.013	-0.043	-0.024	0.019			
S. Dev.	0.06	0.0	0.0	0.053	0.050	0.015	0.077	0.060	0.022			
Avg. Abs. Value				0.046	0.044	0.017	0.062	0.049	0.023			
S. Dev.				0.034	0.023	0.009	0.062	0.040	0.017			

Table A-2 (continued) - 3

Experiment	Initial Concentrations			Final - Init NO			Final - Init NO_2-UNC			Final - Init PROPENE		
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)
5. SAPRC ITC - NO_x-CO-AIR												
ITC625	0.28	0.0	0.1	-0.069	-0.085	-0.015	0.068	0.078	0.010	-0.004	-0.002	0.001
ITC634	0.60	0.0	0.1	-0.040	-0.059	-0.020	0.034	0.051	0.016	-0.004	-0.001	0.002
Group Average	0.44	0.0	0.1	-0.055	-0.072	-0.018	0.051	0.064	0.013	-0.004	-0.002	0.002
S. Dev.	0.22	0.0	0.0	0.021	0.018	0.003	0.024	0.019	0.005	0.000	0.001	0.001
Avg. Abs. Value				0.055	0.072	0.018	0.051	0.064	0.013	0.004	0.002	0.002
S. Dev.				0.021	0.018	0.003	0.024	0.019	0.005	0.000	0.001	0.001
6. SAPRC OTC - NO_x-CO-AIR												
OTC188	0.34	0.0	0.1	-0.090	-0.132	-0.042	0.072	0.121	0.049	-0.003	0.000	0.003
OTC201A	0.37	0.0	0.1	-0.160	-0.152	0.008	0.162	0.139	-0.023	-0.004	0.000	0.004
OTC201B	0.76	0.0	0.1	-0.123	-0.111	0.012	0.096	0.097	0.001	-0.004	0.000	0.004
Group Average	0.49	0.0	0.1	-0.124	-0.132	-0.007	0.110	0.119	0.009	-0.004	0.000	0.003
S. Dev.	0.23	0.0	0.0	0.035	0.021	0.030	0.046	0.021	0.037	0.001	0.000	0.000
Avg. Abs. Value				0.124	0.132	0.021	0.110	0.119	0.024	0.004	0.000	0.003
S. Dev.				0.035	0.021	0.019	0.046	0.021	0.024	0.001	0.000	0.000

Table A-2 (continued) - 4

Experiment	Initial Concentrations			Final - Init NO			Final - Init NO_2-UNC			Final - Init PROPENE		
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)
7. UNC CHAMBER - NO_x-CO-AIR												
JN2782R	0.45	0.0	0.0	-0.320	-0.288	0.032	0.202	0.245	0.043			
AU0282B	0.40	0.0	0.0	-0.054	-0.045	0.009	-0.002	-0.007	-0.005			
AU2082B	0.41	0.0	0.0	-0.111	-0.107	0.004	0.072	0.068	-0.004			
AU2282B	0.46	0.0	0.0	-0.086	-0.084	0.001	0.003	0.019	0.016			
AU2382B	0.43	0.0	0.0	-0.004	-0.029	-0.025	-0.042	-0.012	0.029			
ST0582B	0.50	0.0	0.0	0.019	-0.015	-0.034	-0.086	-0.041	0.045			
JL2783R	0.47	0.0	0.0	-0.289			0.214					
AU0683R	0.39	0.0	0.0	-0.133			0.032					
Group Average	0.44	0.0	0.0	-0.122	-0.095	-0.002	0.049	0.045	0.021			
S. Dev.	0.04	0.0	0.0	0.124	0.101	0.024	0.109	0.104	0.022			
Avg. Abs. Value				0.127	0.095	0.018	0.082	0.065	0.024			
S. Dev.				0.118	0.101	0.015	0.083	0.091	0.018			

Table A-3. Formaldehyde-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Half-Life HCHO			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. SAPRC EC - FORMALDEHYDE-AIR											
EC250	0.02	0.3	14.5	0.215	0.261	0.046	0.22	130	145	15	0.12
EC255	0.02	0.3	20.4	0.203	0.257	0.055	0.27	126	142	16	0.13
Group Average	0.02	0.3	17.4	0.209	0.259	0.050	0.24	128	143	15	0.12
S. Dev.	0.00	0.0	4.2	0.009	0.003	0.006	0.04	2	2	0	0.01
Avg. Abs. Value						0.050	0.24			15	0.12
S. Dev.						0.006	0.04			0	0.01
2. UNC CHAMBER - FORMALDEHYDE-AIR											
JL1782R	0.01	0.5	71.2	0.239	0.368	0.129	0.54	255	172	-83	-0.33
JL1782B	0.01	0.6	86.0	0.264	0.359	0.094	0.36	246	206	-40	-0.16
OC0784R	0.00	0.4	96.1	0.087	0.266	0.179	2.07	415	187	-228	-0.55
OC0784B	0.01	1.0	125.7	0.138	0.341	0.202	1.46	445	261	-184	-0.41
OC1684R	0.00	0.4		0.153	0.291	0.138	0.90	263	193	-70	-0.27
OC1684B	0.00	0.3		0.133	0.238	0.105	0.79	268	173	-95	-0.35
Group Average	0.00	0.5	94.8	0.169	0.310	0.141	1.02	315	198	-116	-0.35
S. Dev.	0.00	0.3	23.0	0.068	0.053	0.042	0.64	89	33	72	0.13
Avg. Abs. Value						0.141	1.02			116	0.35
S. Dev.						0.042	0.64			72	0.13

Table A-4. Acetaldehyde-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Maximum Concentration PAN			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - ACETALDEHYDE-AIR											
EC253	0.02	1.1	53.8	0.137	0.150	0.013	0.09	0.040	0.041	0.002	0.04
Group Average	0.02	1.1	53.8	0.137	0.150	0.013	0.09	0.040	0.041	0.002	0.04
S. Dev.											
Avg. Abs. Value						0.013	0.09			0.002	0.04
S. Dev.											
2. SAPRC ITC - ACETALDEHYDE-AIR											
ITC627	0.03	0.8	26.1	0.060	0.080	0.020	0.33	0.013	0.013	0.000	-0.02
ITC636	0.03	0.7	26.6	0.047	0.081	0.034		0.011	0.013	0.002	0.16
ITC825	0.00	0.0			0.031				0.007		
ITC957	0.04	1.1	27.6	0.076	0.085	0.009	0.12	0.013	0.015	0.002	0.16
ITC974	0.03	0.9	29.8	0.085	0.080	-0.005	-0.06	6.300	0.014	-6.286	-1.00
ITC1009	0.04	0.9	27.0	0.078	0.083	0.006	0.07	0.008	0.014	0.005	0.64
Group Average	0.03	0.7	27.4	0.069	0.073	0.013	0.11	1.269	0.013	-1.255	-0.01
S. Dev.	0.01	0.4	1.4	0.015	0.021	0.015	0.16	2.812	0.003	2.812	0.60
Avg. Abs. Value						0.015	0.15			1.259	0.40
S. Dev.						0.012	0.12			2.810	0.41

Table A-4 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Maximum Concentration PAN			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
3. SAPRC OTC - ACETALDEHYDE-AIR											
OTC200A	0.01	1.1	96.9	0.088	0.096	0.007	0.08	0.008	0.007	-0.001	-0.17
OTC200B	0.01	0.8	68.8	0.076	0.094	0.019	0.25	0.006	0.007	0.001	0.13
OTC206A	0.01	1.3	136.8	0.030	0.074	0.044		0.020	0.011	-0.009	-0.46
OTC206B	0.01	1.0	94.0	0.023	0.103	0.079		0.013	0.009	-0.004	-0.32
OTC234A	0.04	1.0	26.2	0.083	0.160	0.077	0.93	0.004	0.011	0.007	1.63
OTC234B	0.04	1.5	39.3	0.084	0.160	0.076	0.90	0.007	-0.011	0.004	0.58
Group Average	0.02	1.1	77.0	0.064	0.114	0.050	0.54	0.010	0.009	-0.001	0.23
S. Dev.	0.01	0.2	40.8	0.029	0.037	0.032	0.44	0.006	0.002	0.006	0.78
Avg. Abs. Value						0.050	0.54			0.004	0.55
S. Dev.						0.032	0.44			0.003	0.56
4. UNC CHAMBER - ACETALDEHYDE-AIR											
JL2683R	0.02	1.1	48.3	0.422	0.502	0.080	0.19	0.026	0.050	0.024	0.93
JL2683B	0.01	1.1	87.6	0.331	0.370	0.039	0.12	0.027	0.058	0.030	1.11
AU0483R	0.03	1.0	34.3	0.548	0.554	0.007	0.01	0.040	0.047	0.007	0.17
AU0483B	0.02	1.1	47.1	0.431	0.479	0.048	0.11	0.040	0.057	0.017	0.43
OC1584R	0.02	0.0	1.1	0.140	0.268	0.127	0.91	0.023	0.068	0.045	1.92
OC1584B	0.02	0.0	1.1	0.193	0.318	0.125	0.65	0.035	0.066	0.031	0.90
Group Average	0.02	0.7	36.6	0.344	0.415	0.071	0.33	0.032	0.058	0.026	0.91
S. Dev.	0.01	0.5	32.8	0.155	0.113	0.049	0.36	0.007	0.008	0.013	0.60
Avg. Abs. Value						0.071	0.33			0.026	0.91
S. Dev.						0.049	0.36			0.013	0.60

Table A-5. Formaldehyde-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt				Half-Life HCHO			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. SAPRC EC - FORMALDEHYDE - NO_x-AIR															
EC251	0.11	0.2	1.7	0.271	0.303	0.032	0.12	3.25	4.45	1.20	0.37	112	74	-38	-0.34
EC252	0.49	0.4	0.7	0.032	0.025	-0.007		1.94	2.41	0.47	0.24	99	137	38	0.38
EC389	4.75	9.1	1.9	0.002	0.029	0.026		50.01	58.34	8.33	0.17	190	101	-89	-0.47
EC391	4.43	17.7	4.0	2.371	2.371	0.000	0.00	102.89	116.11	13.23	0.13	75	76	1	0.01
EC392	8.05	9.5	1.2	0.000	0.008	0.008		13.52	33.67	20.15	1.49	129	123	-6	-0.05
Group Average	3.57	7.4	1.9	0.535	0.547	0.012	0.06	34.32	43.00	8.68	0.48	121	102	-18	-0.09
S. Dev.	3.30	7.3	1.3	1.032	1.027	0.017	0.08	42.99	46.91	8.30	0.57	43	27	47	0.33
Avg. Abs. Value						0.014	0.06			8.68	0.48			34	0.25
S. Dev.						0.014	0.08			8.30	0.57			35	0.21
2. SAPRC ITC - FORMALDEHYDE - NO_x-AIR															
ITC864	0.54	0.1	0.1	0.001	0.016	0.015		0.60	0.71	0.12	0.19				
Group Average	0.54	0.1	0.1					0.60	0.71	0.12	0.19				
S. Dev.															
Avg. Abs. Value										0.12	0.19				
S. Dev.															

Table A-5 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt				Half-Life HCHO			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
3. SAPRC OTC - FORMALDEHYDE - NO_x-AIR															
OTC235A	0.56	0.1	0.1	0.273	0.149	-0.124	-0.46	2.00	1.80	-0.20	-0.10				
OTC235B	0.58	0.1	0.1	0.308	0.235	-0.073	-0.24	2.16	2.10	-0.06	-0.03				
Group Average	0.57	0.1	0.1	0.291	0.192	-0.099	-0.35	2.08	1.95	-0.13	-0.06				
S. Dev.	0.02	0.0	0.0	0.025	0.061	0.036	0.15	0.11	0.21	0.10	0.05				
Avg. Abs. Value						0.099	0.35			0.13	0.06				
S. Dev.						0.036	0.15			0.10	0.05				
4. UNC CHAMBER - FORMALDEHYDE - NO_x-AIR															
AU0179B	0.35	1.0	2.8	0.618	0.508	-0.110	-0.18	2.06	2.58	0.52	0.26	245	173	-72	-0.29
AU0279B	0.21	1.0	4.7	0.606	0.582	-0.024	-0.04	2.12	3.07	0.94	0.44	233	147	-86	-0.37
AU0479B	0.23	0.5	2.1	0.378	0.284	-0.094	-0.25	1.17	1.31	0.14	0.12	280	180	-100	-0.36
AU0579B	0.54	1.2	2.2	0.508	0.499	-0.009	-0.02	1.95	2.73	0.78	0.40	283	190	-93	-0.33
JL2381B	0.43	1.5	3.5	0.637	0.745	0.108	0.17	2.70	3.73	1.03	0.38	205	174	-31	-0.15
OC0984R	0.56	1.0	1.7	0.666	1.096	0.430	0.65	2.11	2.93	0.82	0.39	328	218	-110	-0.34
OC0984B	0.50	1.0	1.9	0.301	0.345	0.045	0.15	1.51	1.93	0.42	0.28	330	206	-124	-0.38
Group Average	0.40	1.0	2.7	0.531	0.580	0.049	0.07	1.94	2.61	0.66	0.32	272	184	-88	-0.32
S. Dev.	0.14	0.3	1.1	0.141	0.273	0.184	0.30	0.49	0.79	0.32	0.11	47	23	30	0.08
Avg. Abs. Value						0.117	0.21			0.66	0.32			88	0.32
S. Dev.						0.144	0.21			0.32	0.11			30	0.08

Table A-6. Aldehyde or Ketone-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - ACETALDEHYDE											
EC164	0.51	0.7	1.4	0.086	0.068	-0.017	-0.20	2.03	1.82	-0.20	-0.10
EC254	0.11	1.0	8.5	0.264	0.276	0.012	0.05	1.33	1.47	0.14	0.11
Group Average	0.31	0.8	5.0	0.175	0.172	-0.003	-0.08	1.68	1.65	-0.03	0.00
S. Dev.	0.28	0.2	5.0	0.126	0.147	0.021	0.18	0.49	0.25	0.24	0.15
Avg. Abs. Value						0.015	0.12			0.17	0.10
S. Dev.						0.004	0.11			0.05	0.00
2. UNC CHAMBER - ACETALDEHYDE											
AU0179R	0.36	2.0	5.7	0.930	0.868	-0.062	-0.07	1.98	1.87	-0.11	-0.06
JN1482R	0.31	3.1	9.9	0.731	0.518	-0.212	-0.29	1.62	1.59	-0.03	-0.02
AU2482B	0.32	1.9	6.0	0.972	0.768	-0.204	-0.21	1.68	1.54	-0.14	-0.08
Group Average	0.33	2.3	7.2	0.878	0.718	-0.159	-0.19	1.76	1.67	-0.09	-0.05
S. Dev.	0.02	0.7	2.3	0.129	0.180	0.084	0.11	0.19	0.17	0.06	0.03
Avg. Abs. Value						0.159	0.19			0.09	0.05
S. Dev.						0.084	0.11			0.06	0.03

Table A-6 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
3. UNC CHAMBER - PROPANALDEHYDE											
JN1482B	0.30	3.1	10.5	0.733	0.519	-0.215	-0.29	1.75	1.97	0.22	0.13
AU2482R	0.33	1.9	5.6	0.941	0.806	-0.135	-0.14	1.82	1.76	-0.06	-0.03
Group Average	0.32	2.5	8.0	0.837	0.662	-0.175	-0.22	1.79	1.87	0.08	0.05
S. Dev.	0.02	0.9	3.4	0.147	0.203	0.057	0.11	0.05	0.15	0.20	0.11
Avg. Abs. Value						0.175	0.22			0.14	0.08
S. Dev.						0.057	0.11			0.11	0.07
4. UNC CHAMBER - ACETONE											
JN0480R	0.17	4.8	27.5	0.233	0.554	0.321	1.38	0.48	0.67	0.19	0.40
Group Average	0.17	4.8	27.5	0.233	0.554	0.321	1.38	0.48	0.67	0.19	0.40
S. Dev.											
Avg. Abs. Value						0.321	1.38			0.19	0.40
S. Dev.											
5. UNC CHAMBER - METHYL ETHYL KETONE											
OC2079R	0.22	13.6	60.5	0.563	0.539	-0.023	-0.04	1.25	1.27	0.01	0.01
JN0480B	0.18	3.8	21.6	0.652	0.723	0.070	0.11	1.13	1.20	0.07	0.06
Group Average	0.20	8.7	41.0	0.607	0.631	0.024	0.03	1.19	1.23	0.04	0.04
S. Dev.	0.03	6.9	27.5	0.063	0.130	0.066	0.11	0.09	0.05	0.04	0.04
Avg. Abs. Value						0.047	0.07			0.04	0.04
S. Dev.						0.033	0.05			0.04	0.04

Table A-6 (continued) -3

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min) --	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - ACETALDEHYDE											
EC164	116	309	193	1.66	0.026	0.014	-0.012	-0.47	0.050	0.084	0.034	0.67
EC254	297	331	34	0.11	0.071	0.082	0.010	0.15	0.037	0.078	0.041	1.10
Group Average	206	320	113	0.89	0.049	0.048	-0.001	-0.16	0.044	0.081	0.037	0.88
S. Dev.	127	15	112	1.10	0.032	0.048	0.016	0.44	0.009	0.004	0.005	0.31
Avg. Abs. Value			113	0.89			0.011	0.31			0.037	0.88
S. Dev.			112	1.10			0.001	0.23			0.005	0.31
2. UNC CHAMBER - ACETALDEHYDE											
AU0179R	352	381	29	0.08	0.210	0.168	-0.042	-0.20	0.410	0.184	-0.226	-0.55
JN1482R	426				0.226	0.275	0.049	0.22	0.150	0.142	-0.008	-0.05
AU2482B	412	455	43	0.10	0.174	0.189	0.015	0.09	0.190	0.132	-0.058	-0.31
Group Average	396	418	36	0.09	0.203	0.211	0.007	0.03	0.250	0.153	-0.097	-0.30
S. Dev.	39	52	9	0.02	0.027	0.057	0.046	0.21	0.140	0.027	0.114	0.25
Avg. Abs. Value			36	0.09			0.036	0.17			0.097	0.30
S. Dev.			9	0.02			0.018	0.07			0.114	0.25

Table A-6 (continued) - 4

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min) --	Calc -Expt --	Calc -Expt /Expt
1 UNC CHAMBER -											
JN1482B	405	342	-63	-0.16	0.027	0.066	0.040	1.48	0.034	0.223	0.189	5.53
AU2482R	374	352	-22	-0.06	0.077	0.083	0.006	0.07		0.140		
Group Average	389	347	-42	-0.11	0.052	0.075	0.023	0.77	0.034	0.182	0.189	5.53
S. Dev.	21	7	28	0.07	0.036	0.012	0.024	0.99				
Avg. Abs. Value			42	0.11			0.023	0.77			0.189	5.53
S. Dev.			28	0.07			0.024	0.99				
1. UNC CHAMBER - ACETONE											
JN0480R					0.008	0.046	0.038	4.96		0.026		
Group Average					0.008	0.046	0.038	4.96				
S. Dev.												
Avg. Abs. Value							0.038	4.96				
S. Dev.												
1. UNC CHAMBER - METHYL ETHYL KETONE											
OC2079R						0.110			0.155	0.116	-0.039	-0.25
JN0480B					0.070	0.088	0.018	0.26	0.070	0.054	-0.016	-0.23
Group Average					0.070	0.099	0.018	0.26	0.113	0.085	-0.028	-0.24
S. Dev.									0.060	0.044	0.016	0.01
Avg. Abs. Value							0.018	0.26			0.028	0.24
S. Dev.											0.016	0.01

Table A-7. N-Butane-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - BUTANE											
EC130	0.10	17.6	179.3	0.459	0.527	0.068	0.15	4.41	2.76	-1.65	-0.37
EC133	0.50	8.6	17.1	0.249	0.074	-0.175	-0.70	2.42	1.28	-1.14	-0.47
EC134	0.51	8.3	16.3	0.034	0.058	0.024		0.94	1.51	0.58	0.61
EC137	0.50	8.7	17.3	0.042	0.070	0.028		1.02	1.52	0.50	0.50
EC162	0.51	8.2	16.3	0.112	0.079	-0.034	-0.30	1.73	1.46	-0.27	-0.15
EC163	0.49	9.0	18.3	0.454	0.251	-0.203	-0.45	3.31	2.31	-1.00	-0.30
EC168	0.49	8.0	16.2	0.655	0.443	-0.212	-0.32	2.03	1.48	-0.55	-0.27
EC178	0.10	7.8	79.6	0.384	0.471	0.087	0.23	1.61	1.77	0.17	0.10
EC304	0.47	17.1	36.7	0.362	0.640	0.279	0.77	2.09	2.75	0.66	0.32
EC305	0.10	15.7	159.7	0.398	0.632	0.234	0.59	2.39	3.58	1.19	0.50
EC306	0.19	25.8	138.2	0.535	0.795	0.260	0.49	2.38	4.09	1.72	0.72
EC307	0.10	25.8	252.9	0.420	0.685	0.265	0.63	2.61	5.77	3.16	1.21
EC308	0.48	16.2	33.6	0.047	0.267	0.220		1.04	3.14	2.10	2.03
EC309	0.47	17.2	36.3	0.545	0.715	0.170	0.31	2.00	2.79	0.79	0.40
Group Average	0.36	13.9	72.7	0.335	0.408	0.072	0.13	2.14	2.59	0.45	0.34
S. Dev.	0.19	6.4	77.7	0.205	0.270	0.177	0.50	0.94	1.27	1.33	0.69
Avg. Abs. Value						0.161	0.45			1.11	0.57
S. Dev.						0.094	0.20			0.82	0.50

Table A-7 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
2. SAPRC ITC - BUTANE											
ITC507	0.09	15.2	165.0	0.149	0.406	0.257	1.73	0.69	1.39	0.70	1.02
ITC533	0.12	11.9	99.8	0.165	0.395	0.230	1.40	0.61	1.39	0.78	1.28
ITC770	0.52	37.9	72.8	0.042	0.049	0.007		1.56	1.89	0.33	0.21
ITC939	0.51	14.8	28.9	0.017	0.030	0.013		0.36	0.73	0.37	1.02
ITC948	0.26	10.0	38.2	0.054	0.179	0.125	2.32	0.53	1.15	0.62	1.16
Group Average	0.30	18.0	81.0	0.085	0.212	0.126	1.82	0.75	1.31	0.56	0.94
S. Dev.	0.21	11.4	54.8	0.067	0.182	0.118	0.47	0.47	0.42	0.20	0.42
Avg. Abs. Value						0.126	1.82			0.56	0.94
S. Dev.						0.118	0.47			0.20	0.42
3. SAPRC OTC - BUTANE											
OTC211	0.55	42.8	77.5	0.008	0.168	0.160		0.56	1.31	0.74	1.32
Group Average	0.55	42.8	77.5					0.56	1.31	0.74	1.32
S. Dev.											
Avg. Abs. Value										0.74	1.32
S. Dev.											

Table A-7 (continued) - 3

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
4. UNC CHAMBER - BUTANE											
JL2178R	0.24	7.2	29.9	0.763	0.554	-0.209	-0.27	1.17	1.04	-0.13	-0.11
JL2178B	0.24	15.4	63.9	0.986	0.948	-0.038	-0.04	1.64	1.52	-0.11	-0.07
JL2278R	0.55	7.9	14.4	0.166	0.060	-0.107	-0.64	0.90	0.72	-0.18	-0.20
JL2278B	0.55	17.5	31.5	0.788	0.274	-0.514	-0.65	1.55	1.14	-0.41	-0.26
ST1879B	0.21	21.2	103.1	0.185	0.351	0.165	0.89	0.51	0.71	0.20	0.38
OC0979R	0.21	14.6	71.0	0.191	0.459	0.268	1.40	0.60	0.90	0.30	0.51
OC1879B	0.20	14.3	71.8	0.208	0.534	0.326	1.57	0.60	0.92	0.31	0.52
Group Average	0.31	14.0	55.1	0.470	0.454	-0.015	0.32	1.00	0.99	0.00	0.11
S. Dev.	0.16	5.0	31.0	0.359	0.277	0.296	0.95	0.47	0.28	0.28	0.35
Avg. Abs. Value						0.232	0.78			0.23	0.29
S. Dev.						0.157	0.56			0.11	0.18

Table A-7 (continued) - 4

Experiment	Maximum Concentration PAN				Maximum Concentration ACETALD				Maximum Concentration MEK			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - BUTANE												
EC130	0.044	0.049	0.005	0.12	0.130	0.175	0.045	0.34	0.165	0.219	0.054	0.33
EC133	0.031	0.005	-0.026	-0.85	0.096	0.077	-0.019	-0.20	0.122	0.084	-0.038	-0.31
EC134	0.004	0.003	-0.001	-0.13	0.049	0.073	0.024	0.49	0.064	0.079	0.015	0.23
EC137	0.005	0.004	-0.001	-0.18	0.062	0.075	0.013	0.21	0.072	0.081	0.009	0.13
EC162	0.015	0.005	-0.011	-0.69	0.098	0.076	-0.021	-0.22	0.067	0.084	0.016	0.24
EC163	0.106	0.046	-0.060	-0.57	0.526	0.410	-0.116	-0.22	0.077	0.071	-0.006	-0.08
EC168	0.092	0.042	-0.051	-0.55	0.114	0.104	-0.010	-0.09	0.193	0.147	-0.046	-0.24
EC178	0.045	0.050	0.004	0.10	0.092	0.105	0.014	0.15	0.091	0.148	0.057	0.63
EC304	0.027	0.055	0.027	1.00	0.149	0.185	0.036	0.24	0.092	0.227	0.135	1.47
EC305	0.031	0.050	0.019	0.61	0.131	0.173	0.042	0.32	0.085	0.210	0.125	1.48
EC306	0.035	0.067	0.032	0.90	0.166	0.232	0.065	0.39	0.098	0.277	0.179	1.83
EC307	0.026	0.051	0.024	0.93	0.161	0.222	0.061	0.38	0.139	0.258	0.119	0.86
EC308	0.005	0.028	0.023	4.86	0.037	0.125	0.088	2.40	0.076	0.142	0.065	0.86
EC309	0.034	0.039	0.005	0.14	0.226	0.188	-0.038	-0.17	0.115	0.224	0.109	0.95
Group Average	0.036	0.035	-0.001	0.41	0.145	0.159	0.013	0.29	0.104	0.161	0.057	0.60
S. Dev.	0.030	0.022	0.028	1.42	0.121	0.092	0.052	0.66	0.039	0.074	0.069	0.67
Avg. Abs. Value			0.021	0.83			0.042	0.42			0.070	0.69
S. Dev.			0.018	1.21			0.031	0.58			0.055	0.57

Table A-7 (continued) - 5

Experiment	Maximum Concentration PAN				Maximum Concentration ACETALD				Maximum Concentration MEK			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
2. SAPRC ITC - BUTANE												
ITC507	0.004	0.010	0.006	1.56	0.029	0.097	0.068	2.35	0.075	0.101	0.026	0.35
ITC533	0.004	0.014	0.009	2.16	0.033	0.094	0.061	1.85	0.036	0.102	0.065	1.79
ITC770	0.000	0.001	0.001		0.056	0.086	0.030	0.54	0.047	0.081	0.034	0.72
ITC939		0.001			0.014	0.061	0.047	3.35	0.019	0.059	0.041	2.14
ITC948		0.004			0.015	0.078	0.063	4.25	0.021	0.078	0.057	2.75
Group Average	0.003	0.006	0.005	1.86	0.029	0.083	0.054	2.47	0.040	0.084	0.045	1.55
S. Dev.	0.002	0.006	0.004	0.43	0.017	0.015	0.016	1.42	0.023	0.018	0.016	1.00
Avg. Abs. Value			0.005	1.86			0.054	2.47			0.045	1.55
S. Dev.			0.004	0.43			0.016	1.42			0.016	1.00
3. SAPRC OTC - BUTANE												
OTC211	0.013	0.004	-0.009	-0.68	0.100	0.136	0.036	0.36		0.132		
Group Average	0.013	0.004	-0.009	-0.68	0.100	0.136	0.036	0.36				
S. Dev.												
Avg. Abs. Value			0.009	0.68			0.036	0.36				
S. Dev.												

Table A-7 (continued) - 6

Experiment	Maximum Concentration PAN				Maximum Concentration ACETALD				Maximum Concentration MEK			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
4. UNC CHAMBER - BUTANE												
JL2178R						0.001				0.001		
JL2178B						0.002				0.002		
JL2278R						0.001				0.001		
JL2278B						0.001				0.001		
ST1879B	0.010	0.017	0.008	0.80								
OC0979R	1.100	0.020	-1.080	-0.98					0.000	0.120	0.120	
OC1879B	4.590	0.030	-4.560	-0.99					0.052	0.127	0.074	1.42
Group Average	1.900	0.022	-1.878	-0.39					0.026	0.042	0.097	1.42
S. Dev.	2.393	0.007	2.386	1.03								
Avg. Abs. Value			1.883	0.92							0.097	1.42
S. Dev.			2.380	0.11								

Table A-8. Branched Alkane-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d([O3] - [NO])/dt			
	NOx (ppm)	HC (ppmC)	HC/NOx	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - 2,3 DIMETHYL BUTANE											
EC165	0.10	11.3	114.3	0.488	0.676	0.188	0.38	1.77	2.57	0.80	0.45
EC169	0.19	4.5	23.5	0.493	0.537	0.043	0.09	1.00	1.22	0.22	0.22
EC171	0.10	3.5	35.7	0.403	0.469	0.066	0.16	1.30	1.33	0.03	0.02
Group Average	0.13	6.4	57.8	0.462	0.561	0.099	0.21	1.36	1.71	0.35	0.23
S. Dev.	0.05	4.2	49.3	0.051	0.106	0.078	0.15	0.39	0.75	0.40	0.22
Avg. Abs. Value						0.099	0.21			0.35	0.23
S. Dev.						0.078	0.15			0.40	0.22
2. UNC CHAMBER - 2,3 DIMETHYL BUTANE											
OC1879R	0.20	16.4	81.9	0.236	0.676	0.440	1.86	0.64	1.01	0.38	0.59
OC2079B	0.22	12.6	56.5	0.217	0.495	0.278	1.28	0.66	0.97	0.31	0.47
Group Average	0.21	14.5	69.2	0.226	0.585	0.359	1.57	0.65	0.99	0.34	0.53
S. Dev.	0.02	2.7	18.0	0.014	0.128	0.114	0.41	0.02	0.03	0.05	0.08
Avg. Abs. Value						0.359	1.57			0.34	0.53
S. Dev.						0.114	0.41			0.05	0.08
3. UNC CHAMBER - ISO-PENTANE											
AU1983R	0.38	4.7	12.6	0.088	0.098	0.011	0.12	0.61	0.66	0.05	0.09
4. UNC CHAMBER - ISO-OCTANE											
AU1983B	0.37	4.1	10.9	0.057	0.056	-0.001	-0.02	0.53	0.54	0.02	0.03

Table A-8 (continued) - 2

Experiment	Maximum Concentration PAN				Maximum Concentration ACETONE				Maximum Concentration ACETALD			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - 2,3 DIMETHYL BUTANE												
EC165	0.017	0.008	-0.008	-0.50	0.471					0.000		
EC169	0.024	0.011	-0.012	-0.52	0.343				0.018	0.007	-0.012	-0.63
EC171	0.020	0.009	-0.011	-0.56	0.362				0.029	0.006	-0.023	-0.79
Group Average	0.020	0.010	-0.011	-0.53					0.024	0.004	-0.017	-0.71
S. Dev.	0.003	0.002	0.002	0.03					0.008	0.004	0.008	0.11
Avg. Abs. Value			0.011	0.53							0.017	0.71
S. Dev.			0.002	0.03							0.008	0.11
2. UNC CHAMBER - 2,3 DIMETHYL BUTANE												
OC1879R	1.260	0.003	-1.257	-1.00	0.253					0.001		
OC2079B		0.002			0.349					0.001		
3. UNC CHAMBER - ISO-PENTANE												
AU1983R	0.035	0.001	-0.034	-0.98	0.113				0.064	0.051	-0.013	-0.20
4. UNC CHAMBER - ISO-OCTANE												
AU1983B	0.002	0.000	-0.002	-0.91	0.078				0.000	0.012	0.012	

Table A-9. N-Pentane and Higher N-Alkane-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d([O3] - [NO])/dt			
	NOx (ppm)	HC (ppmC)	HC/NOx	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - PENTANE											
EC135	0.10	20.4	212.7	0.435	0.607	0.172	0.39	2.92	2.97	0.05	0.02
2. UNC CHAMBER - PENTANE											
OC0979B	0.21	15.1	73.3	0.184	0.463	0.280	1.52	0.59	0.87	0.28	0.47
3. SAPRC EC - HEXANE											
EC131	0.10	24.6	251.1	0.393	0.596	0.203	0.52	1.92	2.21	0.29	0.15
4. SAPRC ITC - HEXANE											
ITC559	0.19	279.4	1441.1	0.377	0.486	0.109	0.29	1.79	1.43	-0.36	-0.20
5. SAPRC ITC - HEPTANE											
ITC538	0.11	60.3	529.0	0.150	0.250	0.099	0.66	0.74	0.90	0.16	0.22
ITC540	0.11	274.8	2421.3	0.360	0.313	-0.047	-0.13	1.85	0.96	-0.89	-0.48
Group Average	0.11	167.6	1475.2	0.255	0.281	0.026	0.27	1.30	0.93	-0.36	-0.13
S. Dev.	0.00	151.7	1338.1	0.148	0.045	0.104	0.56	0.79	0.04	0.75	0.50
Avg. Abs. Value						0.073	0.40			0.53	0.35
S. Dev.						0.037	0.37			0.52	0.18

Table A-9 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d([O3] - [NO])/dt			
	NOx (ppm)	HC (ppmC)	HC/NOx	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
6. SAPRC ITC - OCTANE											
ITC552	0.13	428.8	3278.4	0.315	0.193	-0.122	-0.39	1.19	0.72	-0.47	-0.40
ITC761	0.52	75.2	145.9	0.030	0.015	-0.015		1.08	0.79	-0.29	-0.27
ITC762	0.27	74.7	280.4	0.105	0.068	-0.037	-0.35	0.83	0.96	0.13	0.16
ITC763	0.28	7.7	27.7	0.041	0.034	-0.007		0.68	0.96	0.28	0.41
ITC797	0.52	7.3	14.0	0.004	0.008	0.003		0.64	0.67	0.03	0.05
Group Average	0.34	118.7	749.3	0.099	0.064	-0.036	-0.37	0.88	0.82	-0.06	-0.01
S. Dev.	0.17	176.6	1417.9	0.126	0.076	0.051	0.02	0.24	0.13	0.31	0.32
Avg. Abs. Value						0.037	0.37			0.24	0.26
S. Dev.						0.050	0.02			0.17	0.15
7. UNC CHAMBER - OCTANE											
ST1879R	0.21	6.3	30.4	0.122	0.654	0.532	4.36	0.40	0.70	0.30	0.75
8. SAPRC EC - NONANE											
EC155	0.10	37.3	385.1	0.264	0.396	0.132	0.50	1.33	0.95	-0.38	-0.29

Table A-10. Ethene-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d([O3] - [NO])/dt				Half-Life ETHENE			
	NOx (ppm)	HC (ppmC)	HC/NOx	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. SAPRC EC - ETHENE															
EC142	0.48	1.9	4.1	0.782	0.541	-0.240	-0.31	3.20	2.48	-0.72	-0.23	222	298	76	0.34
EC143	0.50	4.1	8.1	1.087	0.854	-0.233	-0.21	8.50	5.53	-2.98	-0.35	155	229	74	0.48
EC156	0.50	4.0	8.0	1.105	0.816	-0.289	-0.26	8.89	5.49	-3.40	-0.38	153	229	76	0.50
EC285	1.01	3.9	3.9	0.840	1.048	0.208	0.25	5.05	6.00	0.96	0.19	265	254	-11	-0.04
EC286	0.94	7.5	8.0	1.081	1.290	0.209	0.19	11.76	14.24	2.47	0.21	174	162	-12	-0.07
EC287	0.53	8.0	15.1	0.965	1.098	0.133	0.14	13.89	17.27	3.38	0.24	171	149	-22	-0.13
Group Average	0.66	4.9	7.9	0.977	0.941	-0.036	-0.03	8.55	8.50	-0.05	-0.05	190	220	30	0.18
S. Dev.	0.25	2.4	4.1	0.139	0.261	0.242	0.25	3.99	5.83	2.81	0.30	44	56	49	0.29
Avg. Abs. Value						0.219	0.23			2.32	0.27			45	0.26
S. Dev.						0.051	0.06			1.20	0.08			33	0.21
2. SAPRC ITC - ETHENE															
ITC926	0.51	7.9	15.6	0.982	0.995	0.013	0.01	6.96	8.31	1.35	0.19	227	220	-7	-0.03
ITC936	0.50	3.9	7.8	0.940	0.962	0.022	0.02	2.72	3.22	0.50	0.18	337	323	-14	-0.04
Group Average	0.50	5.9	11.7	0.961	0.978	0.017	0.02	4.84	5.77	0.93	0.19	282	271	-10	-0.04
S. Dev.	0.01	2.8	5.5	0.030	0.023	0.007	0.01	3.00	3.60	0.60	0.01	77	72	4	0.01
Avg. Abs. Value						0.017	0.02			0.93	0.19			10	0.04
S. Dev.						0.007	0.01			0.60	0.01			4	0.01

Table A-10 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d([O3] - [NO])/dt				Half-Life ETHENE			
	NOx (ppm)	HC (ppmC)	HC/NOx	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
3. UNC CHAMBER - ETHENE															
AU0479R	0.23	0.9	3.9	0.729	0.592	-0.137	-0.19	1.60	1.20	-0.39	-0.25	307	377	70	0.23
AU0579R	0.64	4.1	6.4	1.294	1.189	-0.105	-0.08	3.17	3.21	0.04	0.01	333	356	23	0.07
OC0584R	0.36	3.2	8.8	0.856	1.053	0.197	0.23	2.16	2.55	0.38	0.18	394	311	-83	-0.21
OC1184R	0.35	2.9	8.2	0.858	1.142	0.284	0.33	2.22	2.59	0.36	0.16	366	295	-71	-0.19
OC1284R	0.72	2.7	3.7	0.495	0.649	0.154	0.31	1.58	1.72	0.13	0.08		467		
OC0584B	0.37	1.8	5.0	0.675	0.830	0.155	0.23	1.48	1.68	0.20	0.14	465	375	-90	-0.19
Group Average	0.45	2.6	6.0	0.818	0.909	0.091	0.14	2.04	2.16	0.12	0.05	373	363	-30	-0.06
S. Dev.	0.19	1.1	2.2	0.269	0.256	0.172	0.22	0.64	0.74	0.29	0.16	61	60	72	0.20
Avg. Abs. Value						0.172	0.23			0.25	0.14			67	0.18
S. Dev.						0.063	0.09			0.15	0.08			26	0.06

Table A-10 (continued) -3

Experiment	Maximum Concentration HCHO				Experiment	Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt		Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - ETHENE					3. UNC CHAMBER - ETHENE				
EC142	0.207	0.378	0.170	0.82	AU0479R	0.306	0.147	-0.158	-0.52
EC143	0.967	0.852	-0.115	-0.12	AU0579R	1.488	0.718	-0.770	-0.52
EC156	0.735	0.847	0.112	0.15	OC0584R	0.869	0.575	-0.294	-0.34
EC285	0.709	0.731	0.022	0.03	OC1184R	0.707	0.516	-0.191	-0.27
EC286	1.425	1.557	0.132	0.09	OC1284R	0.655	0.456	-0.198	-0.30
EC287	1.426	1.645	0.219	0.15	OC0584B	0.558	0.309	-0.249	-0.45
Group Average	0.912	1.002	0.090	0.19	Group Average	0.764	0.453	-0.310	-0.40
S. Dev.	0.469	0.496	0.120	0.33	S. Dev.	0.401	0.202	0.230	0.11
Avg. Abs. Value			0.128	0.23	Avg. Abs. Value			0.310	0.40
S. Dev.			0.066	0.29	S. Dev.			0.230	0.11
2. SAPRC ITC - ETHENE									
ITC926	1.308	1.632	0.324	0.25					
ITC936	0.697	0.780	0.084	0.12					
Group Average	1.002	1.206	0.204	0.18					
S. Dev.	0.432	0.602	0.170	0.09					
Avg. Abs. Value			0.204	0.18					
S. Dev.			0.170	0.09					

Table A-11. Propene-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt				Half-Life PROPENE			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. SAPRC EC - PROPENE															
EC121	0.51	1.5	2.9	0.506	0.518	0.012	0.02	7.46	4.07	-3.39	-0.45	56	116	60	1.07
EC177	0.46	1.5	3.2	0.540	0.542	0.002	0.00	3.89	3.90	0.01	0.00	95	121	26	0.27
EC216	0.52	1.5	3.0	0.564	0.652	0.088	0.16	4.18	5.55	1.38	0.33	105	94	-11	-0.10
EC217	0.48	0.6	1.2	0.149	0.292	0.143	0.96	0.80	1.55	0.76	0.95	116	120	4	0.03
EC230	0.52	1.9	3.7	0.344	0.316	-0.028	-0.08	3.06	4.66	1.60	0.52	123	128	5	0.04
EC256	0.56	0.4	0.7	0.002	0.010	0.007		0.98	1.06	0.08	0.08	181	166	-15	-0.08
EC257	0.56	0.7	1.3	0.068	0.103	0.035	0.51	3.35	4.29	0.94	0.28	80	80	0	0.00
EC276	0.52	1.6	3.2	0.388	0.483	0.094	0.24	3.24	4.33	1.08	0.33	128	126	-2	-0.02
EC277	0.11	1.7	15.7	0.313	0.398	0.085	0.27	8.27	7.56	-0.72	-0.09	74	69	-5	-0.07
EC278	0.49	3.1	6.2	0.625	0.699	0.074	0.12	7.72	9.03	1.31	0.17	87	85	-2	-0.02
EC279	0.97	3.5	3.5	0.679	0.717	0.038	0.06	6.64	7.99	1.35	0.20	123	121	-2	-0.02
EC314	0.93	3.2	3.5	0.728	0.875	0.147	0.20	7.21	10.08	2.87	0.40	98	91	-7	-0.07
EC315	0.94	2.9	3.1	0.344	0.482	0.137	0.40	4.33	5.54	1.21	0.28	159	140	-19	-0.12
EC316	0.98	3.2	3.3	0.955	1.127	0.172	0.18	10.64	11.81	1.17	0.11	70	78	8	0.11
EC317	0.54	1.5	2.8	0.615	0.663	0.048	0.08	4.06	4.39	0.33	0.08	85	81	-4	-0.05
Group Average	0.61	1.9	3.8	0.455	0.525	0.070	0.22	5.06	5.72	0.67	0.21	105	107	2	0.07
S. Dev.	0.24	1.0	3.5	0.260	0.286	0.061	0.26	2.81	3.02	1.39	0.31	33	27	19	0.30
Avg. Abs. Value						0.074	0.23			1.21	0.29			11	0.14
S. Dev.						0.056	0.25			0.92	0.24			15	0.27

Table A-11 (Continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt				Half-Life PROPENE			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
2. SAPRC ITC - PROPENE															
ITC693	0.49	3.5	7.2	0.779	0.729	-0.050	-0.06	5.07	5.11	0.04	0.01	126	139	13	0.10
ITC810	0.52	2.8	5.4	0.782	0.685	-0.097	-0.12	4.25	4.09	-0.17	-0.04	135	160	25	0.19
ITC860	0.52	3.0	5.8	0.585	0.659	0.075	0.13	3.57	4.50	0.93	0.26	142	145	3	0.02
ITC925	0.54	2.8	5.2	0.779	0.711	-0.068	-0.09	3.72	3.57	-0.15	-0.04	150	166	16	0.11
ITC938	0.52	2.8	5.3	0.729	0.726	-0.003	0.00	3.61	3.69	0.09	0.02	137	160	23	0.17
ITC947	0.53	1.9	3.6	0.710	0.744	0.034	0.05	3.34	3.64	0.31	0.09	157	163	6	0.04
ITC960	0.50	2.8	5.5	0.721	0.678	-0.043	-0.06	4.23	3.82	-0.41	-0.10	133	155	22	0.17
Group Average	0.52	2.8	5.4	0.726	0.705	-0.022	-0.02	3.97	4.06	0.09	0.03	140	155	15	0.11
S. Dev.	0.02	0.5	1.0	0.070	0.031	0.060	0.09	0.59	0.56	0.43	0.12	10	9	8	0.06
Avg. Abs. Value						0.053	0.07			0.30	0.08			15	0.11
S. Dev.						0.030	0.04			0.31	0.09			8	0.06
3. SAPRC OTC - PROPENE															
OTC186	0.55	3.6	6.6	0.822	0.881	0.059	0.07	5.16	6.11	0.95	0.18	104	110	6	0.06
OTC191	0.54	3.7	6.9	0.903	1.148	0.245	0.27	12.18	10.57	-1.60	-0.13	56	72	16	0.29
OTC210	0.57	2.7	4.8	0.972	1.037	0.065	0.07	6.70	5.48	-1.22	-0.18	121	130	9	0.07
OTC233	0.46	0.1	0.2	0.633	0.960	0.327	0.52	3.69	4.75	1.06	0.29	132	130	-2	-0.02
OTC236	0.53	3.3	6.3	0.848	0.978	0.130	0.15	6.91	7.13	0.23	0.03	109	104	-5	-0.05
Group Average	0.53	2.7	5.0	0.836	1.001	0.165	0.22	6.93	6.81	-0.12	0.04	104	109	4	0.07
S. Dev.	0.04	1.5	2.8	0.127	0.099	0.117	0.19	3.21	2.28	1.23	0.20	29	23	8	0.13
Avg. Abs. Value						0.165	0.22			1.01	0.16			7	0.10
S. Dev.						0.117	0.19			0.50	0.09			5	0.11

Table A-11 (continued) - 3

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt				Half-Life PROPENE			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
4. UNC CHAMBER - PROPENE															
JA1078R	0.46	3.1	6.9	0.363	0.377	0.014	0.04	0.46	0.49	0.03	0.06	867			
OC1278B	0.48	1.4	2.9	0.461	0.428	-0.034	-0.07	1.40	1.71	0.31	0.22	303	241	-62	-0.20
OC2078R	0.46	1.3	2.9	0.340	0.317	-0.024	-0.07	1.23	1.44	0.21	0.17	341	263	-78	-0.23
OC2078B	0.46	3.5	7.7	0.727	0.810	0.083	0.11	2.83	3.49	0.66	0.23	233	178	-55	-0.24
OC2178R	0.50	3.9	7.9	0.670	0.788	0.118	0.18	2.53	3.43	0.90	0.36	251	186	-65	-0.26
OC2578B	0.44	1.3	2.9	0.230	0.255	0.025	0.11	1.03	1.34	0.31	0.30	347	266	-81	-0.23
JN1279R	0.50	1.0	2.1	0.382	0.271	-0.111	-0.29	0.85	0.79	-0.06	-0.07	327	312	-15	-0.05
JN1279B	0.49	1.5	3.0	0.673	0.504	-0.168	-0.25	1.24	1.12	-0.12	-0.09	320	315	-5	-0.02
JN1379R	0.45	2.9	6.5	0.974	0.802	-0.171	-0.18	2.69	2.87	0.18	0.07	254	226	-28	-0.11
AU0279R	0.22	1.5	7.0	0.788	0.612	-0.176	-0.22	2.41	2.17	-0.24	-0.10	166	185	19	0.11
AU2780B	0.48	1.9	4.0	1.044	1.134	0.090	0.09	3.26	3.28	0.02	0.01	212	217	5	0.02
ST0482B	0.23	1.1	4.9	0.658	0.657	-0.001	0.00	1.46	1.69	0.23	0.16	266	212	-54	-0.20
ST1382B	0.33	1.1	3.3	0.731	0.684	-0.047	-0.06	1.69	1.62	-0.06	-0.04	236	232	-4	-0.02
JL1783R	0.27	1.1	3.9	0.848	0.710	-0.137	-0.16	2.10	1.74	-0.35	-0.17	194	227	33	0.17
JL2183R	0.22	1.1	5.0	0.804	0.775	-0.029	-0.04	1.76	1.82	0.05	0.03	225	206	-19	-0.08
JL2983B	0.21	1.1	5.3	0.697	0.755	0.058	0.08	1.66	1.84	0.18	0.11	235	204	-31	-0.13
JL3183R	0.21	1.1	5.1	0.719	0.705	-0.013	-0.02	1.81	1.52	-0.29	-0.16	150	166	16	0.11
ST2383B	0.38	1.6	4.3	0.405	0.659	0.255	0.63	1.23	2.00	0.77	0.63	347	220	-127	-0.37
OC0484R	0.36	2.1	5.9	0.645	0.797	0.152	0.24	2.07	2.31	0.24	0.12	293	207	-86	-0.29
OC0484B	0.36	1.0	2.9	0.446	0.506	0.060	0.14	1.25	1.36	0.11	0.08	319	247	-72	-0.23
OC1184B	0.36	2.2	6.3	0.674	0.776	0.102	0.15	2.38	2.64	0.26	0.11	235	185	-50	-0.21
OC1284B	0.68	2.0	2.9	0.432	0.428	-0.004	-0.01	1.67	1.81	0.14	0.08	352	287	-65	-0.18
Group Average	0.39	1.8	4.7	0.623	0.625	0.002	0.02	1.77	1.93	0.16	0.10	294	227	-39	-0.13
S. Dev.	0.12	0.9	1.8	0.214	0.217	0.111	0.20	0.70	0.80	0.32	0.18	141	41	41	0.15
Avg. Abs. Value						0.085	0.14			0.26	0.15			46	0.17
S. Dev.						0.069	0.14			0.23	0.14			32	0.10

Table A-11 (continued) - 4

Experiment	Maximum Concentration PAN				Maximum Concentration ACETALD				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - PROPENE												
EC121	0.167	0.134	-0.033	-0.20	0.162	0.212	0.050	0.31	0.278	0.225	-0.053	-0.19
EC177	0.165	0.162	-0.002	-0.01	0.186	0.218	0.032	0.17	0.091	0.230	0.139	1.54
EC216	0.154	0.177	0.023	0.15	0.202	0.225	0.023	0.11	0.181	0.260	0.078	0.43
EC217	0.019	0.031	0.012	0.65	0.151	0.150	-0.001	-0.01	0.040	0.079	0.039	0.96
EC230	0.110	0.034	-0.076	-0.69	0.260	0.244	-0.015	-0.06	0.282	0.307	0.025	0.09
EC256	0.001	0.001	-0.001	-0.44	0.040	0.045	0.005	0.13	0.042	0.056	0.014	0.32
EC257	0.007	0.008	0.000	0.05	0.037	0.049	0.012	0.33		0.547		
EC276	0.100	0.123	0.023	0.23	0.192	0.239	0.047	0.25	0.192	0.253	0.061	0.32
EC277	0.077	0.102	0.025	0.32	0.192	0.261	0.069	0.36	0.213	0.274	0.062	0.29
EC278	0.260	0.258	-0.002	-0.01	0.378	0.467	0.089	0.24	0.438	0.485	0.047	0.11
EC279	0.340	0.277	-0.063	-0.19	0.470	0.511	0.041	0.09	0.522	0.519	-0.003	-0.01
EC314	0.226	0.336	0.111	0.49	0.441	0.477	0.036	0.08	0.523	0.491	-0.031	-0.06
EC315	0.116	0.230	0.114	0.98	0.382	0.402	0.020	0.05	0.383	0.382	-0.001	0.00
EC316	0.270	0.283	0.012	0.05	0.489	0.493	0.004	0.01	0.586	0.524	-0.062	-0.11
EC317	0.130	0.170	0.039	0.30	0.205	0.219	0.014	0.07	0.268	0.226	-0.042	-0.16
Group Average	0.143	0.155	0.012	0.11	0.252	0.281	0.028	0.14	0.288	0.324	0.019	0.25
S. Dev.	0.100	0.107	0.052	0.42	0.146	0.154	0.028	0.13	0.179	0.160	0.057	0.48
Avg. Abs. Value			0.036	0.32			0.031	0.15			0.047	0.33
S. Dev.			0.038	0.29			0.025	0.12			0.035	0.43

Table A-11 (continued) - 5

Experiment	Maximum Concentration PAN				Maximum Concentration ACETALD				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
2. SAPRC ITC - PROPENE												
ITC693	0.311	0.242	-0.069	-0.22	0.320	0.539	0.218	0.68	0.416	0.516	0.100	0.24
ITC810	0.140	0.192	0.052	0.37	0.174	0.451	0.277	1.59	0.447	0.419	-0.028	-0.06
ITC860		0.182			0.189	0.438	0.249	1.32	0.617	0.412	-0.206	-0.33
ITC925	0.205	0.188	-0.017	-0.08	0.141	0.444	0.303	2.16	0.467	0.411	-0.056	-0.12
ITC938	0.296	0.213	-0.083	-0.28	0.134	0.448	0.314	2.34	0.416	0.416	0.000	0.00
ITC947	0.270	0.210	-0.060	-0.22	0.121	0.448	0.327	2.71		0.415		
ITC960	0.056	0.188	0.133	2.39	0.203	0.448	0.245	1.21	0.255	0.419	0.163	0.64
Group Average	0.213	0.202	-0.007	0.33	0.183	0.459	0.276	1.71	0.436	0.429	-0.004	0.06
S. Dev.	0.100	0.021	0.084	1.04	0.068	0.035	0.040	0.71	0.116	0.038	0.129	0.34
Avg. Abs. Value			0.069	0.59			0.276	1.71			0.092	0.23
S. Dev.			0.038	0.88			0.040	0.71			0.080	0.23
3. Runs IDs = OTC PROPENE												
OTC186	0.260	0.304	0.044	0.17	0.508	0.590	0.083	0.16	0.462	0.585	0.123	0.27
OTC191	0.190	0.244	0.054	0.29	0.433	0.567	0.135	0.31	0.811	0.562	-0.249	-0.31
OTC210	0.126	0.165	0.039	0.31	0.481	0.483	0.002	0.00		0.468		
OTC233	0.037	0.117	0.080	2.17	0.380	0.473	0.092	0.24		0.458		
OTC236	0.095	0.245	0.150	1.58	0.599	0.565	-0.034	-0.06	0.459	0.542	0.083	0.18
Group Average	0.142	0.215	0.074	0.90	0.480	0.536	0.056	0.13	0.577	0.523	-0.015	0.05
S. Dev.	0.086	0.074	0.045	0.91	0.082	0.054	0.069	0.16	0.202	0.057	0.204	0.31
Avg. Abs. Value			0.074	0.90			0.069	0.16			0.151	0.25
S. Dev.			0.045	0.91			0.052	0.13			0.087	0.06

Table A-11 (continued) - 6

Experiment	Maximum Concentration PAN				Maximum Concentration ACETALD				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
4. Runs IDs = UNC PROPENE												
JA1078R						0.003				0.002		
OC1278B	0.069	0.086	0.017	0.25	0.214	0.182	-0.032	-0.15				
OC2078R	0.082	0.073	-0.008	-0.10	0.190	0.183	-0.007	-0.04	0.440	0.159	-0.281	-0.64
OC2078B	0.241	0.297	0.056	0.23	0.460	0.510	0.050	0.11	0.800	0.493	-0.307	-0.38
OC2178R	0.162	0.291	0.129	0.80	0.455	0.496	0.041	0.09	0.840	0.476	-0.364	-0.43
OC2578B	0.050	0.058	0.009	0.18	0.166	0.165	-0.001	0.00		0.142		
JN1279R	0.032	0.034	0.002	0.07	0.122	0.105	-0.017	-0.14	0.142	0.088	-0.054	-0.38
JN1279B	0.134	0.138	0.004	0.03	0.385	0.389	0.004	0.01	0.208	0.105	-0.103	-0.50
JN1379R	0.223	0.271	0.048	0.21	0.419	0.390	-0.029	-0.07	0.410	0.372	-0.038	-0.09
AU0279R		0.093			0.201	0.213	0.011	0.06	0.440	0.221	-0.219	-0.50
AU2780B	0.130	0.144	0.015	0.11		0.278			0.030	0.261	0.231	7.70
ST0482B	0.122	0.119	-0.003	-0.02		0.162				0.158		
ST1382B	0.117	0.095	-0.022	-0.19		0.154				0.152		
JL1783R	0.086	0.085	-0.001	-0.01	0.134	0.156	0.023	0.17	0.174	0.164	-0.010	-0.06
JL2183R	0.093	0.078	-0.016	-0.17	0.124	0.160	0.035	0.29	0.214	0.170	-0.045	-0.21
JL2983B	0.092	0.107	0.015	0.16	0.129	0.156	0.027	0.21	0.185	0.157	-0.027	-0.15
JL3183R	0.088	0.096	0.008	0.09	0.134	0.150	0.015	0.11	0.211	0.155	-0.057	-0.27
ST2383B	0.100	0.198	0.098	0.98	0.215	0.226	0.011	0.05		0.207		
OC0484R	0.167	0.202	0.035	0.21	0.293	0.297	0.004	0.01	0.424	0.285	-0.139	-0.33
OC0484B	0.086	0.081	-0.006	-0.06	0.145	0.142	-0.003	-0.02	0.223	0.134	-0.089	-0.40
OC1184B	0.180	0.220	0.041	0.23	0.287	0.323	0.035	0.12	0.484	0.310	-0.173	-0.36
OC1284B	0.144	0.106	-0.038	-0.26	0.236	0.269	0.034	0.14	0.427	0.240	-0.187	-0.44
Group Average	0.120	0.137	0.019	0.14	0.239	0.232	0.011	0.05	0.353	0.212	-0.116	0.16
S. Dev.	0.054	0.078	0.040	0.30	0.117	0.126	0.024	0.12	0.226	0.121	0.142	2.02
Avg. Abs. Value			0.028	0.22			0.021	0.10			0.145	0.80
S. Dev.			0.034	0.24			0.015	0.08			0.110	1.85

Table A-12. Butene-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d([O3] - [NO])/dt				Half-Life Butene			
	NOx (ppm)	HC (ppmC)	HC/NOx	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. SAPRC EC - 1-BUTENE															
EC122	0.50	0.9	1.7	0.227	0.152	-0.075	-0.33	2.29	1.86	-0.44	-0.19	97	136	39	0.40
EC123	0.51	1.6	3.2	0.506	0.390	-0.116	-0.23	4.16	3.01	-1.15	-0.28	84	135	51	0.61
EC124	0.99	1.7	1.7	0.247	0.260	0.014	0.06	1.99	2.41	0.42	0.21	122	158	36	0.30
Group Average	0.67	1.4	2.2	0.326	0.268	-0.059	-0.17	2.81	2.42	-0.39	-0.09	101	143	42	0.43
S. Dev.	0.28	0.5	0.9	0.155	0.119	0.066	0.20	1.18	0.58	0.79	0.26	19	13	7	0.16
Avg. Abs. Value						0.068	0.20			0.67	0.23			42	0.43
S. Dev.						0.051	0.14			0.42	0.05			7	0.16
2. SAPRC ITC - 1-BUTENE															
ITC927	0.31	3.8	12.3	0.646	0.768	0.122	0.19	3.24	4.90	1.67	0.52	168	127	-41	-0.24
ITC928	0.67	3.8	5.7	0.022	0.109	0.087		1.36	2.14	0.78	0.58				
ITC930	0.32	7.2	22.2	0.717	0.794	0.077	0.11	7.91	12.02	4.12	0.52	92	74	-18	-0.20
ITC935	0.66	7.6	11.6	0.872	0.988	0.116	0.13	5.39	9.12	3.74	0.69	159	117	-42	-0.26
Group Average	0.49	5.6	12.9	0.564	0.665	0.101	0.14	4.47	7.05	2.58	0.58	139	106	-33	-0.23
S. Dev.	0.20	2.1	6.8	0.374	0.383	0.022	0.04	2.82	4.39	1.61	0.08	41	28	13	0.04
Avg. Abs. Value						0.101	0.14			2.58	0.58			33	0.23
S. Dev.						0.022	0.04			1.61	0.08			13	0.04

Table A-12 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d([O3] - [NO])/dt				Half-Life Butene			
	NOx (ppm)	HC (ppmC)	HC/NOx	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
3. UNC CHAMBER - 1-BUTENE															
ST2383R	0.40	1.5	3.7	0.206	0.541	0.335	1.62	0.96	1.60	0.64	0.67	358	221	-137	-0.38
ST2583R	0.46	1.6	3.6	0.266	0.557	0.291	1.09	1.16	1.73	0.57	0.49	330	232	-98	-0.30
ST2583B	0.42	2.9	6.8	0.594	0.761	0.167	0.28	1.78	2.68	0.90	0.50	295	203	-92	-0.31
ST2783R	0.45	1.6	3.6	0.285	0.561	0.276	0.97	1.19	1.70	0.51	0.43	335	234	-101	-0.30
Group Average	0.43	1.9	4.4	0.338	0.605	0.267	0.99	1.27	1.93	0.66	0.52	329	222	-107	-0.32
S. Dev.	0.03	0.6	1.6	0.174	0.104	0.071	0.55	0.36	0.51	0.17	0.11	26	14	20	0.04
Avg. Abs. Value						0.267	0.99			0.66	0.52			107	0.32
S. Dev.						0.071	0.55			0.17	0.11			20	0.04
4. SAPRC EC - TRANS-2-BUTENE															
EC146	0.51	0.9	1.8	0.247	0.173	-0.073	-0.30	5.87	4.24	-1.63	-0.28	23	39	16	0.70
EC147	0.98	1.7	1.7	0.154	0.142	-0.012	-0.08	9.83	8.05	-1.79	-0.18	27	42	15	0.56
EC157	0.53	0.9	1.7	0.205	0.147	-0.058	-0.28	5.96	3.94	-2.02	-0.34	25	40	15	0.60
Group Average	0.67	1.2	1.7	0.202	0.154	-0.048	-0.22	7.22	5.41	-1.81	-0.27	25	40	15	0.62
S. Dev.	0.27	0.5	0.1	0.046	0.017	0.032	0.12	2.26	2.29	0.20	0.08	2	1	0	0.07
Avg. Abs. Value						0.048	0.22			1.81	0.27			15	0.62
S. Dev.						0.032	0.12			0.20	0.08			0	0.07

Table A-12 (continued) - 3

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d([O3] - [NO])/dt				Half-Life Butene			
	NOx (ppm)	HC (ppmC)	HC/NOx	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
5. UNC CHAMBER - TRANS-2-BUTENE															
ST2783B	0.43	2.0	4.7	0.523	0.572	0.049	0.09	3.00	3.14	0.14	0.05	125	98	-27	-0.22
Group Average	0.43	2.0	4.7	0.523	0.572	0.049	0.09	3.00	3.14	0.14	0.05	125	98	-27	-0.22
S. Dev.															
Avg. Abs. Value						0.049	0.09			0.14	0.05			27	0.22
S. Dev.															
6. SAPRC ITC - ISOBUTENE															
ITC694	0.51	4.6	9.1	0.900	0.973	0.073	0.08	8.84	12.78	3.94	0.45	76	59	-17	-0.22

Table A-12 (continued) - 4

Experiment	Maximum Concentration PAN				Maximum Concentration PPN			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - 1-BUTENE								
EC122	0.021	0.008	-0.013	-0.61	0.031	0.021	-0.010	-0.31
EC123	0.065	0.028	-0.038	-0.58	0.085	0.096	0.011	0.13
EC124	0.038	0.027	-0.011	-0.28	0.036	0.055	0.019	0.51
Group Average	0.041	0.021	-0.020	-0.49	0.051	0.057	0.007	0.11
S. Dev.	0.022	0.011	0.015	0.18	0.030	0.037	0.015	0.41
Avg. Abs. Value			0.020	0.49			0.013	0.32
S. Dev.			0.015	0.18			0.005	0.19

Table A-12 (continued) - 5

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO				Maximum Concentration ACETALD			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - TRANS-2-BUTENE												
EC146	0.063	0.040	-0.023	-0.37	0.030	0.083	0.053	1.75	0.204	0.271	0.067	0.33
EC147	0.060	0.050	-0.010	-0.17	0.095	0.150	0.056	0.59	0.389	0.475	0.086	0.22
EC157	0.052	0.033	-0.019	-0.37	0.028	0.084	0.055	1.96	0.220	0.252	0.032	0.15
Group Average	0.058	0.041	-0.018	-0.30	0.051	0.106	0.055	1.43	0.187	0.223	0.036	0.14
S. Dev.	0.006	0.009	0.007	0.12	0.038	0.039	0.002	0.74	0.224	0.215	0.093	0.27
Avg. Abs. Value			0.018	0.30			0.055	1.43			0.036	0.14
S. Dev.			0.007	0.12			0.002	0.74			0.093	0.27
2. UNC CHAMBER - TRANS-2-BUTENE												
ST2783B	0.145	0.183	0.038	0.26	0.158	0.082	-0.076	-0.48				
3. SAPRC ITC - ISOBUTENE												
ITC694	0.137	0.033	-0.104	-0.76	0.644	0.695	0.051	0.08				

Table A-13. Benzene-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC ITC - BENZENE											
ITC560	0.12	332.3	2874.4	0.323	0.369	0.046	0.14	7.01	9.66	2.64	0.38
ITC561	0.11	79.1	694.2	0.273	0.329	0.057	0.21	4.75	4.73	-0.03	-0.01
ITC562	0.56	83.8	149.7	0.412	0.462	0.050	0.12	2.85	2.95	0.10	0.03
ITC698	0.50	83.5	167.4	0.374	0.436	0.062	0.17	2.87	3.00	0.13	0.04
ITC710	0.55	83.6	151.0	0.367	0.448	0.081	0.22	2.70	2.82	0.12	0.04
ITC831	1.01	12.2	12.1	0.021	0.004	-0.017		0.17	0.27	0.10	0.61
Group Average	0.47	112.4	674.8	0.295	0.341	0.046	0.17	3.39	3.90	0.51	0.18
S. Dev.	0.33	111.3	1103.2	0.142	0.173	0.033	0.04	2.30	3.16	1.05	0.25
Avg. Abs. Value						0.052	0.17			0.52	0.19
S. Dev.						0.021	0.04			1.04	0.25

Table A-14. Toluene-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - TOLUENE											
EC264	0.48	8.1	17.0	0.419	0.401	-0.018	-0.04	4.46	5.25	0.80	0.18
EC265	0.48	7.5	15.6	0.393	0.395	0.001	0.00	3.56	5.02	1.46	0.41
EC266	0.49	8.4	17.0	0.405	0.405	-0.001	0.00	4.62	5.41	0.79	0.17
EC269	0.47	4.0	8.4	0.318	0.305	-0.012	-0.04	2.55	2.53	-0.03	-0.01
EC270	0.46	4.2	9.0	0.369	0.364	-0.005	-0.01	3.72	3.98	0.25	0.07
EC271	0.21	8.0	37.4	0.296	0.343	0.047	0.16	6.56	6.03	-0.53	-0.08
EC272	0.48	4.1	8.5	0.410	0.301	-0.109	-0.27	3.69	2.54	-1.15	-0.31
EC273	0.11	4.1	37.2	0.215	0.267	0.052	0.24	5.90	3.86	-2.03	-0.34
EC327	0.45	4.0	8.9	0.376	0.358	-0.018	-0.05	2.49	2.68	0.19	0.08
EC336	0.44	7.2	16.3	0.396	0.442	0.046	0.12	6.06	6.99	0.93	0.15
EC337	0.45	7.9	17.7	0.325	0.345	0.020	0.06	2.55	2.56	0.01	0.00
EC339	0.44	5.0	11.3	0.225	0.144	-0.080	-0.36	1.53	1.44	-0.09	-0.06
EC340	0.43	4.1	9.5	0.344	0.351	0.007	0.02	2.50	2.52	0.02	0.01
Group Average	0.42	5.9	16.5	0.345	0.340	-0.005	-0.01	3.86	3.91	0.05	0.02
S. Dev.	0.12	1.9	9.9	0.068	0.076	0.047	0.16	1.58	1.69	0.92	0.20
Avg. Abs. Value						0.032	0.11			0.64	0.14
S. Dev.						0.033	0.12			0.63	0.14

Table A-14 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
2. SAPRC ITC - TOLUENE											
ITC699	0.51	10.5	20.8	0.485	0.444	-0.041	-0.08	4.72	4.77	0.05	0.01
ITC828	1.02	3.0	3.0	0.021	0.006	-0.015		0.49	0.99	0.49	1.00
Group Average	0.76	6.8	11.9	0.253	0.225	-0.028	-0.08	2.61	2.88	0.27	0.51
S. Dev.	0.36	5.3	12.6					2.99	2.68	0.32	0.70
Avg. Abs. Value						0.028	0.08			0.27	0.51
S. Dev.										0.32	0.70
3. UNC CHAMBER - TOLUENE											
JL3080R	0.18	3.9	21.3	0.273	0.386	0.112	0.41	1.20	1.28	0.09	0.07
AU2780R	0.48	2.3	4.8	0.736	0.716	-0.020	-0.03	1.76	1.52	-0.24	-0.14
AU2782B	0.43	3.0	7.0	0.116	0.171	0.056	0.48	0.63	0.74	0.10	0.16
OC2782R	0.39	4.5	11.7	0.123	0.355	0.232	1.89	0.66	0.91	0.25	0.38
AU0183R	0.39	4.6	11.8	0.458	0.460	0.002	0.01	1.75	1.78	0.02	0.01
Group Average	0.37	3.7	11.3	0.341	0.418	0.076	0.55	1.20	1.25	0.05	0.10
S. Dev.	0.11	1.0	6.4	0.261	0.198	0.101	0.78	0.55	0.43	0.18	0.19
Avg. Abs. Value						0.084	0.56			0.14	0.15
S. Dev.						0.093	0.77			0.10	0.14

Table A-14 (continued) - 3

Experiment	Maximum Concentration PAN			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - TOLUENE				
EC264	0.071	0.077	0.006	0.09
EC265	0.072	0.074	0.003	0.04
EC266	0.075	0.079	0.004	0.06
EC269	0.050	0.039	-0.011	-0.22
EC270	0.057	0.050	-0.007	-0.12
EC271	0.053	0.057	0.004	0.07
EC272	0.132	0.039	-0.093	-0.71
EC273	0.032	0.035	0.003	0.10
EC327	0.041	0.046	0.006	0.15
EC336	0.059	0.069	0.010	0.17
EC337	0.047	0.051	0.004	0.09
EC339	0.024	0.013	-0.011	-0.45
EC340	0.042	0.041	-0.001	-0.03
Group Average	0.058	0.052	-0.006	-0.06
S. Dev.	0.027	0.019	0.027	0.26
Avg. Abs. Value			0.013	0.18
S. Dev.			0.024	0.19

Table A-14 (continued) - 4

Experiment	Maximum Concentration PAN			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
2. SAPRC ITC - TOLUENE				
ITC699	0.145	0.087	-0.058	-0.40
ITC828	0.000	0.000	0.000	
Group Average	0.072	0.044	-0.029	-0.40
S. Dev.				
Avg. Abs. Value			0.029	0.40
S. Dev.				
3. UNC CHAMBER - TOLUENE				
JL3080R	0.037	0.036	0.000	-0.01
AU2780R	0.020	0.013	-0.008	-0.37
AU2782B	0.012	0.009	-0.002	-0.18
OC2782R	0.013	0.062	0.049	3.69
AU0183R	0.043	0.040	-0.003	-0.07
Group Average	0.025	0.032	0.007	0.61
S. Dev.	0.014	0.022	0.024	1.73
Avg. Abs. Value			0.012	0.86
S. Dev.			0.021	1.59

Table A-15. Xylene-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - XYLENE											
EC343	0.28	4.2	14.9	0.283	0.395	0.111	0.39	8.18	11.10	2.91	0.36
EC344	0.67	4.0	5.9	0.589	0.552	-0.037	-0.06	10.72	10.22	-0.51	-0.05
EC345	0.28	3.7	13.3	0.396	0.405	0.010	0.02	11.35	11.32	-0.03	0.00
EC346	0.26	3.9	14.8	0.384	0.389	0.006	0.01	7.65	11.26	3.60	0.47
Group Average	0.37	3.9	12.2	0.413	0.435	0.022	0.09	9.48	10.97	1.50	0.19
S. Dev.	0.20	0.2	4.3	0.128	0.078	0.063	0.20	1.83	0.51	2.06	0.26
Avg. Abs. Value						0.041	0.12			1.76	0.22
S. Dev.						0.049	0.18			1.76	0.23
2. SAPRC ITC - XYLENE											
ITC702	0.52	4.0	7.8	0.627	0.507	-0.120	-0.19	7.79	8.62	0.83	0.11
ITC827	1.07	1.2	1.1	0.021	0.010	-0.011		1.12	1.77	0.65	0.58
Group Average	0.79	2.6	4.4	0.324	0.258	-0.065	-0.19	4.45	5.19	0.74	0.34
S. Dev.	0.39	2.0	4.7					4.71	4.85	0.13	0.33
Avg. Abs. Value						0.065	0.19			0.74	0.34
S. Dev.										0.13	0.33

Table A-15 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
3. UNC CHAMBER - XYLENE											
JL3080B	0.18	2.2	12.4	0.555	0.448	-0.107	-0.19	1.97	2.05	0.08	0.04
AU2782R	0.43	2.0	4.6	0.491	0.514	0.023	0.05	1.31	1.46	0.16	0.12
OC2782B	0.39	2.8	7.0	0.396	0.416	0.020	0.05	1.43	1.68	0.25	0.17
AU0183B	0.37	2.7	7.2	0.688	0.514	-0.174	-0.25	2.39	1.61	-0.78	-0.32
Group Average	0.34	2.4	7.8	0.532	0.473	-0.059	-0.09	1.77	1.70	-0.07	0.00
S. Dev.	0.11	0.4	3.3	0.123	0.049	0.097	0.16	0.50	0.25	0.47	0.22
Avg. Abs. Value						0.081	0.14			0.32	0.16
S. Dev.						0.074	0.10			0.31	0.12

Table A-15 (continued) - 3

Experiment	Half-Life M-XYL			
	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. SAPRC EC - XYLENE				
EC343	83	58	-25	-0.30
EC344	67	71	4	0.06
EC345	55	57	2	0.04
EC346		56		
Group Average	68	60	-6	-0.07
S. Dev.	14	7	16	0.20
Avg. Abs. Value			10	0.13
S. Dev.			12	0.15
2. SAPRAC ITC - XYLENE				
ITC702	87	86	-1	-0.01
ITC827				
Group Average	87	86	-1	-0.01
S. Dev.				
Avg. Abs. Value			1	0.01
S. Dev.				

Table A-15 (continued) - 4

Experiment	Half-Life O-XYL			
	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. UNC CHAMBER - XYLENE				
JL3080B	187	179	-8	-0.04
AU2782R	318	293	-25	-0.08
OC2782B	300	258	-42	-0.14
AU0183B	221	315	94	0.43
Group Average	256	261	4	0.04
S. Dev.	62	59	61	0.26
Avg. Abs. Value			42	0.17
S. Dev.			37	0.17
1. SAPRC EC - XYLENE				
EC343	0.081	0.105	0.025	0.31
EC344	0.175	0.175	0.000	0.00
EC345	0.107	0.104	-0.002	-0.02
EC346	0.102	0.102	0.001	0.01
Group Average	0.116	0.122	0.006	0.07
S. Dev.	0.041	0.035	0.013	0.16
Avg. Abs. Value			0.007	0.08
S. Dev.			0.012	0.15

Table A-15 (continued) - 5

Experiment	Maximum Concentration PAN			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
2. SAPRC ITC - XYLENE				
ITC702	0.390	0.156	-0.234	-0.60
ITC827	0.002	0.002	0.000	-0.09
Group Average	0.196	0.079	-0.117	-0.35
S. Dev.	0.274	0.109	0.165	0.36
Avg. Abs. Value			0.117	0.35
S. Dev.			0.165	0.36
3. UNC CHAMBER - XYLENE				
JL3080B	0.091	0.063	-0.028	-0.30
AU2782R	0.093	0.068	-0.025	-0.27
OC2782B	0.112	0.122	0.011	0.10
AU0183B	0.102	0.069	-0.034	-0.33
Group Average	0.099	0.081	-0.019	-0.20
S. Dev.	0.009	0.028	0.020	0.20
Avg. Abs. Value			0.024	0.25
S. Dev.			0.010	0.11

Table A-16. 1,3,5-Trimethylbenzene-NO_x-Air Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - MESITYLENE											
EC900	0.53	5.4	10.2	0.381	0.463	0.082	0.21	3.85			
EC901	0.51	2.7	5.2	0.384	0.452	0.069	0.18	8.88	7.84	-1.04	-0.12
EC903	1.00	4.7	4.7	0.502	0.633	0.131	0.26	14.96	12.73	-2.22	-0.15
Group Average	0.68	4.3	6.7	0.422	0.516	0.094	0.22	9.23		-1.63	-0.13
S. Dev.	0.28	1.4	3.1	0.069	0.101	0.033	0.04	5.56		0.83	0.02
Avg. Abs. Value						0.094	0.22			1.63	0.13
S. Dev.						0.033	0.04			0.83	0.02
2. SAPRC ITC - MESITYLENE											
ITC703	0.50	5.3	10.6	0.707	0.518	-0.189	-0.27	14.59	19.02	4.44	0.30
ITC706	0.49	2.7	5.4	0.641	0.571	-0.069	-0.11	7.20	9.27	2.07	0.29
ITC709	0.99	4.7	4.7	0.779	0.785	0.006	0.01	11.74	14.58	2.85	0.24
ITC742	0.48	4.6	9.7	0.773	0.523	-0.250	-0.32	13.14	16.15	3.01	0.23
ITC826	0.90	0.8	0.9	0.022	0.013	-0.009		1.68	2.34	0.67	0.40
Group Average	0.67	3.6	6.3	0.584	0.482	-0.102	-0.17	9.67	12.28	2.61	0.29
S. Dev.	0.25	1.9	3.9	0.320	0.284	0.113	0.15	5.26	6.59	1.38	0.07
Avg. Abs. Value						0.105	0.18			2.61	0.29
S. Dev.						0.110	0.14			1.38	0.07

Table A-16 (continued) - 2

Experiment	Half-Life 135-TMB				Maximum Concentration PAN			
	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - MESITYLENE								
EC900		46			0.400	0.164	-0.236	-0.59
EC901	47	44	-3	-0.06	0.293	0.140	-0.153	-0.52
EC903	49	48	-1	-0.02	0.470	0.270	-0.200	-0.43
Group Average	48	46	-2	-0.04	0.388	0.191	-0.196	-0.51
S. Dev.	1	2	1	0.03	0.089	0.069	0.041	0.08
Avg. Abs. Value			2	0.04			0.196	0.51
S. Dev.			1	0.03			0.041	0.08
2. SAPRC ITC - MESITYLENE								
ITC703	45	36	-9	-0.20	0.586	0.185	-0.401	-0.68
ITC706	45	38	-7	-0.16	0.440	0.161	-0.279	-0.63
ITC709	52	46	-6	-0.12	0.590	0.311	-0.279	-0.47
ITC742	42	36	-6	-0.14	0.470	0.180	-0.290	-0.62
ITC826	112				0.003	0.003	0.000	-0.16
Group Average	59	39	-7	-0.15	0.418	0.168	-0.250	-0.51
S. Dev.	29	4	1	0.04	0.241	0.110	0.148	0.21
Avg. Abs. Value			7	0.15			0.250	0.51
S. Dev.			1	0.04			0.148	0.21

Table A-17. Mixtures of Like Compounds

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - Mixed Alkenes											
EC144	0.51	4.7	9.3	1.065	0.831	-0.234	-0.22	10.53	7.23	-3.30	-0.31
EC145	0.99	3.4	3.4	0.777	0.476	-0.301	-0.39	5.11	4.52	-0.60	-0.12
EC160	0.99	3.2	3.3	0.874	0.425	-0.450	-0.51	5.86	4.08	-1.78	-0.30
EC149	0.99	2.0	2.0	0.286	0.173	-0.113	-0.40	10.83	5.54	-5.29	-0.49
EC150	1.00	3.5	3.5	0.799	0.443	-0.356	-0.45	6.30	5.05	-1.24	-0.20
EC151	2.06	5.2	2.5	0.147	0.174	0.027	0.19	8.43	9.36	0.93	0.11
EC152	0.50	3.7	7.3	0.791	0.711	-0.080	-0.10	10.41	8.40	-2.01	-0.19
EC153	0.97	6.6	6.8	1.050	0.882	-0.168	-0.16	19.23	14.60	-4.63	-0.24
EC161	0.51	3.2	6.4	0.857	0.660	-0.197	-0.23	9.94	5.87	-4.07	-0.41
Group Average	0.95	4.0	5.0	0.738	0.531	-0.208	-0.25	9.63	7.18	-2.44	-0.24
S. Dev.	0.48	1.4	2.5	0.316	0.260	0.147	0.22	4.22	3.30	2.03	0.17
Avg. Abs. Value						0.214	0.29			2.65	0.26
S. Dev.						0.136	0.14			1.72	0.13
2. UNC CHAMBER - Mixed Alkenes											
OC1278R	0.48	1.4	3.0	0.260	0.347	0.087	0.33	1.14	1.38	0.25	0.22
OC2578R	0.44	1.4	3.1	0.147	0.180	0.033	0.22	0.94	1.11	0.18	0.19
AU0180R	0.56	0.5	0.8	0.256	0.055	-0.201	-0.78	0.98	0.51	-0.47	-0.48
AU1480R	0.47	1.4	3.0	0.863	0.452	-0.411	-0.48	2.13	1.41	-0.72	-0.34
Group Average	0.49	1.2	2.5	0.382	0.259	-0.123	-0.18	1.30	1.11	-0.19	-0.10
S. Dev.	0.05	0.5	1.1	0.325	0.176	0.229	0.54	0.56	0.42	0.48	0.36
Avg. Abs. Value						0.183	0.45			0.40	0.31
S. Dev.						0.167	0.24			0.24	0.13

Table A-17 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
3. SAPRC EC - Mixed Alkanes											
EC166	0.10	9.2	92.0	0.462	0.489	0.027	0.06	2.11	1.82	-0.29	-0.14
EC172	0.10	2.8	28.9	0.369	0.412	0.043	0.12	1.00	1.03	0.03	0.03
Group Average	0.10	6.0	60.5	0.415	0.450	0.035	0.09	1.55	1.43	-0.13	-0.05
S. Dev.	0.00	4.5	44.6	0.066	0.054	0.011	0.04	0.79	0.56	0.23	0.12
Avg. Abs. Value						0.035	0.09			0.16	0.08
S. Dev.						0.011	0.04			0.18	0.07
4. UNC CHAMBER - Mixed Aromatics											
ST0682R	0.46	2.8	6.2	0.378	0.404	0.026	0.07	1.11	1.17	0.06	0.05
ST0682B	0.45	2.9	6.5	0.478	0.451	-0.026	-0.06	1.35	1.40	0.04	0.03
Group Average	0.46	2.9	6.3	0.428	0.428	0.000	0.01	1.23	1.28	0.05	0.04
S. Dev.	0.01	0.1	0.2	0.070	0.033	0.037	0.09	0.17	0.16	0.01	0.01
Avg. Abs. Value						0.026	0.06			0.05	0.04
S. Dev.						0.000	0.01			0.01	0.01

Table A-17 (continued) - 3

Experiment	Half-Life PROPENE				Half-Life TRANS-2-BUTENE			
	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. SAPRAC EC - Mixed Alkenes								
EC144	63	98	35	0.56				
EC145	102	149	47	0.46				
EC160	86	151	65	0.76				
EC149	75	155	80	1.07	26	52	26	1.00
EC150	102				35	49	14	0.40
EC151	114				34	42	8	0.24
EC152	64				25	34	9	0.36
EC153	58				25	36	11	0.44
EC161	58				23	37	14	0.61
Group Average	80	138	56	0.71	28	41	13	0.51
S. Dev.	21	26	19	0.27	5	7	6	0.27
Avg. Abs. Value			56	0.71			13	0.51
S. Dev.			19	0.27			6	0.27
2. UNC CHAMBER - Mixed Alkenes								
AU148OR					121	150	29	0.24
Group Average					121	150	29	0.24
S. Dev.								
Avg. Abs. Value							29	0.24
S. Dev.								

Table A-17 (continued) - 4

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - Mixed Alkenes								
EC144	0.075	0.121	0.045	0.61	0.846	0.946	0.100	0.12
EC145	0.112	0.080	-0.032	-0.28	0.516	0.559	0.043	0.08
EC160	0.158	0.068	-0.089	-0.57	0.500	0.529	0.030	0.06
EC149	0.112	0.054	-0.058	-0.52	0.105	0.245	0.141	1.34
EC150	0.145	0.078	-0.067	-0.46	0.433	0.514	0.081	0.19
EC151	0.077	0.062	-0.015	-0.19	0.512	0.634	0.122	0.24
EC152	0.115	0.127	0.012	0.11	0.262	0.558	0.297	1.13
EC153	0.175	0.204	0.029	0.17	0.645	1.008	0.363	0.56
EC161	0.125	0.107	-0.019	-0.15	0.423	0.495	0.072	0.17
Group Average	0.121	0.100	-0.021	-0.14	0.471	0.610	0.139	0.43
S. Dev.	0.034	0.047	0.045	0.38	0.211	0.234	0.115	0.48
Avg. Abs. Value			0.041	0.34			0.139	0.43
S. Dev.			0.026	0.20			0.115	0.48
2. UNC CHAMBER - Mixed Alkenes								
OC1278R	0.053	0.099	0.046	0.87				
OC2578R	0.041	0.077	0.037	0.91				
AU018OR	0.013	0.001	-0.011	-0.89	0.230	0.064	-0.166	-0.72
AU148OR	0.058	0.024	-0.034	-0.59	0.402	0.164	-0.238	-0.59
Group Average	0.041	0.050	0.009	0.08	0.316	0.114	-0.202	-0.66
S. Dev.	0.020	0.046	0.038	0.95	0.122	0.071	0.051	0.09
Avg. Abs. Value			0.032	0.82			0.202	0.66
S. Dev.			0.015	0.15			0.051	0.09

Table A-17 (continued) - 5

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
3. SAPRC EC - Mixed Alkanes								
EC166	0.040	0.031	-0.009	-0.22	0.010	0.015	0.005	0.51
EC172	0.029	0.025	-0.004	-0.13	0.010	0.012	0.002	0.16
Group Average	0.034	0.028	-0.006	-0.17	0.010	0.013	0.003	0.34
S. Dev.	0.008	0.004	0.003	0.06	0.000	0.003	0.003	0.25
Avg. Abs. Value			0.006	0.17			0.003	0.34
S. Dev.			0.003	0.06			0.003	0.25
4. UNC CHAMBER - Mixed Aromatics								
ST0682R	0.043	0.039	-0.003	-0.08	0.088	0.026	-0.062	-0.71
ST0682B	0.061	0.057	-0.004	-0.07	0.100	0.033	-0.067	-0.67
Group Average	0.052	0.048	-0.004	-0.08	0.094	0.029	-0.065	-0.69
S. Dev.	0.013	0.012	0.001	0.01	0.008	0.005	0.004	0.02
Avg. Abs. Value			0.004	0.08			0.065	0.69
S. Dev.			0.001	0.01			0.004	0.02

Table A-18. Miscellaneous Simple (Non-Surrogate) Mixtures

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - ALKANE/OLEFIN											
EC106	0.50	9.2	18.3	0.592	0.732	0.140	0.24	3.80	4.16	0.36	0.09
EC113	0.11	9.5	85.0	0.352	0.470	0.119	0.34	5.26	6.39	1.13	0.22
EC114	1.00	17.3	17.3	0.744	0.790	0.046	0.06	8.03	6.37	-1.66	-0.21
EC115	0.51	12.7	25.2	0.590	0.739	0.149	0.25	3.78	3.62	-0.16	-0.04
EC116	0.49	18.6	37.6	0.743	0.841	0.098	0.13	8.28	8.71	0.43	0.05
Group Average	0.52	13.5	36.7	0.604	0.714	0.110	0.20	5.83	5.85	0.02	0.02
S. Dev.	0.31	4.3	28.2	0.160	0.143	0.041	0.11	2.21	2.04	1.05	0.16
Avg. Abs. Value						0.110	0.20			0.75	0.12
S. Dev.						0.041	0.11			0.63	0.08
2. UNC CHAMBER - ALKANE/OLEFIN											
JL1581R	0.27	2.3	8.4	0.485	0.523	0.037	0.08	1.08	1.00	-0.07	-0.07
JL1881R	0.26	2.1	8.0	0.658	0.458	-0.201	-0.30	1.31	1.08	-0.23	-0.18
ST2481R	0.23	1.6	6.7	0.211	0.339	0.128	0.61	0.62	0.84	0.22	0.36
AU2781R	0.23	2.1	9.2	0.554	0.591	0.038	0.07	0.95	1.09	0.13	0.14
OC0382R	0.25	2.7	11.0	0.247	0.504	0.257	1.04	0.76	0.94	0.18	0.23
OC0382B	0.25	1.9	7.7	0.158	0.320	0.162	1.03	0.62	0.76	0.14	0.23
NV1582R	0.18	2.6	14.4	0.061	0.218	0.157	2.58	0.42	0.62	0.20	0.47
Group Average	0.24	2.2	9.3	0.339	0.422	0.083	0.73	0.82	0.90	0.08	0.17
S. Dev.	0.03	0.4	2.6	0.225	0.133	0.146	0.96	0.31	0.17	0.17	0.23
Avg. Abs. Value						0.140	0.81			0.17	0.24
S. Dev.						0.081	0.88			0.06	0.14

Table A-18 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
3. UNC CHAMBER - UNC MIX											
JL2281R	0.26	2.4	9.1	0.626	0.535	-0.091	-0.15	1.18	1.11	-0.07	-0.06
JL2181B	0.24	1.3	5.4	0.237	0.250	0.013	0.05	0.63	0.64	0.00	0.01
NV1582B	0.18	2.7	14.9	0.167	0.348	0.182	1.09	0.71	1.07	0.37	0.52
DE0782B	0.19	3.5	18.7	0.093	0.398	0.305	3.30	0.55	1.20	0.66	1.20
Group Average	0.22	2.5	12.0	0.281	0.383	0.102	1.07	0.77	1.01	0.24	0.42
S. Dev.	0.04	0.9	5.9	0.238	0.119	0.176	1.58	0.28	0.25	0.34	0.58
Avg. Abs. Value						0.148	1.15			0.27	0.45
S. Dev.						0.126	1.51			0.30	0.55
4. SAPRC EC - OLEFIN/AROMATIC											
EC335	0.44	7.7	17.4	0.398	0.425	0.026	0.07	4.64	4.89	0.24	0.05
EC329	0.45	4.2	9.2	0.403	0.407	0.004	0.01	3.27	3.26	-0.01	0.00
EC330	0.29	4.3	14.6	0.344	0.370	0.025	0.07	3.91	3.62	-0.29	-0.07
EC334	0.45	8.1	18.2	0.408	0.427	0.019	0.05	5.59	5.17	-0.41	-0.07
EC338	0.45	15.0	33.7	0.484	0.566	0.082	0.17	5.19	4.78	-0.42	-0.08
Group Average	0.42	7.9	18.6	0.407	0.439	0.031	0.07	4.52	4.34	-0.18	-0.04
S. Dev.	0.07	4.4	9.1	0.050	0.075	0.030	0.06	0.94	0.85	0.29	0.06
Avg. Abs. Value						0.031	0.07			0.27	0.06
S. Dev.						0.030	0.06			0.17	0.03

Table A-18 (continued) - 3

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO				Half-Life PROPENE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
5. UNC CHAMBER - OLEFIN/AROMATIC												
JN1379B	0.44	6.1	13.7	0.756	0.720	-0.036	-0.05		2.44	2.95	0.50	0.21
Group Average	0.44	6.1	13.7	0.756	0.720	-0.036	-0.05		2.44	2.95	0.50	0.21
S. Dev.												
Avg. Abs. Value						0.036	0.05				0.50	0.21
S. Dev.												
6. SAPRC EC - ALKANE/AROMATIC												
EC328	0.45	12.1	27.1	0.523	0.591	0.069	0.13		3.50	3.37	-0.13	-0.04
Group Average	0.45	12.1	27.1	0.523	0.591	0.069	0.13		3.50	3.37	-0.13	-0.04
S. Dev.												
Avg. Abs. Value						0.069	0.13				0.13	0.04
S. Dev.												

Table A-18 (continued) - 4

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO				Half-Life PROPENE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. SAPRC EC - ALKANE/OLEFIN												
EC106	0.162	0.162	0.000	0.00	0.207	0.187	-0.021	-0.10	134	136	2	0.01
EC113	0.060	0.080	0.020	0.33		0.202			82	80	-2	-0.02
EC114	0.231	0.197	-0.034	-0.15	0.433	0.350	-0.083	-0.19	112	153	41	0.37
EC115	0.134	0.135	0.001	0.01	0.201	0.150	-0.051	-0.25	130	154	24	0.18
EC116	0.186	0.206	0.020	0.11	0.463	0.403	-0.060	-0.13	90	96	6	0.07
Group Average	0.155	0.156	0.001	0.06	0.326	0.259	-0.054	-0.17	109	123	14	0.12
S. Dev.	0.064	0.051	0.022	0.18	0.141	0.111	0.026	0.07	23	33	17	0.16
Avg. Abs. Value			0.015	0.12			0.054	0.17			15	0.13
S. Dev.			0.014	0.13			0.026	0.07			17	0.15
2. UNC CHAMBER - ALKANE/OLEFIN												
JL1581R	0.097	0.052	-0.046	-0.47	0.157	0.088	-0.069	-0.44	248	282	34	0.14
JL1881R	0.046	0.052	0.006	0.14	0.080	0.076	-0.004	-0.05	258	264	6	0.02
ST2481R		0.049			0.224	0.066	-0.158	-0.71	312	247	-65	-0.21
AU2781R		0.046			0.164	0.087	-0.078	-0.47	250	243	-7	-0.03
OC0382R	0.008	0.038	0.030	3.90		0.127				259		
OC0382B	0.004	0.018	0.015	4.04		0.081				248		
NV1582R	0.004	0.013	0.009	1.99	0.090	0.065	-0.025	-0.28	435	256	-179	-0.41
Group Average	0.032	0.038	0.003	1.92	0.143	0.084	-0.067	-0.39	300	257	-42	-0.10
S. Dev.	0.041	0.016	0.029	2.08	0.059	0.021	0.060	0.24	79	13	84	0.22
Avg. Abs. Value			0.021	2.11			0.067	0.39			58	0.16
S. Dev.			0.017	1.84			0.060	0.24			71	0.16

Table A-18 (continued) - 5

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO				Half-Life PROPENE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
3. UNC CHAMBER - UNCMIX												
JL2281R	0.055	0.041	-0.014	-0.25	0.174	0.079	-0.095	-0.55				
JL2181B	0.013	0.010	-0.003	-0.20		0.043						
NV1582B	0.008	0.039	0.031	3.66	0.150	0.081	-0.069	-0.46				
DE0782B	0.009	0.045	0.036	4.18	0.100	0.111	0.011	0.11				
Group Average	0.021	0.034	0.013	1.85	0.141	0.079	-0.051	-0.30				
S. Dev.	0.023	0.016	0.025	2.40	0.038	0.028	0.055	0.36				
Avg. Abs. Value			0.021	2.07			0.058	0.37				
S. Dev.			0.015	2.14			0.043	0.23				
4. SAPRC EC - OLEFIN/AROMATIC												
EC335	0.115	0.123	0.008	0.07	0.117	0.107	-0.010	-0.09				
EC329	0.067	0.071	0.004	0.06	0.088	0.072	-0.016	-0.18	73	91	18	0.25
EC330	0.058	0.062	0.004	0.07	0.098	0.074	-0.025	-0.25	59	78	19	0.32
EC334	0.071	0.083	0.012	0.17	0.113	0.099	-0.014	-0.12	63	83	20	0.32
EC338	0.076	0.087	0.011	0.15	0.091	0.052	-0.039	-0.43				
Group Average	0.077	0.085	0.008	0.10	0.101	0.081	-0.021	-0.21	65	84	19	0.30
S. Dev.	0.022	0.023	0.004	0.05	0.013	0.022	0.012	0.14	7	6	1	0.04
Avg. Abs. Value			0.008	0.10			0.021	0.21			19	0.30
S. Dev.			0.004	0.05			0.012	0.14			1	0.04

Table A-18 (continued) - 6

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO				Half-Life PROPENE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
5. UNC CHAMBER - OLEFIN/AROMATIC												
JN1379B	0.181	0.214	0.033	0.18	0.340	0.381	0.041	0.12	249	208	-41	-0.16
Group Average	0.181	0.214	0.033	0.18	0.340	0.381	0.041	0.12	249	208	-41	-0.16
S. Dev.												
Avg. Abs. Value			0.033	0.18			0.041	0.12			41	0.16
S. Dev.												
6. SAPRC EC - ALKARO												
EC328	0.074	0.078	0.004	0.06	0.088	0.034	-0.054	-0.61				
Group Average	0.074	0.078	0.004	0.06	0.088	0.034	-0.054	-0.61				
S. Dev.												
Avg. Abs. Value			0.004	0.06			0.054	0.61				
S. Dev.												

Table A-19. Minimum Surrogate Mixtures

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRAC ITC - MINI SURROGATE											
ITC479	0.09	4.0	43.4	0.332	0.379	0.047	0.14	2.95	4.63	1.69	0.57
ITC584	0.10	4.0	40.7	0.375	0.369	-0.006	-0.02	3.05	3.79	0.74	0.24
ITC579	0.10	3.4	34.7	0.356	0.352	-0.004	-0.01	1.54	2.32	0.79	0.51
ITC472	0.10	3.6	35.1	0.258	0.388	0.130	0.50	1.72	3.07	1.35	0.79
ITC474	0.09	4.2	45.1	0.293	0.381	0.087	0.30	3.40	5.73	2.34	0.69
ITC581	0.09	4.3	50.0	0.352	0.352	0.000	0.00	3.74	4.99	1.26	0.34
ITC585	0.10	4.8	50.8	0.311	0.334	0.023	0.08	5.11	6.62	1.51	0.30
ITC478	0.10	5.0	52.6	0.320	0.355	0.035	0.11	4.73	7.79	3.07	0.65
ITC482	0.10	1.2	12.3	0.279	0.345	0.066	0.24	2.44	4.31	1.87	0.76
ITC488	0.09	6.0	66.2	0.293	0.390	0.097	0.33	3.06	4.89	1.82	0.60
ITC492	0.09	8.1	88.4	0.326	0.416	0.090	0.28	3.28	5.01	1.73	0.53
ITC494	0.09	8.5	92.5	0.321	0.423	0.102	0.32	3.30	4.94	1.64	0.50
ITC498	0.10	3.9	40.2	0.320	0.391	0.070	0.22	2.16	3.47	1.31	0.61
ITC500	0.10	4.1	42.7	0.286	0.377	0.091	0.32	5.18	7.25	2.06	0.40
ITC502	0.09	4.6	49.5	0.271	0.356	0.086	0.32	7.07	12.56	5.48	0.78
ITC462	0.11	7.5	71.3	0.099	0.204	0.105	1.07	0.70	0.69	-0.01	-0.01
ITC466	0.10	6.5	62.7	0.131	0.229	0.098	0.75	0.77	0.95	0.18	0.24
ITC468	0.09	4.6	49.0	0.176	0.284	0.109	0.62	1.19	1.94	0.75	0.63
ITC451	0.10	5.2	52.0	0.312	0.338	0.026	0.08	3.95	5.49	1.54	0.39
ITC455	0.09	4.4	47.8	0.304	0.350	0.046	0.15	3.52	4.90	1.38	0.39
ITC977	0.13	3.2	25.1	0.329	0.381	0.051	0.16	3.94	3.41	-0.52	-0.13
ITC985	0.12	2.7	22.9	0.336	0.352	0.016	0.05	3.95	3.27	-0.68	-0.17
ITC997	0.12	2.7	23.0	0.316	0.346	0.030	0.10	3.89	3.22	-0.67	-0.17
ITC979	0.12	2.9	23.1	0.404	0.474	0.070	0.17	4.88	4.06	-0.82	-0.17
ITC992	0.12	2.6	20.9	0.384	0.452	0.068	0.18	5.57	4.51	-1.06	-0.19
Group Average	0.10	4.5	45.7	0.299	0.361	0.061	0.26	3.40	4.55	1.15	0.36
S. Dev.	0.01	1.8	19.9	0.072	0.058	0.039	0.25	1.55	2.40	1.41	0.33
Avg. Abs. Value						0.062	0.26			1.45	0.43
S. Dev.						0.037	0.25			1.09	0.23

Table A-19 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
2. UNC CHAMBER - PROPENE, BUTANE, AROMATIC SURROGATE											
JL1581B	0.28	2.3	8.0	0.474	0.456	-0.018	-0.04	1.10	0.95	-0.15	-0.14
ST2481B	0.23	1.9	8.1	0.246	0.354	0.108	0.44	0.71	0.87	0.16	0.22
JN0982B	0.28	3.1	11.0	0.667	0.512	-0.155	-0.23	1.37	1.20	-0.16	-0.12
JN1483R	0.22	2.6	11.6	0.585	0.558	-0.027	-0.05	1.10	1.15	0.05	0.04
JN2783B	0.26	2.9	11.1	0.511	0.567	0.056	0.11	1.01	1.10	0.09	0.08
AU1883B	0.28	0.6	2.0	0.556	0.454	-0.102	-0.18	0.70	0.61	-0.09	-0.13
AU2683R	0.32	2.6	8.1	0.646	0.550	-0.096	-0.15	1.24	1.12	-0.12	-0.10
JL1881B	0.27	2.3	8.5	0.693	0.590	-0.103	-0.15	1.91	1.71	-0.21	-0.11
JN0982R	0.29	3.1	10.7	0.714	0.593	-0.121	-0.17	1.77	1.57	-0.20	-0.11
Group Average	0.27	2.4	8.8	0.566	0.515	-0.051	-0.05	1.21	1.14	-0.07	-0.04
S. Dev.	0.03	0.8	2.9	0.145	0.079	0.088	0.21	0.42	0.34	0.13	0.13
Avg. Abs. Value						0.087	0.17			0.14	0.12
S. Dev.						0.045	0.12			0.05	0.05

Table A-19 (continued) - 3

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO				Half-Life PROPENE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. SAPRC ITC - MINI SUSURROGATE												
ITC479	0.050	0.043	-0.007	-0.13		0.059			84	83	-1	-0.01
ITC584	0.080	0.045	-0.035	-0.43		0.052			98	95	-3	-0.03
ITC579	0.058	0.036	-0.022	-0.38		0.007						
ITC472	0.044	0.038	-0.006	-0.14		0.008						
ITC474	0.051	0.048	-0.003	-0.06		0.094			90	82	-8	-0.09
ITC581	0.090	0.047	-0.043	-0.48		0.089			94	90	-4	-0.04
ITC585	0.066	0.053	-0.013	-0.20		0.140			91	89	-2	-0.02
ITC478	0.056	0.054	-0.002	-0.04		0.160			80	81	1	0.01
ITC482	0.052	0.048	-0.004	-0.08		0.065			80	74	-6	-0.08
ITC488	0.051	0.041	-0.010	-0.19		0.056			90	88	-2	-0.02
ITC492	0.054	0.041	-0.013	-0.23		0.055			89	93	4	0.04
ITC494	0.053	0.042	-0.011	-0.21		0.054			92	95	3	0.03
ITC498	0.048	0.043	-0.005	-0.11		0.048			101	95	-6	-0.06
ITC500	0.060	0.051	-0.009	-0.15		0.072			62	73	11	0.18
ITC502	0.066	0.057	-0.009	-0.14		0.089			64	74	10	0.16
ITC462	0.004	0.014	0.010	2.43		0.007			329	278	-51	-0.16
ITC466	0.007	0.018	0.011	1.57		0.008			280	234	-46	-0.16
ITC468	0.021	0.027	0.006	0.31		0.026			160	142	-18	-0.11
ITC451	0.048	0.040	-0.008	-0.17		0.064			70	77	7	0.10
ITC455	0.050	0.039	-0.011	-0.22		0.060			79	79	0	0.00
ITC977	0.035	0.050	0.015	0.42		0.047			80	96	16	0.20
ITC985	0.036	0.042	0.006	0.16		0.044			75	90	15	0.20
ITC997	0.038	0.042	0.003	0.08		0.042			68	91	23	0.34
ITC979	0.027	0.053	0.026	0.95		0.038			89	106	17	0.19
ITC992	0.041	0.046	0.005	0.13		0.032			75	107	32	0.43
Group Average	0.047	0.042	-0.005	0.11					105	104	0	0.05
S. Dev.	0.019	0.010	0.015	0.65					66	50	18	0.15
Avg. Abs. Value			0.012	0.38							12	0.12
S. Dev.			0.010	0.54							13	0.11

Table A-19 (continued) - 4

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO				Half-Life PROPENE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
2. UNC CHAMBER - PROPENE, BUTANE, AROMATIC SURROGATE												
JL1581B	0.079	0.043	-0.035	-0.45	0.166	0.070	-0.096	-0.58	243	283	40	0.16
ST2481B		0.046			0.190	0.050	-0.141	-0.74	278	236	-42	-0.15
JN0982B		0.083				0.081			295	262	-33	-0.11
JN1483R	0.063	0.057	-0.006	-0.09	0.054	0.066	0.012	0.23	281	247	-34	-0.12
JN2783B	0.065	0.053	-0.012	-0.19	0.105	0.073	-0.032	-0.31	295	262	-33	-0.11
AU1883B	0.055	0.032	-0.022	-0.41	0.120	0.058	-0.062	-0.52	285	302	17	0.06
AU2683R		0.057			0.141	0.073	-0.068	-0.48	209	266	57	0.27
JL1881B	0.061	0.092	0.031	0.51	0.150	0.078	-0.072	-0.48	196	194	-2	-0.01
JN0982R		0.131				0.094			245	228	-17	-0.07
Group Average	0.064	0.066	-0.009	-0.13	0.132	0.071	-0.066	-0.41	258	253	-5	-0.01
S. Dev.	0.009	0.031	0.025	0.38	0.045	0.013	0.048	0.31	37	31	35	0.15
Avg. Abs. Value			0.021	0.33			0.069	0.48			30	0.12
S. Dev.			0.012	0.18			0.042	0.17			16	0.07

Table A-20. Full Surrogate Mixtures

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC EC - 7 HYDROCARBON SURROGATE											
EC231	0.49	13.2	26.9	0.620	0.795	0.174	0.28	6.99	8.73	1.74	0.25
EC232	0.49	9.3	18.9	0.342	0.525	0.183	0.54	3.12	3.33	0.21	0.07
EC233	0.10	9.5	92.5	0.330	0.455	0.126	0.38	4.07	5.11	1.04	0.26
EC237	0.48	10.5	21.6	0.652	0.732	0.080	0.12	7.36	6.78	-0.58	-0.08
EC238	0.95	10.1	10.6	0.691	0.827	0.136	0.20	5.10	5.68	0.58	0.11
EC241	0.49	5.0	10.2	0.408	0.471	0.063	0.15	2.87	3.29	0.42	0.15
EC242	0.50	12.9	25.6	0.682	0.707	0.026	0.04	17.53	18.91	1.38	0.08
EC243	0.50	9.7	19.5	0.716	0.745	0.029	0.04	14.50	14.22	-0.28	-0.02
EC245	1.00	12.9	12.9	0.894	0.924	0.030	0.03	13.41	15.00	1.58	0.12
EC246	0.51	8.6	17.0	0.574	0.606	0.031	0.05	2.65	2.47	-0.18	-0.07
EC247	0.51	6.2	12.2	0.657	0.674	0.017	0.03	7.49	7.14	-0.35	-0.05
Group Average	0.55	9.8	24.4	0.597	0.678	0.081	0.17	7.74	8.24	0.51	0.07
S. Dev.	0.24	2.6	23.3	0.173	0.150	0.063	0.17	5.16	5.45	0.83	0.12
Avg. Abs. Value						0.081	0.17			0.76	0.11
S. Dev.						0.063	0.17			0.58	0.08

Table A-20 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
2. SAPRC ITC - SAI SURROGATE											
ITC626	0.30	4.0	13.4	0.618	0.659	0.041	0.07	2.18	2.65	0.47	0.22
ITC630	0.31	1.9	6.3	0.284	0.277	-0.006	-0.02	0.86	1.10	0.24	0.28
ITC631	0.32	1.0	3.2	0.043	0.049	0.006		0.47	0.55	0.09	0.18
ITC633	0.64	4.0	6.2	0.231	0.279	0.048	0.21	1.26	1.77	0.51	0.40
ITC635	1.21	4.0	3.3	0.006	0.016	0.010		0.95	1.25	0.29	0.31
ITC637	0.31	4.0	12.8	0.617	0.657	0.040	0.06	2.31	2.62	0.31	0.13
ITC865	0.28	8.4	29.9	0.632	0.616	-0.016	-0.03	2.60	4.19	1.60	0.61
ITC867	0.28	4.8	17.2	0.631	0.636	0.005	0.01	2.23	4.02	1.80	0.81
ITC868	0.37	2.9	7.8	0.518	0.462	-0.056	-0.11	2.10	1.61	-0.49	-0.23
ITC871	0.37	1.7	4.6	0.376	0.256	-0.120	-0.32	1.18	1.19	0.01	0.01
ITC872	0.38	2.1	5.7	0.213	0.206	-0.006	-0.03	1.20	1.39	0.20	0.16
ITC873	0.39	1.3	3.4	0.160	0.094	-0.065	-0.41	0.85	0.82	-0.03	-0.03
ITC874	0.38	2.1	5.7	0.191	0.141	-0.050	-0.26	0.83	0.91	0.08	0.10
ITC877	0.38	2.3	6.2	0.250	0.217	-0.034	-0.13	1.14	1.38	0.24	0.21
ITC880	0.73	2.2	3.0	0.031	0.033	0.002		0.85	1.07	0.22	0.25
ITC881	0.73	2.3	3.1	0.012	0.022	0.010		1.03	1.11	0.08	0.08
ITC885	0.64	1.5	2.4	0.012	0.020	0.008		0.44	0.82	0.39	0.89
ITC886	0.73	2.3	3.1	0.012	0.017	0.005		1.24	0.73	-0.51	-0.41
ITC888	0.33	4.7	14.5	0.579	0.604	0.024	0.04	1.65	2.20	0.55	0.33
ITC891	0.32	4.4	13.7	0.602	0.614	0.012	0.02	2.67	3.45	0.77	0.29
Group Average	0.47	3.1	8.3	0.301	0.294	-0.007	-0.06	1.40	1.74	0.34	0.23
S. Dev.	0.24	1.7	6.8	0.248	0.254	0.041	0.17	0.70	1.10	0.56	0.30
Avg. Abs. Value						0.028	0.12			0.44	0.30
S. Dev.						0.029	0.13			0.47	0.24

Table A-20 (continued) - 3

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
3. SAPRC OTC - SAI SURROGATE											
OTC189A	0.45	3.3	7.4	0.576	0.750	0.175	0.30	3.79	3.94	0.15	0.04
OTC189B	0.45	4.0	8.9	0.712	0.832	0.119	0.17	3.70	4.00	0.30	0.08
OTC190A	0.41	3.8	9.2	0.702	0.828	0.125	0.18	4.24	3.56	-0.68	-0.16
OTC190B	0.42	3.8	9.0	0.669	0.780	0.111	0.17	3.73	3.12	-0.61	-0.16
OTC192A	0.47	4.2	8.9	0.735	0.849	0.114	0.16	4.25	3.69	-0.57	-0.13
OTC192B	0.47	4.2	8.9	0.754	0.730	-0.024	-0.03	3.84	2.98	-0.87	-0.23
OTC194A	0.38	7.4	19.3	0.737	1.048	0.311	0.42	7.85	9.47	1.61	0.21
OTC194B	0.38	3.7	9.7	0.603	0.705	0.102	0.17	2.95	3.31	0.36	0.12
OTC195A	0.41	1.8	4.5	0.164	0.108	-0.056	-0.34	2.05	1.27	-0.78	-0.38
OTC195B	0.41	4.1	9.9	0.681	0.779	0.098	0.14	4.14	4.20	0.07	0.02
OTC196B	0.41	3.7	9.1	0.597	0.754	0.157	0.26	3.86	3.58	-0.28	-0.07
OTC197A	0.38	3.6	9.5	0.621	0.554	-0.067	-0.11	4.12	2.84	-1.27	-0.31
OTC197B	0.77	3.1	4.1	0.152	0.089	-0.062	-0.41	2.86	2.21	-0.65	-0.23
OTC198A	0.84	5.4	6.4	0.704	0.592	-0.112	-0.16	6.09	4.60	-1.49	-0.25
OTC198B	0.40	3.7	9.4	0.674	0.628	-0.046	-0.07	3.86	2.73	-1.13	-0.29
OTC199A	0.36	3.5	9.6	0.591	0.649	0.058	0.10	3.86	3.28	-0.58	-0.15
OTC199B	0.37	3.5	9.6	0.606	0.633	0.027	0.04	3.40	3.14	-0.25	-0.07
OTC202A	0.73	6.0	8.2	0.714	0.497	-0.217	-0.30	6.95	22.96	16.00	2.30
OTC202B	0.40	2.6	6.7	0.522	0.412	-0.110	-0.21	3.82	3.36	-0.46	-0.12
OTC203A	0.39	3.5	9.0	0.231	0.273	0.042	0.18	2.34	2.62	0.28	0.12
OTC203B	0.19	3.5	18.5	0.394	0.508	0.114	0.29	2.20	2.95	0.75	0.34
OTC204A	0.35	3.6	10.2	0.302	0.382	0.079	0.26	3.27	4.21	0.94	0.29
OTC204B	0.17	3.5	20.3	0.381	0.534	0.153	0.40	2.62	3.25	0.63	0.24
OTC205A	0.84	3.8	4.5	0.039	0.060	0.020		4.85	2.31	-2.55	-0.52
OTC205B	0.14	3.6	26.5	0.392	0.612	0.220	0.56	4.49	4.17	-0.32	-0.07
OTC215A	0.45	3.5	7.8	0.830	0.906	0.075	0.09	4.33	3.92	-0.41	-0.09

Table A-20 (continued) - 4

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
OTC215B	0.44	4.1	9.3	0.868	1.009	0.141	0.16	5.33	5.99	0.66	0.12
OTC217A	0.50	4.9	9.6	0.483	0.583	0.100	0.21	2.55	2.76	0.20	0.08
OTC217B	0.51	4.6	9.0	0.831	0.981	0.149	0.18	4.64	4.66	0.02	0.00
OTC221A	0.41	2.4	5.8	0.235	0.254	0.019	0.08	1.63	1.51	-0.11	-0.07
OTC221B	0.42	2.0	4.7	0.333	0.332	-0.001	0.00	1.63	1.65	0.02	0.01
OTC222A	0.44	3.4	7.8	0.909	0.908	-0.001	0.00	3.83	3.81	-0.03	-0.01
OTC222B	0.43	2.6	6.0	0.940	1.087	0.147	0.16	5.55	6.38	0.82	0.15
OTC223A	0.36	4.8	13.4	0.953	0.910	-0.042	-0.04	4.55	4.40	-0.16	-0.03
OTC223B	0.40	3.5	8.8	0.771	0.704	-0.067	-0.09	3.15	2.94	-0.21	-0.07
OTC224A	0.34	4.4	12.7	0.776	0.812	0.036	0.05	3.67	3.15	-0.53	-0.14
OTC224B	0.34	4.3	12.6	0.813	0.914	0.101	0.12	4.94	4.96	0.02	0.00
OTC226A	0.45	2.5	5.5	0.751	0.488	-0.263	-0.35	3.12	2.35	-0.77	-0.25
OTC228A	0.41	2.4	6.0	0.246	0.385	0.139	0.56	1.49	2.04	0.55	0.37
OTC228B	0.41	2.3	5.6	0.296	0.397	0.101	0.34	1.79	2.66	0.87	0.49
OTC229A	0.46	3.0	6.6	0.253	0.430	0.177	0.70	1.56	2.13	0.57	0.36
OTC229B	0.46	1.7	3.8	0.168	0.360	0.192	1.14	1.38	1.98	0.61	0.44
OTC230A	0.41	3.1	7.6	0.489	0.844	0.355	0.73	2.43	3.31	0.88	0.36
OTC230B	0.41	1.7	4.2	0.271	0.514	0.243	0.90	1.66	2.33	0.68	0.41
OTC237A	0.52	4.3	8.2	0.807	0.832	0.025	0.03	4.10	3.71	-0.39	-0.09
OTC237B	0.52	4.4	8.5	0.757	0.682	-0.075	-0.10	3.48	3.16	-0.32	-0.09
OTC238A	0.50	2.9	5.8	0.406	0.377	-0.029	-0.07	2.58	2.36	-0.22	-0.09
OTC238B	0.50	3.9	7.8	0.702	0.685	-0.017	-0.02	4.06	3.75	-0.31	-0.08
OTC239A	0.49	2.7	5.4	0.343	0.341	-0.002	-0.01	2.66	2.57	-0.09	-0.03
OTC239B	0.50	2.5	5.0	0.234	0.149	-0.085	-0.36	1.85	1.55	-0.29	-0.16
OTC240A	0.50	1.8	3.6	0.034	0.034	0.000		1.08	0.97	-0.11	-0.11
OTC240B	0.50	2.0	4.1	0.217	0.103	-0.114	-0.52	1.79	1.44	-0.35	-0.20
OTC241A	0.32	4.7	14.8	0.671	0.745	0.074	0.11	3.26	3.22	-0.04	-0.01
OTC241B	0.31	4.0	12.9	0.674	0.706	0.032	0.05	3.30	3.46	0.16	0.05
OTC242A	0.45	2.6	5.8	0.182	0.135	-0.047	-0.26	1.47	1.40	-0.07	-0.05

Table A-20 (continued) - 5

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
OTC242B	0.46	2.1	4.7	0.639	0.590	-0.049	-0.08	3.04	2.80	-0.23	-0.08
OTC243A	0.47	4.7	10.0	0.142	0.210	0.068	0.48	1.41	2.07	0.66	0.47
OTC243B	0.38	3.7	9.7	0.152	0.167	0.015	0.10	1.40	2.29	0.89	0.63
OTC248A	0.48	3.7	7.7	0.056	0.065	0.009	0.16	1.40	1.36	-0.05	-0.03
OTC248B	0.46	2.9	6.3	0.081	0.084	0.003	0.04	1.61	1.79	0.18	0.11
OTC249A	0.48	5.6	11.8	0.348	0.335	-0.013	-0.04	2.55	2.57	0.02	0.01
OTC249B	0.46	4.9	10.7	0.325	0.359	0.034	0.11	2.83	3.19	0.36	0.13
Group Average	0.44	3.6	8.8	0.504	0.548	0.045	0.11	3.26	3.46	0.19	0.05
S. Dev.	0.12	1.1	4.2	0.263	0.287	0.113	0.31	1.42	2.86	2.15	0.37
Avg. Abs. Value						0.093	0.23			0.75	0.21
S. Dev.						0.078	0.23			2.02	0.31
4. UNC CHAMBER - UNC MIXTURES											
ST2081R	0.23	2.3	10.0	0.403	0.529	0.125	0.31	0.95	1.23	0.28	0.29
DE0782R	0.19	3.4	18.3	0.076	0.425	0.349	4.57	0.52	1.22	0.70	1.34
AU2681R	0.24	2.0	8.4	0.506	0.574	0.068	0.13	1.18	1.28	0.10	0.08
AU2681B	0.24	2.0	8.5	0.544	0.518	-0.026	-0.05	1.22	1.24	0.01	0.01
AU2781B	0.23	2.0	8.8	0.623	0.543	-0.080	-0.13	1.27	1.26	-0.01	-0.01
ST0381R	0.24	1.8	7.6	0.541	0.503	-0.038	-0.07	1.48	1.31	-0.17	-0.11
ST1081R	0.25	2.8	11.3	0.610	0.671	0.061	0.10	1.59	1.80	0.21	0.13
ST2081B	0.23	2.1	9.2	0.414	0.485	0.071	0.17	1.06	1.14	0.08	0.08
JL2081B	0.42	1.8	4.3	0.165	0.133	-0.031	-0.19	0.82	0.88	0.06	0.08
ST1682R	0.43	3.2	7.5	0.410	0.407	-0.002	0.00	1.28	1.18	-0.10	-0.08
JL2081R	0.41	2.7	6.6	0.635	0.320	-0.315	-0.50	1.55	1.10	-0.45	-0.29
JL2281B	0.26	2.9	11.2	0.722	0.596	-0.125	-0.17	1.80	1.80	-0.01	0.00
OC1481R	0.28	3.3	11.9	0.462	0.608	0.147	0.32	1.53	1.68	0.15	0.10
ST1682B	0.43	3.1	7.2	0.840	0.781	-0.059	-0.07	2.39	2.05	-0.34	-0.14
ST2981R	0.24	2.5	10.3	0.294	0.511	0.217	0.74	0.76	1.03	0.27	0.36

Table A-20 (continued) - 6

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
ST2981B	0.24	2.5	10.4	0.485	0.550	0.066	0.14	1.35	1.39	0.04	0.03
OC1481B	0.29	2.9	9.9	0.458	0.600	0.142	0.31	1.48	1.78	0.30	0.20
ST0381B	0.23	2.0	8.6	0.611	0.548	-0.063	-0.10	1.70	1.77	0.07	0.04
ST1081B	0.24	1.0	4.1	0.626	0.536	-0.090	-0.14	1.36	1.18	-0.17	-0.13
JL0882R	0.29	2.1	7.3	0.598	0.668	0.070	0.12	1.25	1.41	0.16	0.13
JL0882B	0.28	2.1	7.4	0.541	0.657	0.116	0.21	1.12	1.43	0.31	0.28
Group Average	0.28	2.4	9.0	0.503	0.532	0.029	0.27	1.32	1.39	0.07	0.11
S. Dev.	0.08	0.6	3.0	0.175	0.135	0.139	1.02	0.40	0.31	0.25	0.32
Avg. Abs. Value						0.108	0.41			0.19	0.19
S. Dev.						0.089	0.97			0.17	0.28

Table A-20 (continued) - 7

Experiment	Half-Life PROPENE				Half-Life M-XYL			
	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
F. SAPRC EC - 7 HYDROCARBON SURROGATE								
EC231	99	99	0	0.00	136	149	13	0.10
EC232	163	177	14	0.09	204	222	18	0.09
EC233	97	92	-5	-0.05	198	170	-28	-0.14
EC237	85	106	21	0.25	136	156	20	0.15
EC238	141	144	3	0.02	186	189	3	0.02
EC241	142	139	-3	-0.02	180	174	-6	-0.03
EC242	57	60	3	0.05	118	133	15	0.13
EC243	61	69	8	0.13	108	120	12	0.11
EC245	84	85	1	0.01	108	128	20	0.19
EC246	167	174	7	0.04	218	228	10	0.05
EC247	82	94	12	0.15	112	128	16	0.14
Group Average	107	112	5	0.06	154	163	8	0.07
S. Dev.	39	40	7	0.09	42	37	14	0.09
Avg. Abs. Value			7	0.07			14	0.10
S. Dev.			6	0.07			7	0.05

Table A-20 (continued) - 8

Experiment	Half-Life PROPENE				Half-Life M-XYL			
	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
2. SAPRC ITC - SAI SURROGATE								
ITC626	165	154	-11	-0.07	220	216	-4	-0.02
ITC630	230	235	5	0.02	312	309	-3	-0.01
ITC631	267	313	46	0.17	346	387	41	0.12
ITC633	272	282	10	0.04	363	398	35	0.10
ITC635	353	411	58	0.16	490	558	68	0.14
ITC637	151	157	6	0.04	202	219	17	0.08
ITC865	155	111	-44	-0.28	189	151	-38	-0.20
ITC867	133	97	-36	-0.27	181	129	-52	-0.29
ITC868	146	181	35	0.24	186	234	48	0.26
ITC871	224	200	-24	-0.11		244		
ITC872	180	166	-14	-0.08	233	199	-34	-0.15
ITC873	243	226	-17	-0.07	240	266	26	0.11
ITC874	255	219	-36	-0.14	349	259	-90	-0.26
ITC877	210	165	-45	-0.21	258	197	-61	-0.24
ITC880	347	284	-63	-0.18		340		
ITC881	288	244	-44	-0.15		287		
ITC885		282				327		
ITC886	332	312	-20	-0.06		366		
ITC888	193	152	-41	-0.21	262	198	-64	-0.24
ITC891	158	128	-30	-0.19	220	172	-48	-0.22
Group Average	226	215	-13	-0.07	270	272	-10	-0.05
S. Dev.	70	80	33	0.15	86	102	48	0.18
Avg. Abs. Value			30	0.14			41	0.16
S. Dev.			17	0.08			23	0.09

Table A-20 (continued) - 9

Experiment	Half-Life PROPENE				Half-Life M-XYL			
	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
3. SAPRC OTC - SAI SURROGATE								
OTC189A	120	127	7	0.06	151	157	6	0.04
OTC189B	128	126	-2	-0.02	150	153	3	0.02
OTC190A	95	124	29	0.31	132	153	21	0.16
OTC190B	108	137	29	0.27	130	169	39	0.30
OTC192A	101	125	24	0.24	139	158	19	0.14
OTC192B	115	146	31	0.27	151	185	34	0.23
OTC194A	75	73	-2	-0.03	137	102	-35	-0.26
OTC194B	134	127	-7	-0.05	164	160	-4	-0.02
OTC195A	135	176	41	0.30	171	227	56	0.33
OTC195B	93	109	16	0.17	111	136	25	0.23
OTC196B	107	129	22	0.21	146	153	7	0.05
OTC197A	104	134	30	0.29	133	174	41	0.31
OTC197B	109	208	99	0.91	205	260	55	0.27
OTC198A	99	138	39	0.39	140	191	51	0.36
OTC198B	95	124	29	0.31	120	169	49	0.41
OTC199A	108	133	25	0.23	128	166	38	0.30
OTC199B	120	137	17	0.14	145	171	26	0.18
OTC202A	66	99	33	0.50	88	156	68	0.77
OTC202B	182	132	-50	-0.27	154	163	9	0.06
OTC203A	169	189	20	0.12	235	262	27	0.11
OTC203B	153	126	-27	-0.18	181	169	-12	-0.07
OTC204A	86	116	30	0.35	159	179	20	0.13
OTC204B	116	109	-7	-0.06	154	139	-15	-0.10
OTC205A	170	214	44	0.26				
OTC205B	81	87	6	0.07	124	112	-12	-0.10
OTC215A	128	137	9	0.07	152	175	23	0.15

Table A-20 (continued) - 10

Experiment	Half-Life PROPENE				Half-Life M-XYL			
	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
OTC215B	89	91	2	0.02	133	120	-13	-0.10
OTC217A	154	163	9	0.06	188	196	8	0.04
OTC217B	112	126	14	0.12	149	157	8	0.05
OTC221A	188	209	21	0.11	226	239	13	0.06
OTC221B	264	227	-37	-0.14	288	264	-24	-0.08
OTC222A	138	112	-26	-0.19		130		
OTC222B	236	68	-168	-0.71		81		
OTC223A	129	121	-8	-0.06	168	148	-20	-0.12
OTC223B	151	145	-6	-0.04	255	173	-82	-0.32
OTC224A	137	132	-5	-0.04	120	158	38	0.32
OTC224B	99	105	6	0.06	141	131	-10	-0.07
OTC226A	152	166	14	0.09				
OTC228A	198	161	-37	-0.19	280	189	-91	-0.32
OTC228B	151	121	-30	-0.20	283	144	-139	-0.49
OTC229A	142	166	24	0.17		197		
OTC229B		169			276	201	-75	-0.27
OTC230A	162	129	-33	-0.20	187	153	-34	-0.18
OTC230B		149			243	175	-68	-0.28
OTC237A	135	148	13	0.10	156	182	26	0.17
OTC237B	148	158	10	0.07	168	192	24	0.14
OTC238A	160	180	20	0.12	206	223	17	0.08
OTC238B	117	124	7	0.06	172	158	-14	-0.08
OTC239A	136	149	13	0.10	138	180	42	0.30
OTC239B	189	218	29	0.15	273	260	-13	-0.05
OTC240A	232	241	9	0.04		289		
OTC240B	197	213	16	0.08	242	257	15	0.06
OTC241A	107	138	31	0.29	187	174	-13	-0.07
OTC241B	113	111	-2	-0.02	154	140	-14	-0.09
OTC242A	183	201	18	0.10	218	238	20	0.09

Table A-20 (continued) - 11

Experiment	Half-Life PROPENE				Half-Life M-XYL			
	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
OTC242B		156			177	186	9	0.05
OTC243A	230	256	26	0.11				
OTC243B	220	222	2	0.01		344		
OTC248A	313	288	-25	-0.08				
OTC248B	222	210	-12	-0.05		324		
OTC249A	162	189	27	0.17	186	268	82	0.44
OTC249B	155	148	-7	-0.05	209	200	-9	-0.04
Group Average	144	151	6	0.08	175	184	4	0.06
S. Dev.	49	44	33	0.22	49	52	41	0.23
Avg. Abs. Value			23	0.17			31	0.18
S. Dev.			24	0.16			27	0.15

Table A-20 (continued) - 12

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
1. SAPRC EC - 7 HYDROCARBON SURROGATE								
EC231	0.095	0.136	0.041	0.43	0.453	0.505	0.052	0.11
EC232	0.040	0.048	0.009	0.22	0.157	0.131	-0.026	-0.17
EC233	0.037	0.042	0.006	0.15	0.145	0.133	-0.012	-0.08
EC237	0.100	0.127	0.027	0.27	0.387	0.428	0.042	0.11
EC238	0.113	0.152	0.039	0.34	0.404	0.449	0.045	0.11
EC241	0.047	0.050	0.003	0.06	0.137	0.221	0.084	0.61
EC242	0.140	0.166	0.026	0.19	0.673	0.920	0.247	0.37
EC243	0.100	0.157	0.057	0.57	0.571	0.833	0.262	0.46
EC245	0.194	0.262	0.068	0.35	0.778	0.993	0.215	0.28
EC246	0.070	0.065	-0.005	-0.07	0.121	0.129	0.009	0.07
EC247	0.106	0.135	0.029	0.27	0.377	0.475	0.098	0.26
Group Average	0.095	0.122	0.027	0.25	0.382	0.474	0.092	0.19
S. Dev.	0.047	0.067	0.023	0.18	0.228	0.319	0.103	0.23
Avg. Abs. Value			0.028	0.27			0.099	0.24
S. Dev.			0.022	0.15			0.096	0.18

Table A-20 (continued) - 13

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
2. SAPRC ITC - SAI SURROGATE								
ITC626	0.116	0.068	-0.048	-0.42	0.045	0.134	0.089	1.97
ITC630	0.027	0.020	-0.007	-0.26	0.025	0.061	0.036	1.42
ITC631	0.002	0.001	-0.001	-0.45	0.069	0.031	-0.038	-0.56
ITC633	0.034	0.033	-0.001	-0.04	0.031	0.113	0.081	2.59
ITC635	0.001	0.001	0.000	0.25	0.092	0.098	0.006	0.06
ITC637	0.117	0.069	-0.048	-0.41	0.127	0.136	0.008	0.06
ITC865		0.062			0.208	0.169	-0.038	-0.19
ITC867		0.046			0.224	0.214	-0.009	-0.04
ITC868		0.038			0.107	0.090	-0.017	-0.16
ITC871		0.016			0.052	0.066	0.014	0.27
ITC872		0.008			0.111	0.105	-0.006	-0.05
ITC873		0.003			0.028	0.043	0.015	0.54
ITC874		0.005			0.079	0.053	-0.026	-0.33
ITC877		0.009			0.113	0.102	-0.011	-0.10
ITC880		0.001			0.014	0.058	0.044	3.15
ITC881		0.001			0.089	0.085	-0.004	-0.05
ITC885		0.000			0.014	0.037	0.023	1.65
ITC886		0.000			0.067	0.041	-0.026	-0.39
ITC888		0.043			0.154	0.126	-0.028	-0.18
ITC891		0.062			0.069	0.148	0.079	1.14
Group Average	0.049	0.024	-0.018	-0.22	0.086	0.095	0.009	0.54
S. Dev.	0.054	0.026	0.024	0.28	0.059	0.049	0.039	1.07
Avg. Abs. Value			0.018	0.31			0.030	0.75
S. Dev.			0.024	0.15			0.026	0.93

Table A-20 (continued) - 14

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
3. SAPRC OTC - SAI SURROGATE								
OTC189A	0.021	0.072	0.051	2.43	0.199	0.158	-0.041	-0.21
OTC189B	0.025	0.066	0.041	1.64	0.157	0.163	0.006	0.04
OTC190A	0.026	0.052	0.026	0.98	0.276	0.150	-0.126	-0.46
OTC190B	0.018	0.056	0.038	2.10	0.228	0.146	-0.082	-0.36
OTC192A	0.056	0.072	0.016	0.29	0.255	0.165	-0.090	-0.35
OTC192B	0.058	0.073	0.015	0.26	0.284	0.156	-0.128	-0.45
OTC194A	0.100	0.101	0.001	0.01	0.251	0.324	0.073	0.29
OTC194B	0.055	0.063	0.008	0.15	0.190	0.138	-0.052	-0.27
OTC195A	0.007	0.006	-0.001	-0.18	0.069	0.073	0.004	0.06
OTC195B	0.055	0.062	0.007	0.13	0.171	0.163	-0.009	-0.05
OTC196B	0.011	0.009	-0.002	-0.21	0.207	0.164	-0.043	-0.21
OTC197A	0.062	0.061	-0.001	-0.01	0.186	0.131	-0.055	-0.29
OTC197B	0.010	0.005	-0.005	-0.53	0.213	0.125	-0.088	-0.41
OTC198A	0.087	0.093	0.006	0.07	0.426	0.269	-0.157	-0.37
OTC198B	0.059	0.038	-0.021	-0.35	0.253	0.144	-0.109	-0.43
OTC199A	0.057	0.052	-0.005	-0.08	0.205	0.144	-0.061	-0.30
OTC199B	0.055	0.040	-0.015	-0.28	0.215	0.144	-0.072	-0.33
OTC202A	0.086	0.085	-0.001	-0.02	0.219	0.254	0.034	0.16
OTC202B	0.046	0.051	0.005	0.12	0.123	0.135	0.011	0.09
OTC203A	0.016	0.027	0.011	0.72	0.178	0.129	-0.048	-0.27
OTC203B	0.026	0.059	0.033	1.25	0.221	0.139	-0.083	-0.37
OTC204A	0.049	0.041	-0.008	-0.16	0.251	0.141	-0.110	-0.44
OTC204B	0.061	0.048	-0.013	-0.21	0.203	0.141	-0.062	-0.31
OTC205A	0.010	0.004	-0.006	-0.55	0.184	0.128	-0.056	-0.31
OTC205B	0.046	0.043	-0.003	-0.08	0.224	0.156	-0.067	-0.30
OTC215A	0.125	0.094	-0.031	-0.24	0.554	0.203	-0.351	-0.63

Table A-20 (continued) - 15

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
OTC215B	0.123	0.083	-0.040	-0.32	0.831	0.287	-0.544	-0.65
OTC217A	0.068	0.058	-0.010	-0.15	0.237	0.172	-0.065	-0.27
OTC217B	0.121	0.088	-0.033	-0.27	0.291	0.201	-0.090	-0.31
OTC221A	0.036	0.038	0.002	0.06	0.154	0.107	-0.048	-0.31
OTC221B	0.050	0.057	0.007	0.15	0.160	0.120	-0.040	-0.25
OTC222A	0.030	0.039	0.009	0.29	0.261	0.152	-0.109	-0.42
OTC222B	0.031	0.029	-0.002	-0.07	0.253	0.214	-0.039	-0.15
OTC223A	0.054	0.045	-0.009	-0.17	0.421	0.227	-0.195	-0.46
OTC223B	0.051	0.042	-0.009	-0.18	0.198	0.155	-0.043	-0.22
OTC224A	0.046	0.043	-0.003	-0.06	0.267	0.173	-0.094	-0.35
OTC224B	0.062	0.063	0.001	0.02	0.234	0.221	-0.013	-0.05
OTC226A	0.040	0.016	-0.024	-0.59	0.012	0.124	0.112	9.41
OTC228A	0.034	0.040	0.006	0.17	0.063	0.107	0.044	0.69
OTC228B	0.025	0.033	0.008	0.31	0.117	0.129	0.012	0.10
OTC229A	0.027	0.044	0.017	0.62	0.113	0.135	0.022	0.20
OTC229B	0.023	0.044	0.021	0.92	0.059	0.114	0.055	0.93
OTC230A	0.038	0.049	0.011	0.30	0.133	0.161	0.028	0.21
OTC230B	0.024	0.039	0.015	0.61	0.073	0.122	0.049	0.67
OTC237A	0.064	0.082	0.018	0.29	0.216	0.212	-0.004	-0.02
OTC237B	0.046	0.070	0.024	0.51	0.226	0.199	-0.027	-0.12
OTC238A	0.047	0.061	0.014	0.30	0.139	0.141	0.002	0.02
OTC238B	0.053	0.072	0.019	0.35	0.230	0.199	-0.030	-0.13
OTC239A	0.017	0.028	0.011	0.65	0.166	0.150	-0.016	-0.10
OTC239B	0.017	0.010	-0.007	-0.40	0.129	0.109	-0.019	-0.15
OTC240A	0.001	0.001	0.000	-0.39	0.075	0.065	-0.010	-0.14
OTC240B	0.008	0.004	-0.004	-0.56	0.077	0.087	0.010	0.12
OTC241A	0.064	0.069	0.005	0.08	0.218	0.177	-0.041	-0.19
OTC241B	0.047	0.054	0.007	0.16	0.226	0.184	-0.042	-0.19
OTC242A	0.020	0.017	-0.003	-0.16	0.123	0.088	-0.035	-0.28

Table A-20 (continued) - 16

Experiment	Maximum Concentration PAN				Maximum Concentration HCHO			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
OTC242B	0.038	0.053	0.015	0.40	0.129	0.155	0.026	0.20
OTC243A	0.021	0.040	0.019	0.92	0.152	0.171	0.019	0.13
OTC243B	0.022	0.026	0.004	0.17	0.178	0.162	-0.016	-0.09
OTC248A	0.012	0.008	-0.004	-0.32	0.133	0.102	-0.031	-0.23
OTC248B	0.013	0.009	-0.004	-0.31	0.166	0.126	-0.040	-0.24
OTC249A	0.065	0.065	0.000	0.00	0.240	0.199	-0.041	-0.17
OTC249B	0.045	0.051	0.006	0.12	0.265	0.225	-0.041	-0.15
Group Average	0.044	0.047	0.004	0.17	0.208	0.159	-0.049	0.01
S. Dev.	0.028	0.025	0.016	0.59	0.120	0.049	0.093	1.25
Avg. Abs. Value			0.012	0.39			0.066	0.42
S. Dev.			0.011	0.46			0.082	1.17
4. UNC CHAMBER - UNC MIXTURES								
ST2081R		0.063						
DE0782R	0.010	0.073	0.063	6.02				
AU2681R	0.020	0.020	0.000	0.01				
AU2681B	0.014	0.027	0.012	0.86				
AU2781B		0.026						
ST0381R		0.020						
ST1081R		0.056						
ST2081B		0.023						
JL2081B	0.004	0.004	-0.001	-0.12				
ST1682R	0.015	0.022	0.007	0.48				
JL2081R	0.037	0.016	-0.021	-0.56				
JL2281B	0.097	0.076	-0.021	-0.22				
OC1481R	0.137	0.100	-0.037	-0.27				

Table A-20 (continued) - 17

Experiment	Maximum Concentration PAN			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
ST1682B	0.047	0.075	0.027	0.58
ST2981R		0.062		
ST2981B		0.096		
OC1481B	0.117	0.115	-0.002	-0.02
ST0381B		0.096		
ST1081B		0.054		
JL0882R	0.085	0.054	-0.030	-0.36
JL0882B	0.072	0.053	-0.019	-0.26
Group Average	0.055	0.054	-0.002	0.51
S. Dev.	0.046	0.032	0.028	1.78
Avg. Abs. Value			0.020	0.81
S. Dev.			0.018	1.66

Table A-21. UNC Auto Exhaust Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. UNC CHAMBER - VOLARE											
JN2582R	0.65	0.6	0.9	0.003	0.012	0.009		0.64	0.67	0.03	0.05
JN2582B	0.65	0.6	0.9	0.003	0.013	0.009		0.68	0.68	0.00	0.01
JN2982R	0.24	2.5	10.3	0.704	0.782	0.077	0.11	2.32	2.64	0.32	0.14
JN2982B	0.25	2.5	9.8	0.766	0.787	0.021	0.03	2.67	2.70	0.03	0.01
JN3082R	0.32	2.8	8.7	0.811	0.851	0.040	0.05	2.55	3.58	1.04	0.41
JN3082B	0.32	0.6	1.7	0.840	0.866	0.026	0.03	2.68	3.49	0.81	0.30
JL0283B	0.19	1.7	9.1	0.697	0.786	0.089	0.13	1.65	1.98	0.33	0.20
JL0883B	0.37	1.7	4.6	0.879	0.822	-0.057	-0.07	1.76	1.54	-0.21	-0.12
ST2982B	0.39	1.7	4.3	0.205	0.118	-0.086	-0.42	1.12	0.95	-0.17	-0.15
OC0682R	0.46	2.0	4.3	0.355	0.282	-0.073	-0.21	1.37	1.33	-0.04	-0.03
AU1183R	0.22	2.2	9.9	0.850	0.830	-0.020	-0.02	2.55	2.50	-0.04	-0.02
AU1183B	0.23	0.7	3.1	0.601	0.581	-0.019	-0.03	1.26	1.21	-0.05	-0.04
Group Average	0.36	1.6	5.7	0.559	0.561	0.001	-0.04	1.77	1.94	0.17	0.06
S. Dev.	0.16	0.8	3.7	0.330	0.350	0.055	0.16	0.77	1.03	0.39	0.17
Avg. Abs. Value						0.044	0.11			0.26	0.12
S. Dev.						0.031	0.12			0.34	0.13

Table A-21 (continued) - 2

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
2. UNC CHAMBER - CHARGER											
JL0182R	0.37	3.5	9.6	0.740	0.975	0.235	0.32	2.31	3.21	0.90	0.39
JL0182B	0.35	3.6	10.2	0.759	0.927	0.168	0.22	2.41	3.43	1.02	0.43
AU0382R	0.44	2.5	5.7	0.344	0.411	0.066	0.19	1.26	1.40	0.15	0.12
AU0382B	0.16	1.2	7.3	0.576	0.501	-0.074	-0.13	1.06	0.94	-0.12	-0.12
ST1782R	0.26	2.2	8.6	0.562	0.629	0.067	0.12	1.63	1.36	-0.26	-0.16
ST1782B	0.25	2.4	9.5	0.637	0.653	0.016	0.03	1.72	1.47	-0.25	-0.15
ST2982R	0.39	1.7	4.4	0.073	0.100	0.027	0.37	0.86	0.88	0.02	0.02
OC0682B	0.46	2.0	4.3	0.450	0.327	-0.123	-0.27	1.49	1.40	-0.09	-0.06
JL0283R	0.18	1.6	9.0	0.595	0.653	0.058	0.10	1.37	1.53	0.15	0.11
JL0883R	0.37	1.7	4.6	0.756	0.650	-0.106	-0.14	1.52	1.39	-0.13	-0.09
JL1583R	0.35	2.2	6.2	0.866	0.719	-0.147	-0.17	2.10	1.86	-0.23	-0.11
JL1583B	0.35	2.3	6.6	0.922	0.836	-0.086	-0.09	2.20	2.21	0.01	0.00
OC0483R	0.25	2.6	10.3	0.603	0.710	0.107	0.18	1.76	2.01	0.24	0.14
Group Average	0.32	2.3	7.4	0.606	0.622	0.016	0.05	1.67	1.78	0.11	0.04
S. Dev.	0.09	0.7	2.2	0.226	0.242	0.118	0.20	0.48	0.78	0.41	0.19
Avg. Abs. Value						0.099	0.18			0.28	0.15
S. Dev.						0.060	0.10			0.32	0.13

Table A-21 (continued) - 3

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
3. UNC CHAMBER - SYNEXH											
OC0483B	0.25	0.4	1.7	0.642	0.746	0.104	0.16	1.86	2.21	0.35	0.19
OC0783R	0.33	2.7	8.1	0.178	0.498	0.319	1.79	0.94	1.44	0.50	0.54
OC0783B	0.34	2.7	7.9	0.451	0.688	0.237	0.53	1.41	2.24	0.82	0.58
Group Average	0.31	1.9	5.9	0.424	0.644	0.220	0.83	1.40	1.96	0.56	0.44
S. Dev.	0.05	1.3	3.6	0.233	0.130	0.108	0.85	0.46	0.45	0.24	0.21
Avg. Abs. Value						0.220	0.83			0.56	0.44
S. Dev.						0.108	0.85			0.24	0.21

Table A-21 (continued) - 4

Experiment	Maximum Concentration PAN				Half-Life ETHENE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
1. Runs IDs = UNC VOLARE								
JN2582R	0.004	0.001	-0.003	-0.80	692			
JN2582B	0.004	0.001	-0.003	-0.79				
JN2982R	0.065	0.053	-0.012	-0.18		320		
JN2982B	0.070	0.056	-0.014	-0.20		317		
JN3082R	0.068	0.096	0.028	0.42	325	293	-32	-0.10
JN3082B	0.068	0.094	0.025	0.37	339	296	-43	-0.13
JL0283B	0.043	0.033	-0.010	-0.24	345	318	-27	-0.08
JL0883B	0.081	0.031	-0.050	-0.62	433	429	-4	-0.01
ST2982B	0.014	0.005	-0.009	-0.63				
OC0682R	0.024	0.013	-0.011	-0.47		525		
AU1183R	0.032	0.037	0.005	0.17	326	314	-12	-0.04
AU1183B	0.010	0.009	-0.001	-0.08	346	373	27	0.08
Group Average	0.040	0.036	-0.004	-0.25	400	353	-15	-0.05
S. Dev.	0.029	0.034	0.020	0.42	133	77	24	0.07
Avg. Abs. Value			0.014	0.41			24	0.07
S. Dev.			0.014	0.25			14	0.04

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Table A-21 (continued) - 5

Experiment	Maximum Concentration PAN				Half-Life ETHENE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
2. Runs IDs = UNC CHARGR								
JL0182R	0.076	0.084	0.008	0.11	359	309	-50	-0.14
JL0182B	0.079	0.091	0.012	0.15	361	302	-59	-0.16
AU0382R	0.007	0.015	0.008	1.01	513	505	-8	-0.02
AU0382B	0.012	0.016	0.004	0.31	389	387	-2	-0.01
ST1782R	0.042	0.042	0.000	0.01	336	381	45	0.13
ST1782B	0.045	0.044	-0.001	-0.02	354	380	26	0.07
ST2982R	0.006	0.005	-0.001	-0.18	479			
OC0682B	0.026	0.015	-0.012	-0.45	479	506	27	0.06
JL0283R	0.041	0.029	-0.012	-0.29	337	310	-27	-0.08
JL0883R	0.092	0.032	-0.061	-0.66	515	421	-94	-0.18
JL1583R	0.068	0.036	-0.032	-0.47	363	339	-24	-0.07
JL1583B	0.063	0.047	-0.016	-0.26	376	325	-51	-0.14
OC0483R	0.061	0.052	-0.009	-0.15	373	298	-75	-0.20
Group Average	0.048	0.039	-0.009	-0.07	402	371	-24	-0.06
S. Dev.	0.029	0.026	0.020	0.42	67	73	43	0.11
Avg. Abs. Value			0.013	0.31			40	0.10
S. Dev.			0.016	0.28			26	0.06

Table A-21 (continued) - 6

Experiment	Maximum Concentration PAN				Half-Life ETHENE			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt (min)	Calc (min)	Calc -Expt (min)	Calc -Expt /Expt
3. Runs IDs = UNC SYNEXH								
OC0483B	0.060	0.058	-0.002	-0.03	335	293	-42	-0.13
OC0783R	0.056	0.065	0.010	0.17		406		
OC0783B	0.101	0.105	0.004	0.04	408	303	-105	-0.26
Group Average	0.072	0.076	0.004	0.06	371	334	-73	-0.19
S. Dev.	0.025	0.025	0.006	0.10	51	62	44	0.09
Avg. Abs. Value			0.005	0.08			73	0.19
S. Dev.			0.004	0.08			44	0.09

Table A-22. Synthetic Jet Fuel and Jet Exhaust Runs

Experiment	Initial Concentrations			Maximum Concentration OZONE				Average Initial d($[O_3]$ - [NO])/dt			
	NO_x (ppm)	HC (ppmC)	HC/NO_x	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt	Expt --	Calc (ppb/min)	Calc -Expt --	Calc -Expt /Expt
1. SAPRC ITC - SYNTHETIC JET FUEL											
ITC781	0.51	43.0	83.5	0.751	0.811	0.060	0.08	2.77	3.36	0.58	0.21
ITC784	0.50	88.0	177.6	0.746	0.896	0.151	0.20	3.93	4.09	0.16	0.04
ITC785	0.26	45.0	170.7	0.598	0.607	0.008	0.01	2.74	3.08	0.35	0.13
ITC805	0.52	98.0	189.5	0.791	0.929	0.139	0.18	3.27	3.96	0.69	0.21
ITC795	0.50	45.0	89.8	0.761	0.808	0.047	0.06	3.05	4.64	1.58	0.52
ITC796	0.54	97.0	178.9	0.597	0.847	0.250	0.42	4.43	5.37	0.94	0.21
ITC799	0.51	94.0	184.1	0.840	0.985	0.145	0.17	4.59	4.79	0.20	0.04
ITC801	0.55	41.0	75.1	0.881	0.971	0.090	0.10	2.98	3.72	0.74	0.25
Group Average	0.49	68.9	143.7	0.746	0.857	0.111	0.15	3.47	4.13	0.65	0.20
S. Dev.	0.09	27.3	50.8	0.102	0.122	0.076	0.12	0.74	0.77	0.46	0.15
Avg. Abs. Value						0.111	0.15			0.65	0.20
S. Dev.						0.076	0.12			0.46	0.15
2. SAPRC ITC - SYNTHETIC JET EXHAUST											
ITC963	0.49	4.4	9.1	0.822	0.769	-0.053	-0.06	4.00	3.89	-0.11	-0.03
ITC965	0.46	5.2	11.3	0.863	0.781	-0.082	-0.09	5.10	4.76	-0.34	-0.07
ITC967	0.26	4.4	17.2	0.586	0.618	0.032	0.05	5.79	5.03	-0.76	-0.13
ITC968	0.49	8.7	17.8	0.852	0.808	-0.044	-0.05	11.76	9.09	-2.67	-0.23
Group Average	0.42	5.7	13.8	0.781	0.744	-0.037	-0.04	6.66	5.69	-0.97	-0.11
S. Dev.	0.11	2.1	4.3	0.131	0.086	0.048	0.06	3.48	2.31	1.17	0.09
Avg. Abs. Value						0.053	0.07			0.97	0.11
S. Dev.						0.021	0.02			1.17	0.09

Table A-22 (continued) - 2

Experiment	Maximum Concentration PAN			
	Expt (ppm)	Calc (ppm)	Calc -Expt (ppm)	Calc -Expt /Expt
2. SAPRC ITC - SYNTHETIC JET EXHAUST				
ITC963	0.068	0.103	0.035	0.52
ITC965	0.076	0.112	0.036	0.47
ITC967	0.052	0.078	0.026	0.50
ITC968	0.123	0.142	0.019	0.16
Group Average	0.080	0.109	0.029	0.41
S. Dev.	0.031	0.027	0.008	0.17
Avg. Abs. Value			0.029	0.41
S. Dev.			0.008	0.17