Work Order No. 582-23-42327-033
Contract No. 582-19-90500
Tracking No. 2023-04
Task 6.2

Prepared for:

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June 29, 2023

Comparing Ozone Precursor Responses and Volatile Organic Compound (VOC) Reactivity of Carbon Bond Version 7 Revision 1 (CB7r1) to Other Mechanisms

Final Report

PREPARED UNDER A CONTRACT FROM THE
TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

The preparation of this document was financed through a contract from the State of Texas through the Texas Commission on Environmental Quality.
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CONTENTS

Table of Figures

Table of Tables

List of Acronyms and Abbreviations

BC	Boundary Conditions
CAMx	Comprehensive Air Quality Model with Extensions
CB	Carbon Bond mechanism
CB6r5	Carbon Bond mechanism Version 6 Revision 5
CB7r1	Carbon Bond mechanism Version 7 Revision 1
CMAQ	Community Multiscale Air Quality
CMC	Chemical Mechanism Compiler
DDM	Direct Decoupled Method
DFW	Dallas-Fort Worth
DV	Design Value
ELP	El Paso
EPA	Environmental Protection Agency
GEOS-Chem	Goddard Earth Observing System Chemistry
HGB	Houston-Galveston-Brazoria
HO_2	Hydroperoxy radical
IVOC	Intermediate Volatile Organic Compound
MDA1	Maximum Daily 1-hour Average
MDA8	Maximum Daily 8-hour Average
MIR	Maximum Incremental Reactivity
MPE	Model Performance Evaluation
NO	Nitric Oxide
NO_2	Nitrogen Dioxide
NOx	Nitrogen Oxides
O_3	Ozone
OH	Hydroxyl Radical
ON	Organic Nitrate
PANs	Peroxyacetyl Nitrate and higher order Peroxyacyl Nitrates
PBL	Planetary Boundary Layer
RACM2	Regional Atmospheric Chemistry Mechanism version 2
SAN	San Antonio
SAPRC07	Statewide Air Pollution Research Center 2007
SIP	State Implementation Plan
TCEQ	Texas Commission on Environmental Quality
TUV	Tropospheric Visible and Ultraviolet
TYL	Tyler
VOC	Volatile Organic Compound
WRF	Weather Research and Forecasting

Executive Summary

The Texas Commission on Environmental Quality (TCEQ) uses the Comprehensive Air Quality Model with Extensions (CAMx) to assess ozone formation for State Implementation Plan (SIP) purposes. The CAMx chemical mechanism is critical to developing ozone SIP strategies because it determines how ozone responds to precursor (i.e., NOx and VOC) emission changes. The TCEQ uses the Carbon Bond (CB) series of chemical mechanisms and an updated version, Carbon Bond mechanism version 7, revision 1 (CB7r1), was recently developed by Ramboll (Ramboll, 2022). Here, we evaluate CB7r1 against other widely used chemical mechanisms, including the Statewide Air Pollution Research Center 2007 (SAPRC07) mechanism (Carter, 2010a), the Regional Atmospheric Chemistry Mechanism version 2 (RACM2) (Goliff, 2013), and the Goddard Earth Observing System - Chem (GEOS-Chem) mechanism (Harvard University, 2022). CB7r1, SAPRC07, and RACM2 were previously implemented in CAMx and GEOS-Chem was implemented as part of this study. We compare both the response of ozone to precursor emissions and VOC reactivity for all four mechanisms.

For efficiency, CAMx was run as a box model (i.e., a 1-D CAMx simulation with emissions and meteorology that represent a limited area) for several Texas locations (Houston-Galveston-Brazoria (HGB), Dallas-Fort Worth (DFW), San Antonio (SAN), Tyler (TYL), and El Paso (ELP)). Base case simulation results reasonably capture observed MDA8 O_3 values and highlight the similarities and differences between mechanisms. While the mechanisms agree well for many chemical species, significant differences were observed for organic nitrates and peroxyacyl nitrates. For each mechanism and location, 100 CAMx box model simulations were performed by modulating anthropogenic NOx and VOC emissions. All the mechanisms showed a fairly similar O_3 response to varying emissions, with slight differences. RACM2 had a higher O_3 response, indicating that it forms O_3 more efficiently, whereas GEOS-Chem had a lower O_3 response and forms O_3 less efficiently.

VOC reactivity factors (i.e., Maximum Incremental Reactivity (MIR) values) for each mechanism and location were also computed using the Decoupled Direct Method (DDM) in the CAMx box models. MIR values characterize the O_3 forming potential of individual VOCs under atmospheric conditions where adding VOC emission yields the highest incremental increase in O_3 concentration (Carter and Atkinson, 1989). SAPRC07 MIR values have been evaluated against observations (Carter, 2010b) and are used as the standard reference for this analysis. CB7r1, RACM2, and GEOS-Chem agree well with SAPRC07, with correlation coefficients greater than 0.9. GEOS-Chem shows the highest correlation and RACM2 shows the lowest. The similarities in MIR values for most VOCs indicate that O_3 formation resulting from VOC chemistry will be comparable in all four mechanisms. A linear regression of VOC MIR values shows that the slope varies between mechanisms, due primarily to differences in MIR values for individual VOCs. In particular, high MIR values for xylenes, large aromatics, and propane in RACM2 cause a high linear regression slope and more O_3 production in the model. Low MIR values for xylenes, large aromatics, and larger alkanes in GEOS-Chem result in a low slope and less O_3 production.

1.0 Introduction

Tropospheric ozone is formed by the interaction of sunlight with volatile organic compounds (VOC) and nitrogen oxide (NOx). The TCEQ uses the Comprehensive Air Quality Model with Extensions (CAMx) to assess ozone formation for State Implementation Plan (SIP) purposes. The CAMx chemical mechanism is critical to developing ozone SIP strategies because it determines how ozone responds to precursor (i.e., NOx and VOC) emission changes. Ramboll recently developed the Carbon Bond mechanism version 7, revision 1 (CB7r1) and compared its ozone responses to CB6r5 finding that the two mechanisms are similar overall, although CB7r1 is slightly less responsive to NOx reduction than CB6r5 (Ramboll, 2022). The VOC reactivity (i.e., Maximum Incremental Reactivity (MIR) factors) of CB7r1 were not previously compared to CB6r5 or other mechanisms.

The purpose of this project was to further evaluate the CB7r1 chemical mechanism with focus on how ozone responds to precursor (i.e., NOx and VOC) emission changes in Texas, which is critical for the development of ozone State Implementation Plan (SIP) strategies. This project compared both ozone response to precursor emissions changes and VOC reactivity of CB7r1 to other widely used chemical mechanisms including the Statewide Air Pollution Research Center 2007 (SAPRC07) mechanism (Carter, 2010a), the Regional Atmospheric Chemistry Mechanism version 2 (RACM2) (Goliff, 2013), and the Goddard Earth Observing System - Chem (GEOS-Chem) mechanism (Harvard University, 2022). Comparing the VOC reactivity factors of each mechanism (i.e., CB7r1, RACM2, GEOS-Chem) to SAPRC07 is valuable because the SAPRC07 MIRs are well-established and linked to experimental data. Evaluating the GEOS-Chem and RACM2 mechanisms is valuable because the Environmental Protection Agency (EPA) has implemented GEOS-Chem in the Community Multiscale Air Quality (CMAQ) model and RACM2 is widely used for the modeling of regional atmospheric chemistry (e.g., Weather Research & Forecasting Model (WRF)-Chem).

For efficiency, CAMx (i.e., including the implemented GEOS-Chem mechanism) was run as a box model (i.e., a 1-D CAMx simulation with emissions and meteorology that represent a limited area) for several Texas locations (Houston-Galveston-Brazoria (HGB), Dallas-Fort Worth (DFW), San Antonio (SAN), Tyler (TYL), and El Paso (ELP)) to generate ozone response surfaces. For each mechanism and location, 100 CAMx box model simulations were performed by modulating NOx and VOC emissions. VOC reactivity factors (MIR values) for each mechanism and location were computed by using the Decoupled Direct Method (DDM) in the CAMx box models. VOC reactivity factors characterize the O_3 forming potential of individual VOCs under atmospheric conditions where adding VOC emission yields the highest incremental increase in O_3 concentration (Carter and Atkinson, 1989).

2.0 Implementing the GEOS-Chem Mechanism in CAMx

The main objective for implementing the GEOS-Chem mechanism in CAMx was to compare ozone responses to other widely used chemical mechanisms, including CB7r1, SAPRC07 and RACM2. The latest version of GEOS-Chem is version 14.1.0 (DOI: 10.5281/zenodo.7696632) and the chemical mechanism includes 913 reactions and 290 species. We modified and formatted the GEOS-Chem mechanism for input to Ramboll's Chemical Mechanism Compiler (CMC), which produces source code for CAMx. These changes are summarized below.

The CMC requires reactants, products, and stoichiometric coefficients to be formatted in a certain manner. For example, coefficients must be proceeded with a # symbol and species names must be four characters or less. The GEOS-Chem reactions were modified to align with these formatting requirements and species names were changed where needed. Table 2 lists the chemical species, including the original GEOS-Chem name and the corresponding name used in CAMx. Reaction rate constant expressions used in the mechanism must also be defined in CAMx. The latest version of CAMx (v7.2) includes seven rate types. An additional rate type (Type 8) has been defined in this work to more accurately represent some of the GEOS-Chem reactions that depend on pressure but are incompatible with the previously defined rate types. Table 1 lists the CAMx rate constant expressions.

In addition to modifying the reaction formatting and species names, the following changes were made to the GEOS-Chem mechanism.

1. Since this project is focused on tropospheric ozone, the list of reactions was reduced to exclude chemistry occurring in the stratosphere.

2. All halogen reactions were removed from the mechanism. This will allow us to identify ozone response changes that are due to differences in hydrocarbon chemistry between the various mechanisms.

3. Heterogeneous chemistry was reduced to four reactions (Number 585-588 in Table 3) that can be incorporated into CAMx's heterogeneous chemistry scheme.

4. Reaction rate expressions were assigned to one of the eight CAMx rate types listed in Table 1. Some reactions were split into separate reactions to more accurately align with the CAMx defined rate expressions. More complex GEOS-Chem rate expressions were fit into more general expressions when necessary. Rate expressions are provided in Table 3.

5. Photolysis rates were calculated from the Tropospheric Visible and Ultraviolet (TUV) Radiation Model (NCAR, 2022). Rates at 10 different zenith angles are presented for each photolysis reaction in Table 4.

6. Reactions involving the GEOS-Chem species NAP were removed from the mechanism. NAP is a naphthalene intermediate VOC (IVOC) surrogate which corresponds to the CAMx anthropogenic IVOC scheme that operates outside of CMC.

7. GEOS-Chem dummy species used to track oxidation were removed from the reaction listing. Below is an example GEOS-Chem reaction where LISOPNO3 is a dummy species to track isoprene oxidation by NO_3.

ISOP + NO3 = 0.465 INO2B + 0.535 INO2D + LISOPNO3

The final chemical mechanism implemented in CAMx is listed in Table 3 and includes 606 reactions and 193 species. Two species listed in Table 2, HCl and NAP/IVOA, are not included in the mechanism but are necessary to perform gas-aerosol interactions in CAMx which operate outside of CMC.

Table 1. Rate constant expression types supported in CAMx and order of expression parameters for the chemistry parameters file.

Expression Type	Description	Expression
1	Constant	$k = k_{298}$
2	UAM (Arrhenius expression)	$k = k_{298}\, exp\left[E_a\left(\frac{1}{298} - \frac{1}{T}\right)\right]$
3	General temperature dependence	$k = A\left(\frac{T}{T_R}\right)^B exp\left(-\frac{E_a}{T}\right)$
4	Troe-type temperature and pressure dependence	$k = \left(\frac{k^0[M]}{1 + k^0[M]/k^\infty}\right)F^G$ $k^0 = A\left(\frac{T}{T_R}\right)^B exp\left(-\frac{E_a}{T}\right)$ $k^\infty = A'\left(\frac{T}{T_R'}\right)^{B'} exp\left(-\frac{E_a'}{T}\right)$ $G = \left[1 + \left(\frac{log(k^0[M]/k^\infty)}{n}\right)^2\right]^{-1}$
5	Equilibrium with a previously defined reaction (k_{ref})	$k = k_{ref}\left[A\left(\frac{T}{T_R}\right)^B exp\left(-\frac{E_a}{T}\right)\right]^{-1}$
6	Lindemann - Hinshelwood as used for OH + HNO3	$k = k^0 + \frac{k_3[M]}{1 + k_3[M]/k_2}$
7	Simple pressure dependence used for OH + CO	$k = k_1 + k_2[M]$
8	General temperature and pressure dependence	$k = A\left(\frac{T}{T_R}\right)^B exp\left(-\frac{E_a}{T}\right) P^C$

Notes:

T is temperature (K)
T_R is reference temperature of 300 K
E_a is an Arrhenius activation energy (K)
k^0 is the low pressure limit of the rate constant
k^∞ is the high pressure limit of the rate constant
[M] is the concentration of air
P is the air pressure in atmospheres (1 atm = 1013.25 mb)
A, B, and C are reaction specific constants

Table 2. GEOS-Chem species, corresponding CAMx species, molecular formula, and species description.

Number	GEOS-Chem species name	CAMx species name	Molecular formula (when available)	Species description
1	A3O2	A3OO	CH3CH2CH2OO	Primary RO2 from C3H8
2	ACET	ACET	CH3C(O)CH3	Acetone
3	ACTA	AACD	CH3C(O)OH	Acetic acid
4	ALD2	ALD2	CH3CHO	Acetaldehyde
5	ALK4	ALK4		>= C4 alkanes
6	AROMP4	OPN1		Generic C4 product from aromatic oxidation
7	AROMP5	OPN2		Generic C5 product from aromatic oxidation
8	AROMRO2	AROO		Generic peroxy radical from aromatic oxidation
9	ATO2	ATOO	CH3C(O)CH2O2	RO2 from acetone
10	ATOOH	ATPX	CH3C(O)CH2OOH	ATO2 peroxide
11	B3O2	B3OO	CH3CH(OO)CH3	Secondary RO2 from C3H8
12	BALD	BALD		Benzaldehyde and tolualdehyde
13	BENZO2	BZO2	C6H5O2	C6H5O2 radical
14	BENZO	BNZO	C6H5O	C6H5O radical
15	BENZP	BZPX		Hydroperoxide from BENZO2
16	BENZ	BENZ	C6H6	Benzene
17	BRO2	BZOO	C6H5O2	Peroxy radical from BENZ oxidation
18	BZCO3H	BPCD		Perbenzoic acid
19	BZCO3	BCO3		Benzoylperoxy radical
20	BZPAN	BPAN		Peroxybenzoyl nitrate
21	C2H2	C2H2	C2H2	Ethyne
22	C2H4	C2H4	C2H4	Ethylene
23	C2H6	C2H6	C2H6	Ethane
24	C3H8	C3H8	C3H8	Propane
25	C4HVP1	HVP1		C4 hydroxy-vinyl-peroxy radicals from HPALDs
26	C4HVP2	HVP2		C4 hydroxy-vinyl-peroxy radicals from HPALDs
27	CH2OO	CGR1	CH2OO	Criegee intermediate
28	CH2O	HCHO	CH2O	Formaldehyde
29	CH3CHOO	CGR2	CH3CHOO	Criegee intermediate
30	CH4	CH4	CH4	Methane
31	CO	CO	CO	Carbon monoxide
32	CO2	CO2	CO2	Carbon dioxide
33	CSL	CSL		Cresols and xylols
34	DMS	DMS	(CH3)2S	Dimethylsulfide
35	EOH	EOH	C2H5OH	Ethanol
36	ETHLN	ETLN	CHOCH2ONO2	Ethanal nitrate
37	ETHN	ETHN		Stable hydroxy-nitrooxy-ethane
38	ETHP	ETHP		Stable hydroxy-hydroperoxy-ethane

Number	GEOS-Chem species name	CAMx species name	Molecular formula (when available)	Species description
39	ETNO3	ETN	C2H5ONO2	Ethyl nitrate
40	ETOO	HEOO		Hydroxy-peroxy-ethane radical, formed from ethene + OH
41	ETO2	ETOO	CH3CH2OO	Ethylperoxy radical
42	ETO	ETAX		Hydroxy-alkoxy-ethane radical
43	ETP	ETPX	CH3CH2OOH	Ethylhydroperoxide
44	GLYC	GLYC	HOCH2CHO	Glycoaldehyde
45	GLYX	GLY	CHOCHO	Glyoxal
46	H	H	H	Atomic hydrogen
47	H2O	H2O	H2O	Water vapor
48	H2O2	H2O2	H2O2	Hydrogen peroxide
49	H2	H2	H2	Molecular hydrogen
50	HAC	HAC	HOCH2C(O)CH3	Hydroxyacetone
51	HC5A	IHAL	C5H8O2	Isoprene-4,1-hydroxyaldehyde
52	HCl [a]	HCL	HCl	Hydrochloric acid
53	HCOOH	FACD	HCOOH	Formic acid
54	HMHP	HMHP	HOCH2OOH	Hydroxymethyl hydroperoxide
55	HMML	HMML	C4H6O3	Hydroxymethyl-methyl-a-lactone
56	HNO2	HNO2	HONO	Nitrous acid
57	HNO3	HNO3	HNO3	Nitric acid
58	HNO4	HNO4	HNO4	Pernitric acid
59	HO2	HO2	HO2	Hydroperoxyl radical
60	HONIT	TNTR		2nd gen monoterpene organic nitrate
61	HPALD1OO	H1OO		Peroxy radicals from HPALD1
62	HPALD1	HPA1	O=CHC(CH3)=CHCH2OOH	d-4,1-C5-hydroperoxyaldehyde
63	HPALD2OO	H2OO		Peroxy radicals from HPALD2
64	HPALD2	HPA2	HOOCH2C(CH3)=CHCH=O	d-1,4-C5-hydroperoxyaldehyde
65	HPALD3	HPA3	O=CHC(CH3)OOHCH=CH2	b-2,1-C5-hydroperoxyaldehyde
66	HPALD4	HPA4	CH2=C(CH3)CHOOHCH=O	b-3,4-C5-hydroperoxyaldehyde
67	HPETHNL	ELPX	CHOCH2OOH	Hydroperoxyethanal
68	ICHE	ICHE	C5H8O3	Isoprene hydroxy-carbonyl-epoxides
69	ICHOO	IEOO		Peroxy radical from IEPOXD
70	ICNOO	INOO		Peroxy radicals from ICN
71	ICN	ICN	C5H7NO4	Lumped isoprene carbonyl nitrates
72	ICPDH	IDHP	C5H10O5	Isoprene dihydroxy hydroperoxycarbonyl
73	IDCHP	IHDP	C5H8O5	Isoprene dicarbonyl hydroxy dihydroperoxide
74	IDC	IDC	C5H6O2	Lumped isoprene dicarbonyls
75	IDHDP	IDDP	C5H12O6	Isoprene dihydroxy dihydroperoxide
76	IDHNBOO	IBNO		Peroxy radicals from INPB
77	IDHNDOO1	I1OO		Peroxy radicals from INPD

Number	GEOS-Chem species name	CAMx species name	Molecular formula (when available)	Species description
78	IDHNDOO2	I2OO		Peroxy radicals from INPD
79	IDHPE	IHPE	C5H10O5	Isoprene dihydroxy hydroperoxy epoxide
80	IDNOO	IDNO		Peroxy radicals from IDN
81	IDN	IDN	C5H8N2O6	Lumped isoprene dinitrates
82	IEPOXAOO	IEAO		Peroxy radical from trans-Beta isoprene epoxydiol
83	IEPOXA	IEPA	C5H10O3	Trans-Beta isoprene epoxydiol
84	IEPOXBOO	IEBO		Peroxy radical from cis-Beta isoprene epoxydiol
85	IEPOXB	IEPB	C5H10O3	Cis-Beta isoprene epoxydiol
86	IEPOXD	IEPD	C5H10O3	Delta isoprene epoxydiol
87	IHN1	IHN1	C5H9NO4	Isoprene-d-4-hydroxy-1-nitrate
88	IHN2	IHN2	C5H9NO4	Isoprene-b-1-hydroxy-2-nitrate
89	IHN3	IHN3	C5H9NO4	Isoprene-b-4-hydroxy-3-nitrate
90	IHN4	IHN4	C5H9NO4	Isoprene-d-1-hydroxy-4-nitrate
91	IHOO1	IH1O		Peroxy radical from OH addition to isoprene at C1
92	IHOO4	IH4O		Peroxy radical from OH addition to isoprene at C4
93	IHPNBOO	IHBO		Peroxy radicals from INPB
94	IHPNDOO	IHDO		Peroxy radicals from INPD
95	IHPOO1	IP1O		Peroxy radical from ISOPOOH
96	IHPOO2	IP2O		Peroxy radical from ISOPOOH
97	IHPOO3	IP3O		Peroxy radical from ISOPOOH
98	INA	INAX		Alkoxy radical from INO2D
99	INO2B	INBO		Beta-peroxy radicals from isoprene + NO3
100	INO2D	INDO		Delta-peroxy radicals from isoprene + NO3
101	INPB	INPB	C5H9NO5	Lumped isoprene beta-hydroperoxy nitrates
102	INPD	INPD	C5H9NO5	Lumped isoprene delta-hydroperoxy nitrates
103	IONITA	INTR		Aerosol-phase organic nitrate from isoprene precursors
104	IPRNO3	IPRN	C3H8ONO2	Isopropyl nitrate
105	ISOPNOO1	IN1O		Peroxy radicals from IHN2
106	ISOPNOO2	IN2O		Peroxy radicals from IHN3
107	ISOP	ISOP	CH2=C(CH3)CH=CH2	Isoprene
108	ITCN	ITCN	C5H9NO7	Lumped tetrafunctional isoprene carbonyl-nitrates
109	ITHN	ITHN	C5H11NO7	Lumped tetrafunctional isoprene hydroxynitrates
110	KO2	KOO		RO2 from >3 ketones
111	LIMO2	LMOO		RO2 from LIMO
112	LIMO	LIM	C10H16	Limonene
113	LVOC	LVOC	C5H14O5	Gas-phase low-volatility non-IEPOX product of ISOPOOH (RIP) oxidation
114	MACR1OOH	MPCD	CH2=C(CH3)C(O)OOH	Peracid from MACR

Number	GEOS-Chem species name	CAMx species name	Molecular formula (when available)	Species description
115	MCO3	MCO3	CH3C(O)OO	Peroxyacetyl radical
116	MACR1OO	MAC3		Peroxyacyl radical from MACR + OH
117	MACRNO2	MNOO		Product of MCRHN + OH
118	MACR	MACR	CH2=C(CH3)CHO	Methacrolein
119	MAP	APCD	CH3C(O)OOH	Peroxyacetic acid
120	MCRDH	MCDH	C4H8O3	Dihydroxy-MACR
121	MCRENOL	MCRL	C4H6O2	Lumped enols from MVK/MACR
122	MCRHNB	MCNB	O2NOCH2C(OH)(CH3)CHO	Hydroxynitrate from MACR
123	MCRHN	MCHN	HOCH2C(ONO2)(CH3)CHO	Hydroxynitrate from MACR
124	MCRHP	MCHP	HOCH2C(OOH)(CH3)CHO	Hydroxy-hydroperoxy-MACR
125	MCROHOO	MCOO		Peroxy radical from MACR + OH
126	MCT	MCT		Methylcatechols
127	MEK	MEK	RC(O)R	Methyl ethyl ketone
128	MENO3	MENT	CH3ONO2	Methyl nitrate
129	MGLY	MGLY	CH3COCHO	Methylglyoxal
130	MO2	MEOO	CH3O2	Methylperoxy radical
131	MOH	MOH	CH3OH	Methanol
132	MONITS	MTNS		Saturated 1st gen monoterpene organic nitrate
133	MONITU	MTNU		Unsaturated 1st gen monoterpene organic nitrate
134	MPAN	MPAN	CH2=C(CH3)C(O)OONO2	Peroxymethacroyl nitrate (PMN)
135	MPN	MPN	CH3O2NO2	Methyl peroxy nitrate
136	MP	MEPX	CH3OOH	Methylhydroperoxide
137	MSA	MSA	CH4SO3	Methanesulfonic acid
138	MTPA	TRPA		Lumped monoterpenes: a-pinene, b-pinene, sabinene, carene
139	MTPO	OTRP		Other monoterpenes: Terpinene, terpinolene, myrcene, ocimene, other monoterpenes
140	MVKDH	MVDH	HOCH2CH2OHC(O)CH3	Dihydroxy-MVK
141	MVKHCB	MVHB	C4H6O3	MVK hydroxy-carbonyl
142	MVKHC	MVHC	C4H6O3	MVK hydroxy-carbonyl
143	MVKHP	MVPX	C4H8O4	MVK hydroxy-hydroperoxide
144	MVKN	MVKN	HOCH2CH(ONO2)C(=O)CH3	Hydroxynitrate from MVK
145	MVKOHOO	MVOO		Peroxy radical from MVK + OH
146	MVKPC	MVCX	OCHCH(OOH)C(O)CH3	MVK hydroperoxy-carbonyl
147	MVK	MVK	CH2=CHC(=O)CH3	Methyl vinyl ketone
148	N2O5	N2O5	N2O5	Dinitrogen pentoxide
149	NAP [a]	IVOA	C10H8	Naphthalene IVOC surrogate
150	NO2	NO2	NO2	Nitrogen dioxide
151	NO3	NO3	NO3	Nitrate radical
152	NO	NO	NO	Nitric oxide
153	NPHEN	NPHN		Nitrophenols

Number	GEOS-Chem species name	CAMx species name	Molecular formula (when available)	Species description
154	NPRNO3	NPRN	C3H8ONO2	n-propyl nitrate
155	NRO2	NROO		Peroxy radical from NAP oxidation
156	O	O	O(3P)	Ground state atomic oxygen
157	O1D	O1D	O(1D)	Excited atomic oxygen
158	O2	O2	O2	Molecular oxygen
159	O3	O3	O3	Ozone
160	OCS	OCS	COS	Carbonyl sulfide
161	OH	OH	OH	Hydroxyl radical
162	OLND	OLND		Monoterpene-derived NO3-alkene adduct
163	OLNN	OLNN		Monoterpene-derived NO3 adduct
164	OTHRO2	O2OO		Other C2 RO2 not from C2H6 oxidation
165	PAN	PAN	CH3C(O)OONO2	Peroxyacetylnitrate
166	PHEN	PHEN		Phenol
167	PIO2	MTOO		RO2 from MTPA
168	PIP	PIPX		Peroxides from MTPA
169	PO2	POO	HOCH2CH(OO)CH3	RO2 from propene
170	PPN	PPN	CH3CH2C(O)OONO2	Peroxypropionylnitrate
171	PP	PPX	HOCH2CH(OOH)CH3	Peroxide from PO2
172	PRN1	PRNO	O2NOCH2CH(OO)CH3	RO2 from propene + NO3
173	PROPNN	PPNN	CH3C(=O)CH2ONO2	Propanone nitrate
174	PRPE	PRPE	C3H6	>= C3 alkenes
175	PRPN	PNPX	O2NOCH2CH(OOH)CH3	Peroxide from PRN1
176	PYAC	PYAC	CH3COCOOH	Pyruvic acid
177	R4N1	R4NO		RO2 from R4N2
178	R4N2	R4N	RO2NO	>= C4 alkylnitrates
179	R4O2	R4OO		RO2 from ALK4
180	R4P	R4PX	CH3CH2CH2CH2OOH	Peroxide from R4O2
181	RA3P	A3PX	CH3CH2CH2OOH	Peroxide from A3O2
182	RB3P	B3PX	CH3CH(OOH)CH3	Peroxide from B3O2
183	RCHO	RCHO	CH3CH2CHO	>= C3 aldehydes
184	RCO3	RCO3	CH3CH2C(O)OO	Peroxypropionyl radical
185	RCOOH	RACD	C2H5C(O)OH	> C2 organic acids
186	RIPA	RIPA	HOCH2C(OOH)(CH3)CH=CH2	1,2-ISOPOOH
187	RIPB	RIPB	HOCH2C(OOH)(CH3)CH=CH2	4,3-ISOPOOH
188	RIPC	RIPC	C5H10O3	d(1,4)-ISOPOOH
189	RIPD	RIPD	C5H10O3	d(4,1)-ISOPOOH
190	ROH	ROH	C3H7OH	> C2 alcohols
191	RP	RPX	CH3CH2C(O)OOH	Peroxide from RCO3
192	SO2	SO2	SO2	Sulfur dioxide
193	SO4	SULF	SO4	Sulfate
194	TOLU	TOLU	C7H8	Toluene

Number	GEOS-Chem species name	CAMx species name	Molecular formula (when available)	Species description
195	XYLE	XYLE	C8H10	Xylene

(a) Species not included in chemical mechanism but are necessary to perform aerosol chemistry in CAMx

Table 3. GEOS-Chem chemical mechanism implemented in CAMx.

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
1	NO2 = NO + O	Photolysis	6.30E-3
2	O3 = O + O2	Photolysis	3.33E-4
3	O3 = O1D + O2	Photolysis	8.78E-6
4	H2O2 = OH + OH	Photolysis	3.78E-6
5	NO3 = NO2 + O	Photolysis	1.56E-1
6	NO3 = NO + O2	Photolysis	1.98E-2
7	N2O5 = NO3 + NO2	Photolysis	2.52E-5
8	HNO2 = OH + NO	Photolysis	1.04E-3
9	HNO3 = OH + NO2	Photolysis	2.54E-7
10	HNO4 = OH + NO3	Photolysis	6.80E-7
11	HNO4 = HO2 + NO2	Photolysis	2.68E-6
12	PAN = 0.7 MCO3 + 0.7 NO2 + 0.3 MEOO + 0.3 NO3	Photolysis	3.47E-7
13	MEPX = HCHO + HO2 + OH	Photolysis	2.68E-6
14	HCHO = HO2 + H + CO	Photolysis	1.69E-5
15	HCHO = H2 + CO	Photolysis	2.69E-5
16	ALD2 = 0.88 MEOO + HO2 + 0.88 CO + 0.12 MCO3	Photolysis	1.96E-6
17	ALD2 = CH4 + CO	Photolysis	0.00E+0
18	RCHO = 0.5 O2OO + HO2 + CO + 0.07 A3OO + 0.27 B3OO	Photolysis	2.62E-5
19	GLYC = 0.9 HCHO + 1.73 HO2 + CO + 0.07 OH + 0.1 MOH	Photolysis	2.76E-6
20	GLY = 2 HO2 + 2 CO	Photolysis	3.12E-6
21	GLY = H2 + 2 CO	Photolysis	1.57E-5
22	GLY = HCHO + CO	Photolysis	4.53E-5
23	MGLY = MCO3 + CO + HO2	Photolysis	1.46E-4
24	MVK = PRPE + CO	Photolysis	1.72E-7
25	MVK = MCO3 + HCHO + CO + HO2	Photolysis	1.72E-7
26	MVK = MEOO + RCO3	Photolysis	1.72E-7
27	MEK = 0.85 MCO3 + 0.425 O2OO + 0.15 MEOO + 0.15 RCO3 + 0.06 A3OO + 0.23 B3OO	Photolysis	2.27E-7
28	ACET = MCO3 + MEOO	Photolysis	1.04E-7
29	ACET = 2 MEOO + CO	Photolysis	1.04E-7
30	MACR = CO + HO2 + HCHO + MCO3	Photolysis	2.52E-6
31	PIPX = RCHO + OH + HO2	Photolysis	2.68E-6

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
32	ICN = NO2 + 0.839 CO + 0.645 OH + 0.161 HO2 + 0.161 IDC + 0.162 MVCX + 0.481 MCRL + 0.128 HVP2 + 0.068 HVP1	Photolysis	1.48E-5
33	ETLN = NO2 + HCHO + CO + HO2	Photolysis	1.06E-5
34	MVKN = 0.29 HO2 + 0.01 OH + 0.7 NO2 + 1.01 MCO3 + 0.69 GLYC + 0.3 ETLN	Photolysis	1.48E-5
35	MCHN = HAC + CO + HO2 + NO2	Photolysis	2.22E-5
36	MCNB = PPNN + OH + CO + HO2	Photolysis	1.06E-5
37	MTNS = MEK + NO2	Photolysis	1.06E-6
38	MTNU = RCHO + NO2	Photolysis	1.06E-6
39	TNTR = HAC + NO2	Photolysis	1.06E-6
40	MENT = NO2 + HO2 + HCHO	Photolysis	1.06E-6
41	ETN = NO2 + HO2 + ALD2	Photolysis	1.06E-6
42	IPRN = NO2 + HO2 + ACET	Photolysis	1.06E-6
43	NPRN = NO2 + HO2 + RCHO	Photolysis	1.06E-6
44	RIPA = MVK + HCHO + HO2 + OH	Photolysis	2.95E-6
45	RIPB = MACR + HCHO + HO2 + OH	Photolysis	2.95E-6
46	RIPC = OH + HO2 + IHAL	Photolysis	2.95E-6
47	RIPD = OH + HO2 + IHAL	Photolysis	2.95E-6
48	HPA1 = 0.888 CO + 1.662 OH + 0.112 HO2 + 0.112 IDC + 0.112 MVCX + 0.552 MCRL + 0.224 HVP1	Photolysis	1.46E-4
49	HPA2 = 0.818 CO + 1.637 OH + 0.182 HO2 + 0.182 IDC + 0.182 MVCX + 0.455 MCRL + 0.182 HVP2	Photolysis	1.46E-4
50	HPA3 = CO + OH + HO2 + MVK	Photolysis	1.46E-4
51	HPA4 = CO + OH + HO2 + MACR	Photolysis	1.46E-4
52	IHN1 = NO2 + 0.45 IHAL + 0.45 HO2 + 0.55 MVPX + 0.55 CO + 0.55 OH	Photolysis	1.48E-5
53	IHN2 = NO2 + MVK + HO2 + HCHO	Photolysis	1.48E-5
54	IHN3 = NO2 + MACR + HO2 + HCHO	Photolysis	1.48E-5
55	IHN4 = NO2 + 0.45 IHAL + 0.45 HO2 + 0.55 MCHP + 0.55 CO + 0.55 OH	Photolysis	1.48E-5
56	INPB = NO2 + HCHO + 0.097 MACR + 0.903 MVK + 0.67 OH + 0.33 HO2	Photolysis	1.48E-5
57	INPD = OH + 0.159 HO2 + 0.159 ICN + 0.841 INAX	Photolysis	2.68E-5
58	INPD = NO2 + 0.841 IH1O + 0.159 IH4O	Photolysis	1.48E-5
59	IDHP = CO + 1.5 HO2 + 0.5 OH + 0.5 MCHP + 0.35 MVDH + 0.15 MCDH	Photolysis	1.46E-4
60	IDHP = OH + HO2 + 0.122 CO + 0.1 HCHO + 0.1 MVHB + 0.438 HAC + 0.438 GLY + 0.088 GLYC + 0.088 MGLY + 0.122 MCDH	Photolysis	1.42E-5
61	IDDP = 1.25 OH + 0.25 GLYC + 0.25 HAC + 0.75 IDHP + 0.75 HO2	Photolysis	2.84E-5

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
62	IHPE = OH + HO2 + 0.429 MGLY + 0.429 GLYC + 0.571 GLY + 0.571 HAC	Photolysis	1.42E-5
63	IHDP = 0.546 OH + CO + 1.454 HO2 + 0.391 MVHC + 0.155 MVHB + 0.454 MVCX	Photolysis	1.42E-5
64	ITHN = OH + 0.7 HO2 + 0.55 HCHO + 0.5 MCHN + 0.3 GLYC + 0.45 HAC + 0.3 NO2 + 0.15 ETLN + 0.05 MVKN	Photolysis	2.68E-5
65	ITHN = NO2 + 0.8 HAC + 0.7 HO2 + 0.5 ELPX + 0.35 GLYC + 0.15 HCHO + 0.15 MCHP + 0.05 ATPX + 0.3 OH	Photolysis	1.48E-5
66	ITCN = MGLY + OH + NO2 + GLYC	Photolysis	2.96E-5
67	ITCN = 0.5 MVPX + 0.5 MCHP + CO + NO2 + HO2	Photolysis	1.46E-4
68	ETHP = ETAX + OH	Photolysis	2.68E-6
69	BALD = BZO2 + CO + HO2	Photolysis	2.92E-5
70	BPCD = BZO2 + OH + CO2	Photolysis	3.78E-7
71	BZPX = BNZO	Photolysis	2.68E-6
72	NPHN = HNO2 + CO + CO2 + OPN1 + HO2	Photolysis	9.45E-5
73	HAC = MCO3 + HCHO + HO2	Photolysis	1.89E-5
74	IDN = 1.555 NO2 + 0.5 GLYC + 0.5 HAC + 0.05 MVK + 0.005 MACR + 0.055 HCHO + 0.227 INAX + 0.228 ICN + 0.228 HO2	Photolysis	2.96E-5
75	PNPX = OH + HO2 + RCHO + NO2	Photolysis	1.06E-6
76	ETPX = OH + HO2 + ALD2	Photolysis	2.68E-6
77	A3PX = OH + HO2 + RCHO	Photolysis	2.68E-6
78	B3PX = OH + HO2 + ACET	Photolysis	2.68E-6
79	R4PX = OH + HO2 + RCHO	Photolysis	2.68E-6
80	PPX = OH + HO2 + ALD2 + HCHO	Photolysis	2.68E-6
81	RPX = OH + HO2 + ALD2	Photolysis	3.78E-7
82	HMHP = 2 OH + HCHO	Photolysis	2.68E-6
83	ELPX = OH + CO + HO2 + HCHO	Photolysis	2.62E-5
84	PYAC = MCO3 + CO2 + HO2	Photolysis	1.46E-4
85	PPNN = NO2 + HCHO + MCO3	Photolysis	1.06E-5
86	MVHC = CO + HO2 + HCHO + MCO3	Photolysis	1.42E-5
87	MVHB = 0.5 GLY + 1.5 HO2 + 0.5 MCO3 + 0.5 CO + 0.5 MGLY	Photolysis	1.42E-5
88	MVPX = 0.53 MCO3 + 0.53 GLYC + OH + 0.47 HO2 + 0.47 HCHO + 0.47 MGLY	Photolysis	1.42E-5
89	MVCX = OH + 0.571 CO + 0.571 MGLY + 0.571 HO2 + 0.429 GLY + 0.429 MCO3	Photolysis	1.60E-4
90	MCRL = 0.875 CO + 0.75 PYAC + 1.75 OH + 0.125 MGLY + 0.125 HO2 + 0.125 MCO3 + 0.125 GLY	Photolysis	1.60E-4
91	MCHP = OH + 0.77 CO + HO2 + 0.77 HAC + 0.23 MGLY + 0.23 HCHO	Photolysis	1.42E-5

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
92	MPCD = 0.75 OH + 1.238 CO2 + 0.488 MEOO + 0.75 HCHO + 0.262 MAC3 + 0.25 MPCD	Photolysis	1.42E-5
93	ATPX = OH + HCHO + MCO3	Photolysis	3.78E-7
94	R4N = NO2 + 0.32 ACET + 0.19 MEK + 0.18 MEOO + 0.27 HO2 + 0.32 ALD2 + 0.13 RCHO + 0.05 A3OO + 0.18 B3OO + 0.32 O2OO	Photolysis	1.06E-6
95	APCD = OH + MEOO	Photolysis	3.78E-7
96	O + O2 + M = O3 + M	k = 6.00E-34 (T/300)^-2.4	6.10E-34
97	O + OH = O2 + H	k = 1.80E-11 exp(180/T)	3.29E-11
98	O + O3 = 2 O2	k = 8.00E-12 exp(-2060/T)	7.96E-15
99	O3 + HO2 = OH + O2 + O2	k = 1.00E-14 exp(-490/T)	1.93E-15
100	O3 + NO2 = O2 + NO3	k = 1.20E-13 exp(-2450/T)	3.23E-17
101	O3 + OH = HO2 + O2	k = 1.70E-12 exp(-940/T)	7.25E-14
102	O3 + MEOO = HCHO + HO2 + O2	k = 2.90E-16 exp(-1000/T)	1.01E-17
103	O3 + NO = NO2 + O2	k = 3.00E-12 exp(-1500/T)	1.95E-14
104	OH + H2O2 = H2O + HO2	k = 1.80E-12	1.80E-12
105	OH + OH = H2O + O	k = 1.80E-12	1.80E-12
106	OH + NO3 = HO2 + NO2	k = 2.20E-11	2.20E-11
107	OH + H2 = H2O + H	k = 2.80E-12 exp(-1800/T)	6.67E-15
108	OH + HO2 = H2O + O2	k = 4.80E-11 exp(250/T)	1.11E-10
109	OH + OH = H2O2	Falloff: F=0.6; n=1 k(0) = 6.90E-31 (T/300)^-1 k(inf) = 2.60E-11	6.29E-12
110	O1D + H2O = 2 OH	k = 1.63E-10 exp(60/T)	1.99E-10
111	O1D + N2 = O + N2	k = 2.15E-11 exp(110/T)	3.11E-11
112	O1D + O2 = O + O2	k = 3.30E-11 exp(55/T)	3.97E-11
113	HO2 + NO3 = OH + NO2 + O2	k = 3.50E-12	3.50E-12
114	HO2 + HO2 = H2O2 + O2	k = k1 + k2 [M] k1 = 2.20E-13 exp(600/T) k2 = 1.90E-33 exp(980/T)	2.90E-12
115	HO2 + HO2 + H2O = H2O2 + O2	k = k1 + k2 [M] k1 = 3.08E-34 exp(2800/T) k2 = 2.66E-54 exp(3180/T)	6.53E-30
116	HO2 + O = OH + O2	k = 3.00E-11 exp(200/T)	5.87E-11
117	HO2 + NO = OH + NO2	k = 3.30E-12 exp(270/T)	8.17E-12
118	HO2 + NO2 = HNO4	Falloff: F=0.6; n=1 k(0) = 1.90E-31 (T/300)^-3.4 k(inf) = 4.00E-12 (T/300)^0.3	1.31E-12
119	H2O2 + O = OH + HO2	k = 1.40E-12 exp(-2000/T)	1.70E-15
120	H + O2 = HO2	Falloff: F=0.6; n=1 k(0) = 4.40E-32 (T/300)^-1.3 k(inf) = 7.50E-11 (T/300)^-0.2	9.59E-13
121	NO + NO3 = 2 NO2	k = 1.50E-11 exp(170/T)	2.65E-11
122	NO + O = NO2	Falloff: F=0.6; n=1 k(0) = 9.00E-32 (T/300)^-1.5 k(inf) = 3.00E-11	1.66E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
123	NO + OH = HNO2	Falloff: F=0.6; n=1 k(0) = 7.00E-31 (T/300)^-2.6 k(inf) = 3.60E-11 (T/300)^0.1	7.40E-12
124	NO2 + NO3 = NO + NO2 + O2	k = 4.50E-14 exp(-1260/T)	6.56E-16
125	NO2 + O = NO + O2	k = 5.10E-12 exp(210/T)	1.03E-11
126	NO2 + OH = HNO3	Falloff: F=0.6; n=1 k(0) = 1.80E-30 (T/300)^-3 k(inf) = 2.80E-11	1.06E-11
127	NO2 + NO3 = N2O5	Falloff: F=0.6; n=1 k(0) = 2.40E-30 (T/300)^-3 k(inf) = 1.60E-12 (T/300)^-0.1	1.35E-12
128	NO2 + O = NO3	Falloff: F=0.6; n=1 k(0) = 2.50E-31 (T/300)^-1.8 k(inf) = 2.20E-11 (T/300)^0.7	3.27E-12
129	NO3 + O = NO2 + O2	k = 1.00E-11	1.00E-11
130	NO3 + NO3 = 2 NO2 + O2	k = 8.50E-13 exp(-2450/T)	2.28E-16
131	N2O5 = NO2 + NO3	Falloff: F=0.6; n=1 k(0) = 4.14E-4 (T/300)^-3 exp(-10840/T) k(inf) = 2.76E+14 (T/300)^0.1 exp(-10840/T)	3.70E-2
132	HNO2 + OH = H2O + NO2	k = 1.80E-11 exp(-390/T)	4.86E-12
133	HNO3 + OH = H2O + NO3	k = k1 + k3 [M] / (1 + k3 [M] / k2) k1 = 2.41E-14 exp(460/T) k2 = 2.69E-17 exp(2199/T) k3 = 6.51E-34 exp(1335/T)	1.55E-13
134	HNO4 + OH = H2O + NO2 + O2	k = 1.30E-12 exp(380/T)	4.65E-12
135	HNO4 = HO2 + NO2	Falloff: F=0.6; n=1 k(0) = 9.05E-5 (T/300)^-3.4 exp(-10900/T) k(inf) = 1.90E+15 (T/300)^-0.3 exp(-10900/T)	8.13E-2
136	SO2 + OH = SULF + HO2	Falloff: F=0.6; n=1 k(0) = 3.30E-31 (T/300)^-4.3 k(inf) = 1.60E-12	9.59E-13
137	MCO3 + NO2 = PAN	Falloff: F=0.6; n=1 k(0) = 9.70E-29 (T/300)^-5.6 k(inf) = 9.30E-12 (T/300)^1.5	8.52E-12
138	PAN = MCO3 + NO2	k = k(ref) K k(ref) = k(137) K = 9.30E-29 exp(14000/T)	3.62E-4
139	OH + CO = HO2 + CO2	k = k1 + k2 [M] k1 = 1.44E-13 k2 = 3.43E-33	2.28E-13
140	A3OO + MEOO = HO2 + 0.75 HCHO + 0.75 RCHO + 0.25 MOH + 0.25 ROH	k = 5.92E-13	5.92E-13
141	A3OO + HO2 = A3PX	k = 1.51E-13 exp(1300/T)	1.19E-11
142	A3OO + NO = NPRN	k = 1.14E-14 (P/1013.0)^0.767 exp(1100/T)	4.56E-13
143	A3OO + NO = NO2 + HO2 + RCHO	k = 3.18E-12 (P/1013.0)^-0.026 exp(308/T)	8.93E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
144	ACET + OH = ATOO + H2O	k = 1.33E-13	1.33E-13
145	ACET + OH = ATOO + H2O	k = 3.82E-11 exp(-2000/T)	4.65E-14
146	AACD + OH = MEOO + CO2 + H2O	k = 3.15E-14 exp(920/T)	6.90E-13
147	ALD2 + NO3 = HNO3 + MCO3	k = 1.40E-12 exp(-1900/T)	2.38E-15
148	ALD2 + OH = 0.95 MCO3 + 0.05 HCHO + 0.05 CO + 0.05 HO2 + H2O	k = 4.63E-12 exp(350/T)	1.50E-11
149	ALK4 + NO3 = HNO3 + R4OO	k = 2.80E-12 exp(-3280/T)	4.65E-17
150	ALK4 + OH = R4OO	k = 9.10E-12 exp(-405/T)	2.34E-12
151	OPN1 = 0.2 HO2 + 0.2 GLY + 1.2 RCHO	k = 1.50E-3	1.50E-3
152	OPN1 + OH = 0.6 GLY + 0.25 CO + 0.25 FACD + 0.25 OH + 0.33 HO2 + 0.33 RCO3 + 0.45 RACD	k = 5.00E-11	5.00E-11
153	OPN1 + O3 = 0.5 FACD + 0.5 CO + 0.6 GLY + 0.9 GLYC + 0.1 HO2 + 0.1 OH	k = 8.00E-16	8.00E-16
154	OPN2 = 0.2 HO2 + 0.2 R4OO + 0.2 MGLY + 1.2 RCHO	k = 1.50E-3	1.50E-3
155	OPN2 + OH = 0.6 MGLY + 0.15 AACD + 0.1 FACD + 0.25 OH + 0.33 HO2 + 0.33 RCO3 + 0.25 CO + 0.52 RACD	k = 5.00E-11	5.00E-11
156	OPN2 + O3 = 0.6 MGLY + 0.3 AACD + 0.2 FACD + 0.5 CO + 0.95 GLYC + 0.1 HO2 + 0.1 OH	k = 8.00E-16	8.00E-16
157	AROO + NO3 = NO2 + HO2	k = 2.30E-12	2.30E-12
158	AROO + HO2 = OH + HO2	k = 2.39E-13 exp(1300/T)	1.87E-11
159	AROO + MEOO = HCHO + HO2 + HO2	k = 1.70E-14 exp(220/T)	3.56E-14
160	AROO + NO = NO2 + HO2	k = 2.60E-12 exp(365/T)	8.85E-12
161	AROO + MCO3 = MEOO + HO2	k = 4.20E-14 exp(220/T)	8.79E-14
162	ATOO + MCO3 = MEOO + MCO3 + HCHO	k = 1.68E-12 exp(500/T)	8.99E-12
163	ATOO + MCO3 = MGLY + AACD	k = 1.87E-13 exp(500/T)	1.00E-12
164	ATOO + NO = NO2 + HCHO + MCO3	k = 2.80E-12 exp(300/T)	7.66E-12
165	ATOO + MEOO = 0.3 HO2 + 0.3 HCHO + 0.3 MCO3 + 0.2 HAC + 0.2 HCHO + 0.5 MGLY + 0.5 MOH	k = 7.50E-13 exp(500/T)	4.02E-12
166	ATOO + HO2 = 0.15 MCO3 + 0.15 OH + 0.15 HCHO + 0.85 ATPX	k = 8.60E-13 exp(700/T)	9.01E-12
167	ATPX + OH = MGLY + OH + H2O	k = 1.14E-12 exp(200/T)	2.23E-12
168	ATPX + OH = ATOO + H2O	k = 2.66E-12 exp(200/T)	5.20E-12
169	B3OO + MEOO = 0.5 HO2 + 0.5 ACET + 0.25 ACET + 0.75 HCHO + 0.25 MOH + 0.25 ROH + 0.5 HO2	k = 8.37E-14	8.37E-14
170	B3OO + HO2 = B3PX	k = 1.51E-13 exp(1300/T)	1.19E-11
171	B3OO + NO = IPRN	k = 1.06E-14 (P/1013.0)^0.767 exp(1110/T)	4.39E-13
172	B3OO + NO = NO2 + HO2 + ACET	k = 2.96E-12 (P/1013.0)^-0.026 exp(318/T)	8.60E-12
173	B3OO + MCO3 = MEOO + HO2 + ACET	k = 1.68E-12 exp(500/T)	8.99E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
174	B3OO + MCO3 = ACET + AACD	k = 1.87E-13 exp(500/T)	1.00E-12
175	BALD + NO3 = BCO3 + HNO3	k = 2.40E-15	2.40E-15
176	BALD + OH = BCO3	k = 5.90E-12 exp(225/T)	1.26E-11
177	BENZ + OH = BZOO + 0.54 PHEN + 0.54 HO2 + 0.46 AROO + 0.18 GLY + 0.2 CO + 0.56 OPN1	k = 2.30E-12 exp(-193/T)	1.20E-12
178	BNZO + NO2 = NPHN	k = 2.08E-12	2.08E-12
179	BNZO + O3 = BZO2	k = 2.86E-13	2.86E-13
180	BZO2 + NO3 = BNZO + NO2	k = 2.30E-12	2.30E-12
181	BZO2 + NO2 = BNZO + NO3	k = 7.00E-12	7.00E-12
182	BZO2 + HO2 = BZPX	k = 2.24E-13 exp(1300/T)	1.76E-11
183	BZO2 + NO = BNZO + NO2	k = 2.67E-12 exp(365/T)	9.09E-12
184	BZO2 + MEOO = BNZO + HO2 + HCHO	k = 2.67E-13 exp(365/T)	9.09E-13
185	BZPX + OH = BZO2	k = 3.60E-12	3.60E-12
186	BCO3 + NO2 = BPAN	k = 2.16E-12 (P/1013.0)^0.072 exp(423/T)	8.95E-12
187	BCO3 + HO2 = 0.35 CO2 + 0.2 BZO2 + 0.15 O3 + 0.2 OH + 0.15 BZPX + 0.65 BPCD	k = 1.10E-11 exp(340/T)	3.44E-11
188	BCO3 + MEOO = BZO2 + CO2 + HO2 + HCHO	k = 2.67E-12 exp(365/T)	9.09E-12
189	BCO3 + NO = NO2 + CO2 + BZO2	k = 7.50E-12 exp(290/T)	1.98E-11
190	BPCD + OH = BCO3	k = 4.66E-12	4.66E-12
191	BPAN + OH = BZPX + CO2 + NO2	k = 1.06E-12	1.06E-12
192	BPAN = BCO3 + NO2	k = 7.93E+16 (P/1013.0)^0.066 exp(-13906/T)	4.30E-4
193	C2H2 + OH = 0.636 GLY + 0.636 OH + 0.364 CO + 0.364 HO2 + 0.364 FACD	Falloff: F=0.5; n=1.13 k(0) = 5.50E-30 k(inf) = 8.30E-13 (T/300)^-2	7.24E-13
194	C2H4 + O3 = HCHO + CGR1	k = 9.10E-15 exp(-2580/T)	1.58E-18
195	C2H4 + OH = HEOO	Falloff: F=0.5; n=1.13 k(0) = 1.10E-28 (T/300)^-3.5 k(inf) = 8.40E-12 (T/300)^1.75	7.37E-12
196	C2H6 + NO3 = ETOO + HNO3	k = 1.40E-18	1.40E-18
197	C2H6 + OH = ETOO + H2O	k = 7.66E-12 exp(-1020/T)	2.50E-13
198	C3H8 + OH = A3OO	k = 1.01E-11 exp(-1052/T)	2.95E-13
199	C3H8 + OH = B3OO	k = 3.16E-12 exp(-420/T)	7.73E-13
200	HVP1 + NO2 = MVKN	k = 9.00E-12	9.00E-12
201	HVP1 + HO2 = OH + MVOO	k = 1.93E-13 exp(1300/T)	1.51E-11
202	HVP1 + NO = NO2 + MVOO	k = 2.70E-12 exp(350/T)	8.74E-12
203	HVP2 + NO2 = MCHN	k = 9.00E-12	9.00E-12
204	HVP2 + HO2 = OH + MCOO	k = 1.93E-13 exp(1300/T)	1.51E-11
205	HVP2 + NO = NO2 + MCOO	k = 2.70E-12 exp(350/T)	8.74E-12
206	HCHO + O = CO + HO2 + OH	k = 3.40E-11 exp(-1600/T)	1.58E-13
207	HCHO + OH = CO + HO2 + H2O	k = 5.50E-12 exp(125/T)	8.37E-12
208	CGR1 + NO = HCHO + NO2	k = 1.00E-14	1.00E-14
209	CGR1 + NO2 = HCHO + NO3	k = 1.00E-15	1.00E-15

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
210	CGR1 + CO = HCHO	k = 1.20E-15	1.20E-15
211	CGR1 + O3 = HCHO	k = 1.40E-12	1.40E-12
212	CGR1 + H2O = 0.73 HMHP + 0.21 FACD + 0.06 HCHO + 0.06 H2O2	k = 1.70E-15	1.70E-15
213	CGR1 + SO2 = HCHO + SULF	k = 3.70E-11	3.70E-11
214	CGR1 + H2O + H2O = 0.4 HMHP + 0.54 FACD + 0.06 HCHO + 0.06 H2O2	k = 2.88E-35 exp(1391/T)	3.07E-33
215	CGR2 + NO = ALD2 + NO2	k = 1.00E-14	1.00E-14
216	CGR2 + NO2 = ALD2 + NO3	k = 1.00E-15	1.00E-15
217	CGR2 + H2O = AACD	k = 1.00E-17	1.00E-17
218	CGR2 + CO = ALD2	k = 1.20E-15	1.20E-15
219	CGR2 + H2O = ALD2 + H2O2	k = 6.00E-18	6.00E-18
220	CGR2 + SO2 = ALD2 + SULF	k = 7.00E-14	7.00E-14
221	CSL + NO3 = 0.5 NPHN + 0.2 AROO + 0.5 HNO3 + 0.3 BNZO + 0.44 OPN2	k = 1.40E-11	1.40E-11
222	CSL + OH = 0.727 MCT + 0.727 HO2 + 0.2 AROO + 0.073 BNZO + 0.44 OPN2	k = 4.70E-11	4.70E-11
223	DMS + OH + O2 = 0.75 SO2 + 0.25 MSA + MEOO	k = 1.28E-37 exp(4480/T)	4.33E-31
224	DMS + OH = SO2 + MEOO + HCHO	k = 1.20E-11 exp(-280/T)	4.69E-12
225	DMS + NO3 = SO2 + HNO3 + MEOO + HCHO	k = 1.90E-13 exp(530/T)	1.13E-12
226	EOH + OH = HO2 + ALD2	k = 3.35E-12	3.35E-12
227	ETLN + OH = HCHO + CO2 + NO2	k = 2.40E-12	2.40E-12
228	ETLN + NO3 = HNO3 + NO2 + MCO3	k = 1.40E-12 exp(-1860/T)	2.73E-15
229	ETHN + OH = GLYC + NO2	k = 8.40E-13	8.40E-13
230	ETHP + OH = OH + GLYC	k = 1.38E-11	1.38E-11
231	ETHP + OH = HEOO	k = 1.90E-12 exp(190/T)	3.59E-12
232	ETN + OH = ALD2 + NO2	k = 1.00E-12 exp(-490/T)	1.93E-13
233	ETAX + O2 = GLYC + HO2	k = 2.50E-14 exp(-300/T)	9.14E-15
234	ETAX = HO2 + 2 HCHO	k = 9.50E+13 exp(-5988/T)	1.78E+5
235	ETOO + ETOO = EOH + ALD2	k = 2.70E-14	2.70E-14
236	ETOO + ETOO = 2 ALD2 + 2 HO2	k = 4.10E-14	4.10E-14
237	ETOO + NO = ETN	k = 9.52E-15 (P/1013.0)^0.872 exp(916/T)	2.06E-13
238	ETOO + NO = ALD2 + NO2 + HO2	k = 2.66E-12 (P/1013.0)^-0.013 exp(351/T)	8.65E-12
239	HEOO + NO3 = ETAX + NO2	k = 2.30E-12	2.30E-12
240	HEOO + MEOO = 0.6 ETAX + 0.6 HO2 + 0.8 HCHO + 0.2 MOH + 0.2 ETHP + 0.2 GLYC	k = 6.00E-13	6.00E-13
241	HEOO + HO2 = ETHP	k = 1.53E-13 exp(1300/T)	1.20E-11
242	HEOO + NO = 0.995 ETAX + 0.995 NO2 + 0.005 ETHN	k = 2.70E-12 exp(360/T)	9.04E-12
243	ETPX + OH = 0.64 OH + 0.36 O2OO + 0.64 ALD2	k = 5.18E-12 exp(200/T)	1.01E-11

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
244	GLYC + OH = 0.732 HCHO + 0.361 CO2 + 0.505 CO + 0.227 OH + 0.773 HO2 + 0.134 GLY + 0.134 FACD	k = 1.85E-11 exp(-311/T)	6.51E-12
245	GLYC + OH = FACD + OH + CO	k = 3.32E-14 exp(1135/T)	1.50E-12
246	GLY + NO3 = HNO3 + HO2 + 2 CO	k = 1.01E-12 (P/1013.0)^-0.166 exp(-1903/T)	1.71E-15
247	GLY + OH = HO2 + 2 CO	k = 3.10E-12 exp(340/T)	9.70E-12
248	HAC + OH = MGLY + HO2	k = 1.53E-11 exp(-393/T)	4.09E-12
249	HAC + OH = 0.5 FACD + OH + 0.5 AACD + 0.5 CO2 + 0.5 CO + 0.5 MEOO	k = 1.21E-14 exp(1506/T)	1.89E-12
250	IHAL + OH = 1.065 OH + 0.355 CO2 + 0.638 CO + 0.355 MGLY + 0.283 HO2 + 0.294 IEAO + 0.125 MVPX + 0.158 MCHP + 0.068 IEBO	k = 4.64E-12 exp(650/T)	4.11E-11
251	FACD + OH = H2O + CO2 + HO2	k = 4.00E-13	4.00E-13
252	HMHP + OH = 0.5 HCHO + 0.5 HO2 + 0.5 FACD + 0.5 OH	k = 1.30E-12 exp(500/T)	6.96E-12
253	HMML + OH = 0.7 MGLY + 0.7 OH + 0.3 MCO3 + 0.3 FACD	k = 4.33E-12	4.33E-12
254	HO2 + ETOO = ETPX	k = 7.40E-13 exp(700/T)	7.75E-12
255	HO2 + O2OO = ETPX	k = 7.40E-13 exp(700/T)	7.75E-12
256	TNTR + OH = NO3 + HAC	k = k1 + k3 [M] / (1 + k3 [M] / k2) k1 = 2.41E-14 exp(460/T) k2 = 2.69E-17 exp(2199/T) k3 = 6.51E-34 exp(1335/T)	1.55E-13
257	HPA1 + OH = 0.035 MVK + 0.315 H1OO + 0.15 IDC + 0.33 MVPX + 0.085 HO2 + 0.085 HCHO + 0.085 MGLY + 0.085 ICHE + 1.085 OH + 0.45 CO	k = 1.17E-11 exp(450/T)	5.30E-11
258	H1OO + HO2 = OH + OH + CO2 + MVK	k = 2.38E-13 exp(1300/T)	1.87E-11
259	H1OO + NO = NO2 + OH + CO2 + MVK	k = 2.70E-12 exp(350/T)	8.74E-12
260	HPA2 + OH = 0.035 MACR + 0.315 H2OO + 0.15 IDC + 0.17 MCHP + 0.165 HO2 + 0.165 HCHO + 0.165 MGLY + 0.165 ICHE + 1.165 OH + 0.37 CO	k = 1.17E-11 exp(450/T)	5.30E-11
261	H2OO + HO2 = OH + OH + CO2 + MACR	k = 2.38E-13 exp(1300/T)	1.87E-11
262	H2OO + NO = NO2 + OH + CO2 + MACR	k = 2.70E-12 exp(350/T)	8.74E-12
263	HPA3 + OH = OH + 0.23 MVK + 0.42 CO + 0.19 MVPX + 0.58 ICHE	k = 2.20E-11 exp(390/T)	8.14E-11
264	HPA4 + OH = OH + 0.77 ICHE + 0.23 CO + 0.09 MCHP + 0.14 MACR	k = 3.50E-11 exp(390/T)	1.30E-10
265	ELPX + OH = GLY + OH	k = 2.91E-11	2.91E-11
266	ELPX + OH = CO + OH + HCHO	k = 1.55E-12 exp(340/T)	4.85E-12
267	ICHE + OH = OH + 1.5 CO + 0.5 HCHO + 0.5 MGLY + 0.5 HAC	k = 9.85E-12 exp(410/T)	3.90E-11
268	IEOO + NO = NO2 + 0.8 HAC + 0.8 CO + HCHO + HO2 + 0.2 MVHC	k = 3.23E-12 exp(290/T)	8.54E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
269	IEOO + NO = ITCN	k = 1.00E-16 (P/1013.0)^0.188 exp(2277/T)	2.09E-13
270	IEOO = HO2 + 2 CO + HAC + OH	k = 1.88E+13 exp(-10000/T)	5.00E-2
271	IEOO + HO2 = 0.35 IDHP + 0.65 OH + 0.52 CO + 0.13 MVHC + 0.65 HCHO + 0.65 HO2 + 0.52 HAC	k = 2.38E-13 exp(1300/T)	1.87E-11
272	ICN + OH = NO2 + ICHE	k = 8.98E-13 (P/1013.0)^-0.789 exp(139/T)	1.43E-12
273	ICN + OH = 0.244 OH + 0.539 CO + 0.295 HO2 + 0.378 MCNB + 0.461 INOO + 0.161 MVKN	k = 9.35E-12 exp(390/T)	3.46E-11
274	INOO + HO2 = 0.67 INOO + 0.33 CO2 + 0.33 CO + 0.33 HO2 + 0.231 PPNN + OH + 0.099 ETLN	k = 2.54E-13 exp(1300/T)	1.99E-11
275	INOO + NO = 0.67 INOO + 0.33 CO2 + 0.33 CO + 0.33 HO2 + 0.231 PPNN + NO2 + 0.099 ETLN	k = 2.70E-12 exp(350/T)	8.74E-12
276	IDHP + OH = CO + 0.5 HO2 + 0.5 OH + 0.5 MCHP + 0.35 MVDH + 0.15 MCDH	k = 1.00E-11	1.00E-11
277	IDC + OH = CO + HO2 + MVCX	k = 3.00E-12 exp(650/T)	2.66E-11
278	IHDP + OH = 0.888 CO + 0.444 OH + 0.444 HO2 + 0.318 MVHC + 0.08 IEAO + 0.126 MVHB + 0.444 MVCX + 0.032 IEBO	k = 2.25E-11	2.25E-11
279	IDDP + OH = OH + 0.333 IDHP + 0.667 IHPE	k = 3.00E-12	3.00E-12
280	IBNO + NO = 0.355 MCNB + 0.546 PPNN + 0.546 GLYC + 0.028 MVKN + 0.071 ETLN + 0.071 HAC + HO2 + NO2 + 0.383 HCHO	k = 1.14E-11 exp(-136/T)	7.22E-12
281	IBNO + NO = IDN	k = 1.31E-15 (P/1013.0)^0.03 exp(2103/T)	1.52E-12
282	IBNO + HO2 = 0.379 HO2 + 0.379 OH + 0.621 ITHN + 0.094 MCNB + 0.242 GLYC + 0.242 PPNN + 0.01 MVKN + 0.033 HAC + 0.033 ETLN + 0.104 HCHO	k = 2.60E-13 exp(1300/T)	2.04E-11
283	I1OO + NO = 0.935 PPNN + 0.935 GLYC + 0.065 MCNB + 0.065 HCHO + HO2 + NO2	k = 5.23E-12 exp(130/T)	8.09E-12
284	I1OO + NO = IDN	k = 2.36E-16 (P/1013.0)^0.034 exp(2368/T)	6.66E-13
285	I1OO = ITCN + HO2	k = 1.26E+13 exp(-10000/T)	3.35E-2
286	I1OO + HO2 = 0.418 ITHN + 0.551 PPNN + 0.551 GLYC + 0.031 MCNB + 0.031 HCHO + 0.582 HO2 + 0.582 OH	k = 2.60E-13 exp(1300/T)	2.04E-11
287	I2OO + NO = 0.858 HAC + 0.858 ETLN + 0.142 MVKN + 0.142 HCHO + HO2 + NO2	k = 9.27E-12 exp(-65/T)	7.45E-12
288	I2OO + NO = IDN	k = 8.72E-16 (P/1013.0)^0.031 exp(2174/T)	1.29E-12
289	I2OO + HO2 = 0.494 ITHN + 0.441 HAC + 0.441 ETLN + 0.065 MVKN + 0.065 HCHO + 0.506 OH + 0.506 HO2	k = 2.60E-13 exp(1300/T)	2.04E-11
290	I2OO = ITCN + HO2	k = 5.09E+12 exp(-10000/T)	1.36E-2

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
291	IHPE + OH = OH + CO2 + 0.571 MCHP + 0.429 MVPX	k = 3.00E-12	3.00E-12
292	IDN + OH = 0.565 NO2 + 0.565 ITHN + 0.435 IDNO	k = 1.00E-11	1.00E-11
293	IDNO + NO = PPNN + 1.11 NO2 + 0.11 GLYC + 0.89 ETLN + 0.89 HO2	k = 2.70E-12 exp(350/T)	8.74E-12
294	IDNO + HO2 = 0.18 IDN + 0.09 NO2 + 0.09 GLYC + 0.82 OH + 0.73 HO2 + 0.82 PPNN + 0.73 ETLN	k = 2.71E-13 exp(1300/T)	2.13E-11
295	IEPA + OH = 0.67 IEAO + 0.33 IEBO	k = 5.65E-11 (P/1013.0)^-0.143 exp(-465/T)	1.19E-11
296	IEPA + OH = ICHE + HO2	k = 1.05E-11 exp(-400/T)	2.74E-12
297	IEAO + NO = 0.2 MVDH + HO2 + NO2 + 0.2 CO + 0.8 GLYC + 0.8 MGLY	k = 3.23E-12 exp(290/T)	8.54E-12
298	IEAO + NO = ITCN	k = 1.00E-16 (P/1013.0)^0.188 exp(2277/T)	2.09E-13
299	IEAO = OH + CO + MVDH	k = 1.00E+7 exp(-5000/T)	5.17E-1
300	IEAO = IHDP + HO2	k = 1.88E+13 exp(-10000/T)	5.00E-2
301	IEAO + HO2 = 0.13 CO + 0.65 OH + 0.65 HO2 + 0.13 MVDH + 0.52 GLYC + 0.52 MGLY + 0.35 IDHP	k = 2.38E-13 exp(1300/T)	1.87E-11
302	IEPB + OH = 0.81 IEAO + 0.19 IEBO	k = 3.68E-11 (P/1013.0)^-0.116 exp(-453/T)	8.04E-12
303	IEPB + OH = ICHE + HO2	k = 8.25E-12 exp(-400/T)	2.16E-12
304	IEBO + NO = NO2 + HO2 + 0.8 GLY + 0.8 HAC + 0.2 CO + 0.2 MCDH	k = 3.12E-12 exp(302/T)	8.58E-12
305	IEBO + NO = ITCN	k = 7.70E-17 (P/1013.0)^0.189 exp(2289/T)	1.67E-13
306	IEBO = CO + OH + MCDH	k = 1.00E+7 exp(-5000/T)	5.17E-1
307	IEBO = IHDP + HO2	k = 1.88E+13 exp(-10000/T)	5.00E-2
308	IEBO + HO2 = 0.13 CO + 0.65 OH + 0.65 HO2 + 0.13 MCDH + 0.52 HAC + 0.52 GLY + 0.35 IDHP	k = 2.38E-13 exp(1300/T)	1.87E-11
309	IEPD + OH = 0.75 ICHE + 0.75 HO2 + 0.25 IEOO	k = 3.22E-11 exp(-400/T)	8.41E-12
310	IHN1 + OH = IEPD + NO2	k = 4.69E-12 (P/1013.0)^-0.789 exp(139/T)	7.48E-12
311	IHN1 + OH = I1OO	k = 2.04E-11 exp(390/T)	7.55E-11
312	IHN1 + OH = 0.6 OH + 0.6 CO + 0.6 MCNB + 0.4 HO2 + 0.4 ICN	k = 7.50E-12 exp(20/T)	8.02E-12
313	IHN2 + OH = 0.67 IEPA + 0.33 IEPB + NO2	k = 2.75E-12 (P/1013.0)^-0.692 exp(158/T)	4.67E-12
314	IHN2 + OH = IN1O	k = 7.14E-12 exp(390/T)	2.64E-11
315	IHN3 + OH = 0.67 IEPA + 0.33 IEPB + NO2	k = 3.39E-12 (P/1013.0)^-0.774 exp(141/T)	5.44E-12
316	IHN3 + OH = IN2O	k = 1.02E-11 exp(390/T)	3.78E-11

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
317	IHN4 + OH = IEPD + NO2	k = 2.88E-12 (P/1013.0)^-0.789 exp(139/T)	4.59E-12
318	IHN4 + OH = I2OO	k = 2.95E-11 exp(390/T)	1.09E-10
319	IHN4 + OH = 0.6 OH + 0.6 CO + 0.6 MVKN + 0.4 HO2 + 0.4 ICN	k = 7.50E-12 exp(20/T)	8.02E-12
320	IH1O = HCHO + OH + MVK	k = 8.10E+10 exp(-9685/T)	6.22E-4
321	IH1O + HO2 = RIPC	k = 1.64E-12 exp(-230/T)	7.59E-13
322	IH1O + HO2 = 0.063 MVK + 0.063 OH + 0.063 HO2 + 0.063 HCHO + 0.937 RIPA	k = 1.65E-13 exp(1361/T)	1.59E-11
323	IH1O + IH4O = HO2 + IHAL + CO + OH + 0.5 MVPX + 0.5 MCHP	k = 1.97E-11 exp(-1413/T)	1.72E-13
324	IH1O + IH4O = MACR + MVK + 2 HO2 + 2 HCHO	k = 2.30E-12 exp(70/T)	2.91E-12
325	IH1O + MEOO = HCHO + 0.5 IHAL + 1.5 HO2 + 0.5 MVPX + 0.5 CO + 0.5 OH	k = 1.55E-11 exp(-1530/T)	9.13E-14
326	IH1O + MEOO = MVK + 2 HO2 + 2 HCHO	k = 1.56E-12 exp(61/T)	1.91E-12
327	IH1O + IH1O = HO2 + IHAL + CO + OH + MVPX	k = 1.93E-11 exp(-1530/T)	1.14E-13
328	IH1O + IH1O = 2 MVK + 2 HO2 + 2 HCHO	k = 5.39E-14 exp(61/T)	6.61E-14
329	IH1O + NO = NO2 + MVK + HO2 + HCHO	k = 3.75E-12 (P/1013.0)^-0.054 exp(194/T)	7.19E-12
330	IH1O + NO = NO2 + 0.45 IHAL + 0.45 HO2 + 0.55 MVPX + 0.55 CO + 0.55 OH	k = 3.44E-11 (P/1013.0)^-0.046 exp(-1365/T)	3.52E-13
331	IH1O + NO = IHN2	k = 6.20E-15 (P/1013.0)^0.444 exp(1557/T)	1.15E-12
332	IH1O + NO = IHN4	k = 4.76E-14 (P/1013.0)^0.452 exp(-2/T)	4.72E-14
333	IH1O = 0.15 HPA3 + 0.25 HPA1 + 0.4 HO2 + 0.6 CO + 1.5 OH + 0.3 HCHO + 0.3 MGLY + 0.3 ELPX + 0.3 MCO3	k = 4.86E+12 exp(-10793/T)	9.06E-4
334	IH4O = MACR + OH + HCHO	k = 1.35E+11 exp(-9673/T)	1.08E-3
335	IH4O + HO2 = RIPD	k = 1.22E-12 exp(-34/T)	1.09E-12
336	IH4O + HO2 = 0.063 MACR + 0.063 OH + 0.063 HO2 + 0.063 HCHO + 0.937 RIPB	k = 1.52E-13 exp(1379/T)	1.55E-11
337	IH4O + MEOO = HCHO + 0.5 IHAL + 1.5 HO2 + 0.5 MCHP + 0.5 CO + 0.5 OH	k = 1.15E-11 exp(-1334/T)	1.31E-13
338	IH4O + MEOO = MACR + 2 HO2 + 2 HCHO	k = 1.43E-12 exp(79/T)	1.87E-12
339	IH4O + IH4O = HO2 + IHAL + CO + OH + MCHP	k = 2.27E-11 exp(-1334/T)	2.59E-13
340	IH4O + IH4O = 2 MACR + 2 HO2 + 2 HCHO	k = 4.11E-12 exp(79/T)	5.36E-12
341	IH4O + NO = NO2 + MACR + HO2 + HCHO	k = 3.32E-12 (P/1013.0)^-0.05 exp(228/T)	7.13E-12
342	IH4O + NO = NO2 + 0.45 HO2 + 0.45 IHAL + 0.55 MCHP + 0.55 CO + 0.55 OH	k = 2.58E-11 (P/1013.0)^-0.046 exp(-1172/T)	5.06E-13
343	IH4O + NO = IHN3	k = 5.03E-15 (P/1013.0)^0.448 exp(1591/T)	1.05E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
344	IH4O + NO = IHN1	k = 3.57E-14 (P/1013.0)^0.452 exp(191/T)	6.78E-14
345	IH4O = 0.15 HPA4 + 0.25 HPA2 + 1.5 OH + 0.3 HCHO + 0.9 CO + 0.7 HO2 + 0.3 MGLY + 0.3 ATPX	k = 4.09E+10 exp(-8613/T)	1.15E-2
346	IHBO + NO = 0.384 GLYC + 0.17 MCNB + 0.303 ELPX + 0.014 MVKN + 0.051 HAC + 0.013 ATPX + 0.059 MVPX + 0.006 MCHP + 0.687 PPNN + 0.064 ETLN + 0.249 HCHO + 1.065 NO2 + 0.5 HO2 + 0.435 OH	k = 4.64E-12 exp(170/T)	8.21E-12
347	IHBO + NO = IDN	k = 1.54E-16 (P/1013.0)^0.022 exp(2430/T)	5.37E-13
348	IHBO + HO2 = 0.234 ITHN + 0.06 MCNB + 0.34 GLYC + 0.249 ELPX + 0.004 MCHP + 0.008 MVKN + 0.009 ATPX + 0.054 MVPX + 0.042 HAC + 1.147 OH + 0.326 HO2 + 0.058 NO2 + 0.126 HCHO + 0.589 PPNN + 0.051 ETLN	k = 2.64E-13 exp(1300/T)	2.07E-11
349	IHBO = OH + 0.5 ITCN + 0.5 ITHN	k = 8.72E+12 exp(-10000/T)	2.33E-2
350	IHDO + NO = 0.291 MCNB + 0.59 ELPX + 0.07 ATPX + 0.049 MVKN + 0.59 PPNN + 0.07 ETLN + 0.34 HCHO + 1 NO2 + 0.904 HO2 + 0.096 OH	k = 5.60E-12 exp(107/T)	8.01E-12
351	IHDO + NO = IDN	k = 2.59E-16 (P/1013.0)^0.022 exp(2367/T)	7.28E-13
352	IHDO + HO2 = 0.387 ITHN + 0.073 MCNB + 0.471 ELPX + 0.015 MVKN + 0.054 ATPX + 0.646 OH + 0.58 HO2 + 0.088 HCHO + 0.471 PPNN + 0.054 ETLN	k = 2.64E-13 exp(1300/T)	2.07E-11
353	IHDO = OH + ITCN	k = 6.55E+12 exp(-10000/T)	1.75E-2
354	IP1O + NO = 0.716 MCHP + 0.716 HCHO + 0.284 ELPX + 0.284 HAC + NO2 + HO2	k = 8.36E-12 (P/1013.0)^-0.014 exp(-33/T)	7.49E-12
355	IP1O + NO = ITHN	k = 1.12E-15 (P/1013.0)^0.09 exp(2095/T)	1.26E-12
356	IP1O = 0.176 IDHP + 0.824 IHPE + OH	k = 1.59E+13 exp(-10000/T)	4.24E-2
357	IP1O + HO2 = 0.725 IDDP + 0.14 MCHP + 0.14 HCHO + 0.135 ELPX + 0.135 HAC + 0.275 OH + 0.275 HO2	k = 2.47E-13 exp(1300/T)	1.94E-11
358	IP2O + NO = 0.706 MVPX + 0.706 HCHO + 0.294 GLYC + 0.294 ATPX + NO2 + HO2	k = 7.68E-12 exp(-4/T)	7.57E-12
359	IP2O + NO = ITHN	k = 9.28E-16 (P/1013.0)^0.092 exp(2125/T)	1.16E-12
360	IP2O + HO2 = 0.725 IDDP + 0.14 MVPX + 0.14 HCHO + 0.135 GLYC + 0.135 ATPX + 0.275 OH + 0.275 HO2	k = 2.47E-13 exp(1300/T)	1.94E-11
361	IP2O = 0.548 IDHP + 0.452 IHPE + OH	k = 2.91E+13 exp(-10000/T)	7.77E-2
362	IP3O + NO = GLYC + HAC + NO2 + OH	k = 6.15E-12 (P/1013.0)^-0.01 exp(72/T)	7.83E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
363	IP3O + NO = ITHN	k = 5.59E-16 (P/1013.0)^0.095 exp(2201/T)	9.02E-13
364	IP3O = IHPE	k = 1.88E+13 exp(-10000/T)	5.00E-2
365	IP3O + HO2 = 0.35 IDDP + 0.65 GLYC + 0.65 HAC + 1.3 OH	k = 2.47E-13 exp(1300/T)	1.94E-11
366	INAX = IBNO	k = 1.00E+20 exp(-10000/T)	2.67E+5
367	INAX + O2 = ICN + HO2	k = 2.50E-14 exp(-300/T)	9.14E-15
368	INBO + INBO = 1.737 MVK + 0.123 MACR + 1.86 HCHO + 1.86 NO2 + 0.07 INPB + 0.07 ICN	k = 1.61E-12	1.61E-12
369	INBO + MCO3 = HCHO + NO2 + MEOO + 0.903 MVK + 0.097 MACR	k = 1.92E-12	1.92E-12
370	INBO + NO3 = HCHO + 2 NO2 + 0.903 MVK + 0.097 MACR	k = 2.30E-12	2.30E-12
371	INBO + INDO = 0.399 INPB + 0.544 MVK + 0.532 ICN + 0.563 NO2 + 0.474 INAX + 0.089 HO2 + 0.019 MACR + 0.563 HCHO + 0.032 IHN1	k = 2.56E-12	2.56E-12
372	INBO + MEOO = 0.355 INPB + 0.583 MVK + 0.028 MACR + 0.034 ICN + 0.611 HO2 + 1.577 HCHO + 0.611 NO2 + 0.034 MOH	k = 2.80E-13	2.80E-13
373	INBO + NO = 2 NO2 + HCHO + 0.096 MACR + 0.904 MVK	k = 3.36E-12 exp(276/T)	8.49E-12
374	INBO + NO = IDN	k = 7.29E-17 (P/1013.0)^0.102 exp(2405/T)	2.33E-13
375	INBO + HO2 = 0.473 INPB + 0.048 MACR + 0.479 MVK + 0.527 OH + 0.527 HCHO + 0.527 NO2	k = 2.47E-13 exp(1300/T)	1.94E-11
376	INDO + MEOO = 0.298 IHN1 + 0.057 IHN4 + 0.244 INAX + 0.401 ICN + 0.355 MOH + 0.336 HO2 + 0.645 HCHO	k = 1.18E-12	1.18E-12
377	INDO + NO3 = NO2 + 0.841 INAX + 0.159 HO2 + 0.159 ICN	k = 2.30E-12	2.30E-12
378	INDO + INDO = 0.064 HO2 + 0.34 INAX + 0.861 ICN + 0.671 IHN1 + 0.127 IHN4	k = 3.71E-12	3.71E-12
379	INDO + MCO3 = MEOO + 0.841 INAX + 0.159 HO2 + 0.159 ICN	k = 7.71E-12	7.71E-12
380	INDO + NO = NO2 + 0.159 HO2 + 0.159 ICN + 0.841 INAX	k = 1.25E-11 exp(-174/T)	6.98E-12
381	INDO + NO = IDN	k = 2.48E-15 (P/1013.0)^0.085 exp(1955/T)	1.75E-12
382	INDO + HO2 = INPD	k = 2.47E-13 exp(1300/T)	1.94E-11
383	INPB + OH = OH + ITHN	k = 4.08E-12 (P/1013.0)^-0.249 exp(284/T)	1.06E-11
384	INPB + OH = INBO	k = 2.28E-12 exp(200/T)	4.46E-12
385	INPB + OH = 0.67 IHBO + 0.33 IBNO	k = 5.88E-12 exp(390/T)	2.18E-11

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
386	INPD + OH = NO2 + ICHE	k = 4.52E-12 (P/1013.0)^-0.789 exp(139/T)	7.20E-12
387	INPD + OH = OH + ITHN	k = 8.06E-12 (P/1013.0)^-0.241 exp(287/T)	2.11E-11
388	INPD + OH = IHDO	k = 1.61E-11 exp(390/T)	5.96E-11
389	INPD + OH = INDO	k = 3.40E-12 exp(200/T)	6.65E-12
390	INPD + OH = ICN + OH	k = 7.50E-12 exp(20/T)	8.02E-12
391	IPRN + OH = ACET + NO2	k = 1.20E-12 exp(-320/T)	4.10E-13
392	ISOP + O3 = 0.416 MACR + 0.177 MVK + 0.28 OH + 0.407 CO2 + 0.407 CO + 0.407 MEOO + 0.16 HO2 + 0.58 CGR1 + 0.827 HCHO + 0.013 H2O2	k = 1.30E-17	1.30E-17
393	ISOP + OH = + IH4O	k = 2.71E-11 exp(76/T)	3.50E-11
394	ISOP + OH = + IH1O	k = 1.70E-11 exp(390/T)	6.29E-11
395	ISOP + OH = 0.3 HCHO + 0.15 HPA4 + 0.25 HPA2 + 1.5 OH + 0.9 CO + 0.7 HO2 + 0.3 MGLY + 0.3 ATPX	k = 6.46E-18 exp(3771/T)	2.02E-12
396	ISOP + OH = 0.3 MCO3 + 0.3 MGLY + 0.3 HCHO + 0.15 HPA3 + 0.25 HPA1 + 0.4 HO2 + 0.6 CO + 1.5 OH + 0.3 ELPX	k = 1.01E-14 exp(643/T)	8.75E-14
397	ISOP + NO3 = 0.465 INBO + 0.535 INDO	k = 2.95E-12 exp(450/T)	1.34E-11
398	IN1O + NO = 0.272 MCHN + 0.272 HCHO + 0.728 GLYC + 0.728 HAC + 0.272 HO2 + 1.728 NO2	k = 4.48E-12 exp(181/T)	8.22E-12
399	IN1O + NO = IDN	k = 1.51E-16 (P/1013.0)^0.035 exp(2420/T)	5.07E-13
400	IN1O = ITCN + HO2	k = 1.88E+13 exp(-10000/T)	5.00E-2
401	IN1O + HO2 = 0.482 ITHN + 0.059 MCHN + 0.059 HCHO + 0.459 GLYC + 0.459 HAC + 0.059 HO2 + 0.459 NO2 + 0.518 OH	k = 2.60E-13 exp(1300/T)	2.04E-11
402	IN2O + NO = MVKN + HCHO + HO2 + NO2	k = 4.07E-12 exp(214/T)	8.34E-12
403	IN2O + NO = IDN	k = 1.09E-16 (P/1013.0)^0.035 exp(2452/T)	4.08E-13
404	IN2O = ITCN + HO2	k = 1.88E+13 exp(-10000/T)	5.00E-2
405	IN2O + HO2 = 0.401 ITHN + 0.599 MVKN + 0.599 HCHO + 0.599 HO2 + 0.599 OH	k = 2.60E-13 exp(1300/T)	2.04E-11
406	ITCN + OH = CO + NO2 + 0.75 MVPX + 0.25 MCHP	k = 1.00E-11	1.00E-11
407	ITHN + OH = 0.3 OH + 0.62 HO2 + 0.92 ITCN + 0.037 IBNO + 0.041 INOO + 0.022 MCRL + 0.022 NO2 + 0.022 HCHO	k = 3.00E-12	3.00E-12
408	KOO + MEOO = 0.5 ALD2 + 0.5 MCO3 + 0.25 MEK + 0.75 HCHO + 0.25 MOH + 0.25 ROH + 0.5 HO2	k = 8.37E-14	8.37E-14
409	KOO + HO2 = 0.15 OH + 0.15 ALD2 + 0.15 MCO3 + 0.85 ATPX	k = 1.82E-13 exp(1300/T)	1.43E-11
410	KOO + MCO3 = MEOO + ALD2 + MCO3	k = 1.68E-12 exp(500/T)	8.99E-12
411	KOO + MCO3 = MEK + AACD	k = 1.87E-13 exp(500/T)	1.00E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
412	KOO + NO = 0.93 NO2 + 0.93 ALD2 + 0.93 MCO3 + 0.07 R4N	k = 2.70E-12 exp(350/T)	8.74E-12
413	LIM + NO3 = 0.5 OLNN + 0.5 OLND	k = 1.22E-11	1.22E-11
414	LIM + O3 = 0.85 OH + 0.1 HO2 + 0.16 O2OO + 0.42 KOO + 0.02 H2O2 + 0.14 CO + 0.46 PRPE + 0.04 HCHO + 0.79 MACR + 0.01 FACD + 0.07 RACD	k = 2.95E-15 exp(-783/T)	2.13E-16
415	LIM + OH = LMOO	k = 4.20E-11 exp(401/T)	1.61E-10
416	LMOO + NO3 = HO2 + NO2 + 0.385 PRPE + 0.385 HCHO + 0.615 MACR	k = 1.20E-12	1.20E-12
417	LMOO + HO2 = PIPX	k = 1.50E-11	1.50E-11
418	LMOO + NO = 0.686 HO2 + 0.78 NO2 + 0.22 MTNU + 0.289 PRPE + 0.231 HCHO + 0.491 RCHO + 0.058 HAC + 0.289 MEK	k = 4.00E-12	4.00E-12
419	LMOO + MEOO = HO2 + 0.192 PRPE + 1.04 HCHO + 0.308 MACR + 0.25 MOH + 0.25 ROH	k = 3.56E-14 exp(708/T)	3.83E-13
420	LMOO + MCO3 = 0.5 HO2 + 0.5 MEOO + 0.192 PRPE + 0.385 HCHO + 0.308 MACR + 0.5 RACD	k = 7.40E-13 exp(765/T)	9.64E-12
421	LVOC + OH = OH	k = 4.82E-11 exp(-400/T)	1.26E-11
422	MACR + O3 = 0.88 MGLY + 0.88 CGR1 + 0.12 HCHO + 0.12 OH + 0.12 CO + 0.12 MCO3	k = 1.40E-15 exp(-2100/T)	1.22E-18
423	MACR + NO3 = 0.32 HNO3 + 0.32 MAC3 + 0.68 OH + 0.68 CO + 0.68 PPNN	k = 1.80E-13 exp(-1190/T)	3.32E-15
424	MACR + OH = MAC3	k = 2.70E-12 exp(470/T)	1.31E-11
425	MACR + OH = 0.036 ATPX + 0.036 CO + 0.036 HO2 + 0.964 MCOO	k = 4.40E-12 exp(380/T)	1.57E-11
426	MAC3 + NO2 = MPAN	k = 2.07E-12 (P/1013.0)^0.079 exp(432/T)	8.82E-12
427	MAC3 + HO2 = 0.5 MPCD + 0.5 HCHO + 0.325 CO + 0.325 MEOO + 0.175 MCO3 + 0.5 CO2 + 0.5 OH + 0.13 O3	k = 3.14E-12 exp(580/T)	2.20E-11
428	MAC3 + NO = 0.35 MCO3 + 0.65 MEOO + 0.65 CO + HCHO + CO2 + NO2	k = 8.70E-12 exp(290/T)	2.30E-11
429	MPCD + OH = 0.165 MAC3 + 0.585 OH + 0.488 HAC + 0.488 CO + 0.098 HMML + 0.415 CO2 + 0.25 HCHO + 0.087 MCO3 + 0.162 MEOO	k = 1.66E-11	1.66E-11
430	MNOO + NO3 = HAC + 2 NO2 + CO2	k = 4.00E-12	4.00E-12
431	MNOO + NO2 = MPAN + NO2	k = 2.07E-12 (P/1013.0)^0.079 exp(432/T)	8.82E-12
432	MNOO + MEOO = 0.7 HAC + 0.7 CO2 + 0.7 NO2 + 0.7 HO2 + HCHO + 0.3 MCNB	k = 2.90E-12 exp(500/T)	1.55E-11
433	MNOO + HO2 = 0.5 HAC + 0.5 OH + 0.5 CO2 + 0.5 NO2 + 0.13 O3 + 0.37 MCHN + 0.13 MCNB	k = 3.14E-12 exp(580/T)	2.20E-11
434	MNOO + NO = HAC + 2 NO2 + CO2	k = 7.50E-12 exp(290/T)	1.98E-11
435	MCO3 + A3OO = MEOO + RCHO + HO2	k = 1.68E-12 exp(500/T)	8.99E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
436	MCO3 + ETOO = MEOO + ALD2 + HO2	k = 1.68E-12 exp(500/T)	8.99E-12
437	MCO3 + O2OO = MEOO + ALD2 + HO2	k = 1.68E-12 exp(500/T)	8.99E-12
438	MCO3 + POO = MEOO + ALD2 + HCHO + HO2	k = 1.68E-12 exp(500/T)	8.99E-12
439	MCO3 + MEOO = HCHO + MEOO + HO2	k = 1.80E-12 exp(500/T)	9.64E-12
440	MCO3 + A3OO = AACD + RCHO	k = 1.87E-13 exp(500/T)	1.00E-12
441	MCO3 + ETOO = AACD + ALD2	k = 1.87E-13 exp(500/T)	1.00E-12
442	MCO3 + O2OO = AACD + ALD2	k = 1.87E-13 exp(500/T)	1.00E-12
443	MCO3 + POO = AACD + 0.35 RCHO + 0.65 HAC	k = 1.87E-13 exp(500/T)	1.00E-12
444	MCO3 + MEOO = AACD + HCHO	k = 2.00E-13 exp(500/T)	1.07E-12
445	MCO3 + MCO3 = 2 MEOO	k = 2.50E-12 exp(500/T)	1.34E-11
446	MCO3 + HO2 = 0.13 O3 + 0.13 AACD + 0.37 APCD + 0.5 MEOO + 0.5 CO2 + 0.5 OH	k = 3.14E-12 exp(580/T)	2.20E-11
447	MCO3 + NO = MEOO + NO2 + CO2	k = 8.10E-12 exp(270/T)	2.00E-11
448	MCDH + OH = 0.16 MVHB + HO2 + 0.84 HAC + 0.84 CO	k = 2.40E-11 exp(70/T)	3.04E-11
449	MCRL + OH = 0.75 CO + 0.285 OH + 0.715 HO2 + 0.653 PYAC + 0.097 CO2 + 0.097 MCO3 + 0.063 MVHB + 0.187 MGLY + 0.187 FACD	k = 3.71E-12 exp(983/T)	1.00E-10
450	MCHN + OH = MNOO	k = 1.39E-11 exp(380/T)	4.98E-11
451	MCNB + OH = 0.25 CO + OH + PPNN + 0.75 CO2	k = 2.70E-12 exp(470/T)	1.31E-11
452	MCHP + OH = 0.77 CO + OH + 0.77 HAC + 0.23 ATPX + 0.23 CO2	k = 2.70E-12 exp(470/T)	1.31E-11
453	MCOO + NO = 0.86 HAC + 0.86 CO + 0.86 HO2 + NO2 + 0.14 MGLY + 0.14 HCHO	k = 3.50E-12 (P/1013.0)^-0.023 exp(254/T)	8.21E-12
454	MCOO + NO = MCHN	k = 2.31E-15 (P/1013.0)^0.475 exp(1617/T)	5.24E-13
455	MCOO + HO2 = 0.41 MCHP + 0.507 HAC + 0.507 CO + 0.507 HO2 + 0.59 OH + 0.59 O2 + 0.083 MGLY + 0.083 HCHO	k = 2.12E-13 exp(1300/T)	1.66E-11
456	MCOO = HAC + CO + OH	k = 2.90E+7 exp(-5297/T)	5.53E-1
457	MCT + OH = 0.3 BNZO + 0.7 AROO + 1.05 OPN1	k = 2.00E-11	2.00E-11
458	MCT + O3 = GLYC + HO2 + OH + OPN1	k = 9.20E-18	9.20E-18
459	MCT + NO3 = 0.5 NPHN + 0.5 HNO3 + 0.3 BNZO + 0.2 AROO + 0.3 OPN1	k = 9.90E-11	9.90E-11
460	MEK + NO3 = HNO3 + KOO	k = 8.00E-16	8.00E-16
461	MEK + OH = KOO + H2O	k = 1.30E-12 exp(-25/T)	1.20E-12
462	MENT + OH = HCHO + NO2	k = 8.00E-13 exp(-1000/T)	2.79E-14
463	MGLY + OH = MCO3 + CO	k = 1.50E-11	1.50E-11
464	MGLY + NO3 = HNO3 + CO + MCO3	k = 3.36E-12 exp(-1860/T)	6.54E-15
465	MEOO + OH = 0.13 MOH + 0.87 HCHO + 1.74 HO2	k = 1.60E-10	1.60E-10
466	MEOO + ETOO = 0.75 HCHO + 0.75 ALD2 + HO2 + 0.25 MOH + 0.25 EOH	k = 3.00E-13	3.00E-13

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
467	MEOO + O2OO = 0.75 HCHO + 0.75 ALD2 + HO2 + 0.25 MOH + 0.25 EOH	k = 3.00E-13	3.00E-13
468	MEOO + NO = MENT	k = 8.40E-16 exp(300/T)	2.30E-15
469	MEOO + NO = HCHO + HO2 + NO2	k = 2.80E-12 exp(300/T)	7.66E-12
470	MEOO + MEOO = MOH + HCHO + O2	k = 1.64E-14 exp(775/T)	2.21E-13
471	MEOO + MEOO = 2 HCHO + 2 HO2	k = 4.35E-13 exp(-367/T)	1.27E-13
472	MEOO + HO2 = MEPX + O2	k = 4.10E-13 exp(750/T)	5.08E-12
473	MEOO + NO2 = MPN	Falloff: F=0.6; n=1 k(0) = 1.00E-40 (T/300)^-4.8 k(inf) = 1.00E-18 (T/300)^2.1	2.37E-21
474	MOH + OH = HO2 + HCHO	k = 2.90E-12 exp(-345/T)	9.11E-13
475	MTNS + OH = TNTR	k = 4.80E-12	4.80E-12
476	MTNS + NO3 = TNTR	k = 3.15E-13 exp(-448/T)	7.01E-14
477	MTNU + O3 = TNTR	k = 1.67E-16	1.67E-16
478	MTNU + OH = TNTR	k = 7.29E-11	7.29E-11
479	MTNU + NO3 = TNTR	k = 3.15E-13 exp(-448/T)	7.01E-14
480	MEPX + OH = HCHO + OH + H2O	k = 1.14E-12 exp(200/T)	2.23E-12
481	MEPX + OH = MEOO + H2O	k = 2.66E-12 exp(200/T)	5.20E-12
482	MPAN + OH = 0.75 HMML + NO3 + 0.25 HAC + 0.25 CO	k = 2.90E-11	2.90E-11
483	MPAN = MAC3 + NO2	k = 1.58E+16 exp(-13500/T)	3.34E-4
484	TRPA + OH = MTOO	k = 1.21E-11 exp(440/T)	5.30E-11
485	TRPA + O3 = 0.85 OH + 0.1 HO2 + 0.62 KOO + 0.14 CO + 0.02 H2O2 + 0.65 RCHO + 0.53 MEK	k = 5.00E-16 exp(-530/T)	8.44E-17
486	TRPA + NO3 = 0.1 OLNN + 0.9 OLND	k = 8.33E-13 exp(490/T)	4.31E-12
487	OTRP + OH = MTOO	k = 1.21E-11 exp(440/T)	5.30E-11
488	OTRP + O3 = 0.85 OH + 0.1 HO2 + 0.62 KOO + 0.14 CO + 0.02 H2O2 + 0.65 RCHO + 0.53 MEK	k = 5.00E-16 exp(-530/T)	8.44E-17
489	OTRP + NO3 = 0.1 OLNN + 0.9 OLND	k = 8.33E-13 exp(490/T)	4.31E-12
490	MVK + OH = MVOO	k = 2.60E-12 exp(610/T)	2.01E-11
491	MVK + O3 = 0.545 MGLY + 0.5 CGR1 + 0.6 HCHO + 0.38 MCO3 + 0.1 HO2 + 0.08 OH + 0.18 CO + 0.075 PYAC + 0.045 H2O2	k = 8.50E-16 exp(-1520/T)	5.18E-18
492	MVDH + OH = 0.4 MVHB + 0.6 MVHC + HO2	k = 8.70E-12 exp(70/T)	1.10E-11
493	MVHC + OH = 2 CO + HO2 + MCO3	k = 2.00E-12 exp(70/T)	2.53E-12
494	MVHB + OH = OH + MGLY	k = 5.00E-12 exp(470/T)	2.42E-11
495	MVPX + OH = 0.53 MVHC + 0.47 MVHB + OH	k = 5.77E-11	5.77E-11
496	MVKN + OH = 0.241 HCHO + 0.69 NO3 + 0.02 OH + 0.449 MGLY + 0.449 FACD + 0.241 PYAC + 0.29 MVHB + 0.31 NO2 + 0.04 MCO3	k = 1.24E-12 exp(380/T)	4.44E-12
497	MVOO + NO = 0.758 MCO3 + 0.758 GLYC + 0.242 MGLY + 0.242 HCHO + 0.242 HO2 + NO2	k = 3.21E-12 (P/1013.0)^-0.015 exp(286/T)	8.39E-12
498	MVOO + NO = 0.438 MVKN	k = 1.38E-15 (P/1013.0)^0.483 exp(1649/T)	3.50E-13

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
499	MVOO + HO2 = 0.36 MCO3 + 0.36 GLYC + 0.665 OH + 0.305 HO2 + 0.255 MVHC + 0.335 MVPX + 0.05 MGLY + 0.05 HCHO	k = 2.12E-13 exp(1300/T)	1.66E-11
500	MVCX + OH = OH + CO + MGLY	k = 5.00E-12 exp(470/T)	2.42E-11
501	NO3 + HCHO = HNO3 + HO2 + CO	k = 5.80E-16	5.80E-16
502	NPHN + NO3 = 0.5 HNO3 + NO2 + 0.5 R4NO + OPN1	k = 2.60E-12	2.60E-12
503	NPHN + OH = 0.5 R4NO + OPN1 + 0.5 NO2	k = 3.47E-12	3.47E-12
504	NPRN + OH = RCHO + NO2	k = 7.10E-13	7.10E-13
505	NROO + HO2 = + HO2	k = 1.40E-12 exp(700/T)	1.47E-11
506	NROO + NO = + NO	k = 2.60E-12 exp(350/T)	8.41E-12
507	OCS + OH = CO2 + SO2	k = 1.10E-13 exp(-1200/T)	1.96E-15
508	OCS + O = CO + SO2	k = 2.10E-11 exp(-2200/T)	1.31E-14
509	OH + CH4 = MEOO + H2O	k = 2.45E-12 exp(-1775/T)	6.34E-15
510	OH + ECH4 = MEOO + H2O	k = 2.45E-12 exp(-1775/T)	6.34E-15
511	OH + RCHO = RCO3 + H2O	k = 6.00E-12 exp(410/T)	2.38E-11
512	OH + APCD = MCO3	k = 6.13E-13 exp(200/T)	1.20E-12
513	OLND + NO3 = 2 NO2 + 0.287 HCHO + 1.24 RCHO + 0.464 MEK	k = 1.20E-12	1.20E-12
514	OLND + NO = 2 NO2 + 0.287 HCHO + 1.24 RCHO + 0.464 MEK	k = 4.00E-12	4.00E-12
515	OLND + HO2 = 0.7 MTNS + 0.3 MTNU	k = 1.66E-13 exp(1300/T)	1.30E-11
516	OLND + OLND = NO2 + 0.504 HCHO + 1.21 RCHO + 0.285 MEK + 0.7 MTNS + 0.3 MTNU	k = 2.96E-14 exp(1000/T)	8.49E-13
517	OLND + MCO3 = 0.5 MEOO + NO2 + 0.287 HCHO + 1.24 RCHO + 0.464 MEK + 0.5 RACD	k = 5.37E-13 exp(765/T)	7.00E-12
518	OLND + MEOO = 0.5 HO2 + 0.5 NO2 + 0.965 HCHO + 0.93 RCHO + 0.348 MEK + 0.25 MOH + 0.25 ROH + 0.35 MTNS + 0.15 MTNU	k = 9.68E-14 exp(708/T)	1.04E-12
519	OLNN + NO3 = HO2 + NO2 + 0.7 MTNS + 0.3 MTNU	k = 1.20E-12	1.20E-12
520	OLNN + NO = HO2 + NO2 + MTNS	k = 4.00E-12	4.00E-12
521	OLNN + MEOO = 2 HO2 + HCHO + 0.7 MTNS + 0.3 MTNU	k = 1.60E-13 exp(708/T)	1.72E-12
522	OLNN + HO2 = 0.7 MTNS + 0.3 MTNU	k = 1.66E-13 exp(1300/T)	1.30E-11
523	OLNN + OLND = 0.5 HO2 + 0.5 NO2 + 0.202 HCHO + 0.64 RCHO + 0.149 MEK + 1.05 MTNS + 0.45 MTNU	k = 4.25E-14 exp(1000/T)	1.22E-12
524	OLNN + OLNN = HO2 + 1.4 MTNS + 0.6 MTNU	k = 7.00E-14 exp(1000/T)	2.01E-12
525	OLNN + MCO3 = HO2 + MEOO + 0.7 MTNS + 0.3 MTNU	k = 8.85E-13 exp(765/T)	1.15E-11
526	O2OO + O2OO = EOH + ALD2	k = 2.70E-14	2.70E-14
527	O2OO + O2OO = 2 ALD2 + 2 HO2	k = 4.10E-14	4.10E-14
528	O2OO + NO = ALD2 + NO2 + HO2	k = 2.60E-12 exp(365/T)	8.85E-12
529	PHEN + NO3 = 0.258 NPHN + 0.742 HNO3 + 0.742 BNZO	k = 3.80E-12	3.80E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
530	PHEN + OH = 0.06 BNZO + 0.06 GLY + 0.18 OPN1 + 0.14 AROO + 0.8 MCT + 0.8 HO2	k = 4.70E-13 exp(1220/T)	2.82E-11
531	MTOO + NO3 = HO2 + NO2 + RCHO + MEK	k = 1.20E-12	1.20E-12
532	MTOO + HO2 = PIPX	k = 1.50E-11	1.50E-11
533	MTOO + NO = 0.82 HO2 + 0.82 NO2 + 0.23 HCHO + 0.43 RCHO + 0.11 ACET + 0.44 MEK + 0.07 FACD + 0.12 MTNS + 0.06 MTNU	k = 4.00E-12	4.00E-12
534	MTOO + MEOO = HO2 + 0.75 HCHO + 0.25 MOH + 0.25 ROH + 0.75 RCHO + 0.75 MEK	k = 3.56E-14 exp(708/T)	3.83E-13
535	MTOO + MCO3 = 0.5 HO2 + 0.5 MEOO + RCHO + MEK + RACD	k = 7.40E-13 exp(765/T)	9.64E-12
536	PIPX + OH = 0.49 OH + 0.44 R4OO + 0.08 RCHO + 0.41 MEK	k = 3.40E-12 exp(190/T)	6.43E-12
537	POO + MEOO = HO2 + 0.5 ALD2 + 1.25 HCHO + 0.16 HAC + 0.09 RCHO + 0.25 MOH + 0.25 ROH	k = 5.92E-13	5.92E-13
538	POO + HO2 = PPX	k = 1.51E-13 exp(1300/T)	1.19E-11
539	POO + NO = NO2 + HO2 + HCHO + ALD2	k = 2.70E-12 exp(350/T)	8.74E-12
540	PPX + OH = 0.791 OH + 0.209 POO + 0.791 HAC	k = 8.78E-12 exp(200/T)	1.72E-11
541	RCO3 + NO2 = PPN	Falloff: F=0.6; n=1 k(0) = 9.00E-28 (T/300)^-8.9 k(inf) = 7.70E-12 (T/300)^0.2	7.39E-12
542	PPN = RCO3 + NO2	k = k(ref) K k(ref) = k(541) K = 9.00E-29 exp(14000/T)	3.25E-4
543	PRNO + MEOO = NO2 + 0.5 HCHO + 0.5 ALD2 + 0.25 RCHO + 0.75 HCHO + 0.25 MOH + 0.25 ROH + 0.5 HO2	k = 8.37E-14	8.37E-14
544	PRNO + HO2 = PNPX	k = 1.51E-13 exp(1300/T)	1.19E-11
545	PRNO + MCO3 = MEOO + NO2 + HCHO + ALD2	k = 1.68E-12 exp(500/T)	8.99E-12
546	PRNO + MCO3 = RCHO + AACD + NO2	k = 1.87E-13 exp(500/T)	1.00E-12
547	PRNO + NO = 2 NO2 + HCHO + ALD2	k = 2.70E-12 exp(350/T)	8.74E-12
548	PPNN + OH = NO2 + MGLY	k = 6.70E-13	6.70E-13
549	PRPE + NO3 = PRNO	k = 4.59E-13 exp(-1156/T)	9.49E-15
550	PRPE + O3 = 0.5 ALD2 + 0.5 HCHO + 0.12 CGR2 + 0.1 CH4 + 0.12 CGR1 + 0.28 MEOO + 0.56 CO + 0.28 HO2 + 0.36 OH	k = 5.50E-15 exp(-1880/T)	1.00E-17
551	PRPE + OH = POO	Falloff: F=0.5; n=1.13 k(0) = 4.60E-27 (T/300)^-4 k(inf) = 2.60E-11 (T/300)^1.3	2.43E-11
552	PNPX + OH = 0.209 PRNO + 0.791 OH + 0.791 PPNN	k = 8.78E-12 exp(200/T)	1.72E-11
553	PYAC + OH = MCO3 + CO2	k = 8.00E-13	8.00E-13
554	R4NO + MEOO = NO2 + 0.2 HCHO + 0.38 ALD2 + 0.29 RCHO + 0.15 R4OO + 0.25 RCHO + 0.75 HCHO + 0.25 MOH + 0.25 ROH + 0.5 HO2	k = 8.37E-14	8.37E-14

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
555	R4NO + MCO3 = MEOO + NO2 + 0.39 HCHO + 0.75 ALD2 + 0.57 RCHO + 0.3 R4OO	k = 1.68E-12 exp(500/T)	8.99E-12
556	R4NO + MCO3 = RCHO + AACD + NO2	k = 1.87E-13 exp(500/T)	1.00E-12
557	R4NO + NO = 2 NO2 + 0.57 RCHO + 0.86 ALD2 + 0.57 HCHO	k = 2.70E-12 exp(350/T)	8.74E-12
558	R4NO + HO2 = R4N	k = 7.40E-13 exp(700/T)	7.75E-12
559	R4N + OH = R4NO + H2O	k = 1.60E-12	1.60E-12
560	R4OO + MEOO = 0.16 ACET + 0.1 MEK + 0.09 MEOO + 0.14 HO2 + 0.16 ALD2 + 0.07 RCHO + 0.03 A3OO + 0.09 B3OO + 0.16 O2OO + 0.25 MEK + 0.75 HCHO + 0.25 MOH + 0.25 ROH + 0.5 HO2	k = 8.37E-14	8.37E-14
561	R4OO + NO = R4N	k = 6.37E-15 (P/1013.0)^0.511 exp(1487/T)	9.35E-13
562	R4OO + NO = NO2 + 0.32 ACET + 0.19 MEK + 0.19 MEOO + 0.27 HO2 + 0.32 ALD2 + 0.14 RCHO + 0.05 A3OO + 0.18 B3OO + 0.32 O2OO	k = 4.12E-12 (P/1013.0)^-0.046 exp(190/T)	7.80E-12
563	R4OO + MCO3 = MEOO + 0.32 ACET + 0.19 MEK + 0.27 HO2 + 0.32 ALD2 + 0.13 RCHO + 0.05 A3OO + 0.18 B3OO + 0.32 O2OO	k = 1.68E-12 exp(500/T)	8.99E-12
564	R4OO + MCO3 = MEK + AACD	k = 1.87E-13 exp(500/T)	1.00E-12
565	R4OO + HO2 = R4PX	k = 7.40E-13 exp(700/T)	7.75E-12
566	R4PX + OH = 0.791 OH + 0.209 R4OO + 0.791 RCHO	k = 8.78E-12 exp(200/T)	1.72E-11
567	A3PX + OH = 0.64 OH + 0.36 A3OO + 0.64 RCHO	k = 5.18E-12 exp(200/T)	1.01E-11
568	B3PX + OH = 0.791 OH + 0.209 B3OO + 0.791 ACET	k = 8.78E-12 exp(200/T)	1.72E-11
569	RCHO + NO3 = HNO3 + RCO3	k = 6.50E-15	6.50E-15
570	RCO3 + MEOO = HCHO + HO2 + 0.5 O2OO + 0.07 A3OO + 0.27 B3OO	k = 1.68E-12 exp(500/T)	8.99E-12
571	RCO3 + MEOO = RACD + HCHO	k = 1.87E-13 exp(500/T)	1.00E-12
572	RCO3 + MCO3 = MEOO + 0.5 O2OO + 0.07 A3OO + 0.27 B3OO	k = 2.50E-12 exp(500/T)	1.34E-11
573	RCO3 + HO2 = 0.41 RPX + 0.15 RACD + 0.15 O3 + 0.44 OH + 0.22 O2OO + 0.03 A3OO + 0.12 B3OO	k = 4.30E-13 exp(1040/T)	1.41E-11
574	RCO3 + NO = NO2 + 0.5 O2OO + 0.07 A3OO + 0.27 B3OO	k = 6.70E-12 exp(340/T)	2.10E-11
575	RIPA + OH = 0.67 IEPA + 0.33 IEPB + OH + 0.005 LVOC	k = 1.61E-11 (P/1013.0)^-0.066 exp(359/T)	5.37E-11
576	RIPA + OH = 0.655 IP3O + 0.345 IP1O + 0.005 LVOC	k = 2.47E-12 exp(390/T)	9.14E-12
577	RIPA + OH = 0.75 IH1O + 0.125 MVK + 0.25 CO + 0.125 MVPX + 0.25 HO2 + 0.005 LVOC	k = 6.10E-12 exp(200/T)	1.19E-11
578	RIPB + OH = 0.68 IEPA + 0.32 IEPB + OH + 0.005 LVOC	k = 2.83E-11 (P/1013.0)^-0.066 exp(359/T)	9.45E-11
579	RIPB + OH = 0.51 IH4O + 0.16 IEOO + 0.33 CO + 0.33 HO2 + 0.165 MACR + 0.165 MCHP + 0.005 LVOC	k = 4.10E-12 exp(200/T)	8.02E-12

Number	Reactants and Products [a]	Rate Constant Expression	k_{298} [b,c]
580	RIPB + OH = 0.655 IP3O + 0.345 IP2O + 0.005 LVOC	k = 4.35E-12 exp(390/T)	1.61E-11
581	RIPC + OH = 0.595 IP1O + 0.03 IH1O + 0.06 IHAL + 0.024 HO2 + 0.009 HPA3 + 0.015 HPA1 + 0.405 OH + 0.036 CO + 0.018 HCHO + 0.018 MGLY + 0.018 ELPX + 0.018 MCO3 + 0.255 IEPD + 0.005 LVOC	k = 3.53E-11 exp(390/T)	1.31E-10
582	RIPD + OH = 0.255 IP2O + 0.03 IH4O + 0.745 OH + 0.06 IHAL + 0.009 HPA4 + 0.015 HPA2 + 0.042 HO2 + 0.018 HCHO + 0.054 CO + 0.018 MGLY + 0.018 ATPX + 0.595 IEPD + 0.005 LVOC	k = 3.53E-11 exp(390/T)	1.31E-10
583	ROH + OH = HO2 + RCHO	k = 4.60E-12 exp(70/T)	5.82E-12
584	RPX + OH = RCO3	k = 6.13E-13 exp(200/T)	1.20E-12
585	TOLU + OH = 0.19 CSL + 0.19 HO2 + 0.81 AROO + 0.06 BALD + 0.12 GLY + 0.12 MGLY + 0.27 CO + 0.04 MVK + 0.3 OPN2 + 0.68 OPN1	k = 1.80E-12 exp(340/T)	5.63E-12
586	XYLE + OH = 0.15 CSL + 0.15 HO2 + 0.85 AROO + 0.06 BALD + 0.1 GLYX + 0.2 MGLY + 0.3 CO + 0.04 MVK + 0.56 OPN2 + 0.28 OPN1 + 0.45 RACD	k = 1.70E-11	1.70E-11
587	NO + NO + O2 = 2. NO2	k = 4.25E-39 exp(664/T)	3.95E-38
588	N2O5 + H2O = 2 HNO3	k = 1.00E-22	1.00E-22
589	SO2 = SULF	k = 0.00E+0	0.00E+0
590	R4N = HNO3	k = 2.30E-5	2.30E-5
591	NPHN = HNO3	k = 2.30E-5	2.30E-5
592	MVKN = HNO3	k = 2.30E-5	2.30E-5
593	MCHN = HNO3	k = 2.30E-5	2.30E-5
594	MCNB = HNO3	k = 2.30E-5	2.30E-5
595	IHN1 = HNO3	k = 2.30E-5	2.30E-5
596	IHN2 = HNO3	k = 2.30E-5	2.30E-5
597	IHN3 = HNO3	k = 2.30E-5	2.30E-5
598	IHN4 = HNO3	k = 2.30E-5	2.30E-5
599	INPB = HNO3	k = 2.30E-5	2.30E-5
600	INPD = HNO3	k = 2.30E-5	2.30E-5
601	ITCN = HNO3	k = 2.30E-5	2.30E-5
602	ITHN = HNO3	k = 2.30E-5	2.30E-5
603	IDN = HNO3	k = 2.30E-5	2.30E-5
604	MTNS = HNO3	k = 2.30E-5	2.30E-5
605	MTNU = HNO3	k = 2.30E-5	2.30E-5
606	TNTR = HNO3	k = 2.30E-5	2.30E-5

(a) Products O2, CO2 and H2O are sometimes listed
(b) k_{298} is the rate constant at 298 K and 1 atmosphere using units in molecules/cm^3 and 1/s.
(c) For photolysis reactions k_{298} shows the photolysis rate at a solar zenith angle of 60° and height of 600 m MSL/AGL.

Table 4. Photolysis rates (s^{-1}) at several zenith angles.[a]

No.	Reactant	Zenith Angle 0°	Zenith Angle 20°	Zenith Angle 40°	Zenith Angle 60°	Zenith Angle 78°
1	NO2	1.01E-02	9.77E-03	8.75E-03	6.30E-03	2.09E-03
2	O3	4.26E-04	4.19E-04	3.94E-04	3.33E-04	1.79E-04
3	O3	4.55E-05	3.99E-05	2.54E-05	8.78E-06	9.20E-07
4	H2O2	8.79E-06	8.26E-06	6.64E-06	3.78E-06	8.81E-07
5	NO3	1.88E-01	1.86E-01	1.79E-01	1.56E-01	8.22E-02
6	NO3	2.32E-02	2.31E-02	2.23E-02	1.98E-02	1.12E-02
7	N2O5	5.54E-05	5.23E-05	4.26E-05	2.52E-05	6.30E-06
8	HNO2	1.74E-03	1.68E-03	1.49E-03	1.04E-03	3.29E-04
9	HNO3	8.47E-07	7.70E-07	5.57E-07	2.54E-07	4.20E-08
10	HNO4	1.58E-06	1.49E-06	1.19E-06	6.80E-07	1.59E-07
11	HNO4	6.24E-06	5.87E-06	4.71E-06	2.68E-06	6.26E-07
12	PAN	9.53E-07	8.81E-07	6.72E-07	3.47E-07	7.05E-08
13	MEPX	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
14	HCHO	4.16E-05	3.90E-05	3.10E-05	1.69E-05	3.55E-06
15	HCHO	5.43E-05	5.18E-05	4.35E-05	2.69E-05	7.06E-06
16	ALD2	7.29E-06	6.59E-06	4.65E-06	1.96E-06	2.54E-07
17	ALD2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
18	RCHO	6.88E-05	6.41E-05	4.99E-05	2.62E-05	5.17E-06
19	GLYC	9.03E-06	8.24E-06	6.01E-06	2.76E-06	4.40E-07
20	GLY	7.87E-06	7.35E-06	5.78E-06	3.12E-06	6.63E-07
21	GLY	3.52E-05	3.32E-05	2.70E-05	1.57E-05	3.83E-06
22	GLY	7.99E-05	7.69E-05	6.67E-05	4.53E-05	1.43E-05
23	MGLY	2.36E-04	2.29E-04	2.04E-04	1.46E-04	4.92E-05
24	MVK	3.85E-07	3.63E-07	2.95E-07	1.72E-07	4.17E-08
25	MVK	3.85E-07	3.63E-07	2.95E-07	1.72E-07	4.17E-08
26	MVK	3.85E-07	3.63E-07	2.95E-07	1.72E-07	4.17E-08
27	MEK	1.16E-06	1.02E-06	6.50E-07	2.27E-07	2.34E-08
28	ACET	5.12E-07	4.51E-07	2.92E-07	1.04E-07	1.13E-08
29	ACET	5.12E-07	4.51E-07	2.92E-07	1.04E-07	1.13E-08

No.	Reactant	Zenith Angle 0°	Zenith Angle 20°	Zenith Angle 40°	Zenith Angle 60°	Zenith Angle 78°
30	MACR	4.64E-06	4.46E-06	3.84E-06	2.52E-06	7.22E-07
31	PIPX	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
32	ICN	4.60E-05	4.22E-05	3.11E-05	1.48E-05	2.59E-06
33	ETLN	3.29E-05	3.01E-05	2.22E-05	1.06E-05	1.85E-06
34	MVKN	4.60E-05	4.22E-05	3.11E-05	1.48E-05	2.59E-06
35	MCHN	6.91E-05	6.32E-05	4.67E-05	2.22E-05	3.88E-06
36	MCNB	3.29E-05	3.01E-05	2.22E-05	1.06E-05	1.85E-06
37	MTNS	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07
38	MTNU	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07
39	TNTR	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07
40	MENT	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07
41	ETN	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07
42	IPRN	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07
43	NPRN	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07
44	RIPA	6.62E-06	6.24E-06	5.07E-06	2.95E-06	7.17E-07
45	RIPB	6.62E-06	6.24E-06	5.07E-06	2.95E-06	7.17E-07
46	RIPC	6.62E-06	6.24E-06	5.07E-06	2.95E-06	7.17E-07
47	RIPD	6.62E-06	6.24E-06	5.07E-06	2.95E-06	7.17E-07
48	HPA1	2.36E-04	2.29E-04	2.04E-04	1.46E-04	4.92E-05
49	HPA2	2.36E-04	2.29E-04	2.04E-04	1.46E-04	4.92E-05
50	HPA3	2.36E-04	2.29E-04	2.04E-04	1.46E-04	4.92E-05
51	HPA4	2.36E-04	2.29E-04	2.04E-04	1.46E-04	4.92E-05
52	IHN1	4.60E-05	4.22E-05	3.11E-05	1.48E-05	2.59E-06
53	IHN2	4.60E-05	4.22E-05	3.11E-05	1.48E-05	2.59E-06
54	IHN3	4.60E-05	4.22E-05	3.11E-05	1.48E-05	2.59E-06
55	IHN4	4.60E-05	4.22E-05	3.11E-05	1.48E-05	2.59E-06
56	INPB	4.60E-05	4.22E-05	3.11E-05	1.48E-05	2.59E-06
57	INPD	6.02E-05	5.68E-05	4.61E-05	2.68E-05	6.52E-06
58	INPD	4.60E-05	4.22E-05	3.11E-05	1.48E-05	2.59E-06
59	IDHP	2.36E-04	2.29E-04	2.04E-04	1.46E-04	4.92E-05

No.	Reactant	Zenith Angle 0°	Zenith Angle 20°	Zenith Angle 40°	Zenith Angle 60°	Zenith Angle 78°
60	IDHP	3.19E-05	3.01E-05	2.44E-05	1.42E-05	3.46E-06
61	IDDP	6.38E-05	6.02E-05	4.88E-05	2.84E-05	6.91E-06
62	IHPE	3.19E-05	3.01E-05	2.44E-05	1.42E-05	3.46E-06
63	IHDP	3.19E-05	3.01E-05	2.44E-05	1.42E-05	3.46E-06
64	ITHN	6.02E-05	5.68E-05	4.61E-05	2.68E-05	6.52E-06
65	ITHN	4.60E-05	4.22E-05	3.11E-05	1.48E-05	2.59E-06
66	ITCN	9.21E-05	8.43E-05	6.22E-05	2.96E-05	5.18E-06
67	ITCN	2.36E-04	2.29E-04	2.04E-04	1.46E-04	4.92E-05
68	ETHP	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
69	BALD	4.86E-05	4.71E-05	4.18E-05	2.92E-05	9.20E-06
70	BPCD	8.79E-07	8.26E-07	6.64E-07	3.78E-07	8.81E-08
71	BZPX	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
72	NPHN	1.51E-04	1.47E-04	1.31E-04	9.45E-05	3.13E-05
73	HAC	3.07E-05	2.98E-05	2.65E-05	1.89E-05	6.39E-06
74	IDN	9.21E-05	8.43E-05	6.22E-05	2.96E-05	5.18E-06
75	PNPX	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07
76	ETPX	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
77	A3PX	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
78	B3PX	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
79	R4PX	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
80	PPX	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
81	RPX	8.79E-07	8.26E-07	6.64E-07	3.78E-07	8.81E-08
82	HMHP	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07
83	ELPX	6.88E-05	6.41E-05	4.99E-05	2.62E-05	5.17E-06
84	PYAC	2.36E-04	2.29E-04	2.04E-04	1.46E-04	4.92E-05
85	PPNN	3.29E-05	3.01E-05	2.22E-05	1.06E-05	1.85E-06
86	MVHC	3.19E-05	3.01E-05	2.44E-05	1.42E-05	3.46E-06
87	MVHB	3.19E-05	3.01E-05	2.44E-05	1.42E-05	3.46E-06
88	MVPX	3.19E-05	3.01E-05	2.44E-05	1.42E-05	3.46E-06
89	MVCX	2.60E-04	2.52E-04	2.24E-04	1.60E-04	5.41E-05

No.	Reactant	Zenith Angle 0°	Zenith Angle 20°	Zenith Angle 40°	Zenith Angle 60°	Zenith Angle 78°
90	MCRL	2.60E-04	2.52E-04	2.24E-04	1.60E-04	5.41E-05
91	MCHP	3.19E-05	3.01E-05	2.44E-05	1.42E-05	3.46E-06
92	MPCD	3.19E-05	3.01E-05	2.44E-05	1.42E-05	3.46E-06
93	ATPX	8.79E-07	8.26E-07	6.64E-07	3.78E-07	8.81E-08
94	R4N	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07
95	APCD	8.79E-07	8.26E-07	6.64E-07	3.78E-07	8.81E-08

(a) Photolysis rates calculated with TUV at 0.600 km above the surface using an O_3 column of 0.300 (equivalent to 300 Dobson units) and an albedo of 0.040

3.0 Texas Box Model Scenarios

CAMx box model runs are effectively 1-D simulations with emissions and meteorology that represent a limited area. Although box models are limited in their ability to represent spatial variations in concentrations, they have advantages of simplicity and are useful to investigate atmospheric chemistry such as the response of O_3 to NOx and VOC changes (Finlayson-Pitts and Pitts, 1999).

The modeling domains for the CAMx box model used in this study are each 3 x 3 x 2 grid cells (in the x, y, and z dimensions). This is the smallest allowable CAMx domain since edge grid cells containing boundary conditions (BCs) are required by CAMx and 2 layers is the minimum allowed by the solution of vertical transport. All 9 grid cells in each layer have identical meteorological input data. The center grid cells of each domain, i.e. (2,2,1) and (2,2,2), form a 1-D column with layer 1 representing the planetary boundary layer (PBL) and layer 2 representing a residual layer between the PBL and the CAMx top. The PBL depth varies in time, as modeled by WRF for the TCEQ 2019 modeling platform, whereas the top of layer 2 is constant in time at 3,000 m. Horizontal wind speeds in layer 1 are set to zero, preventing horizontal exchange between grid cells and ensuring BCs are not used to compute concentrations. In layer 2, there is a constant horizontal wind speed to purge the layer with a 12-hour lifetime to limit the accumulation of pollutants over time. In this study, the model was run at a 4 km resolution. Since achieving spatial resolution is not a goal of the box model, the grid size is nominal.

Box model simulations were conducted for five Texas locations: Houston-Galveston-Brazoria (HGB), Dallas-Fort Worth (DFW), San Antonio (SAN), El Paso (ELP), and Tyler (TYL). A rectangular area was chosen to represent each of the five locations, shown in Figure 1. The HGB location is defined by a rectangular area containing Harris County, DFW contains Dallas and Tarrant Counties, SAN contains Bexar County, and TYL contains Smith County. A smaller area containing downtown El Paso was used for ELP due to the proximity of the Mexico border and the complex terrain in the region. CAMx box model input data (i.e., meteorology and initial conditions) were derived from the TCEQ 2019 modeling platform (TCEQ, 2022). Data was averaged over the grid cells within each of the rectangular location areas shown in Figure 1.

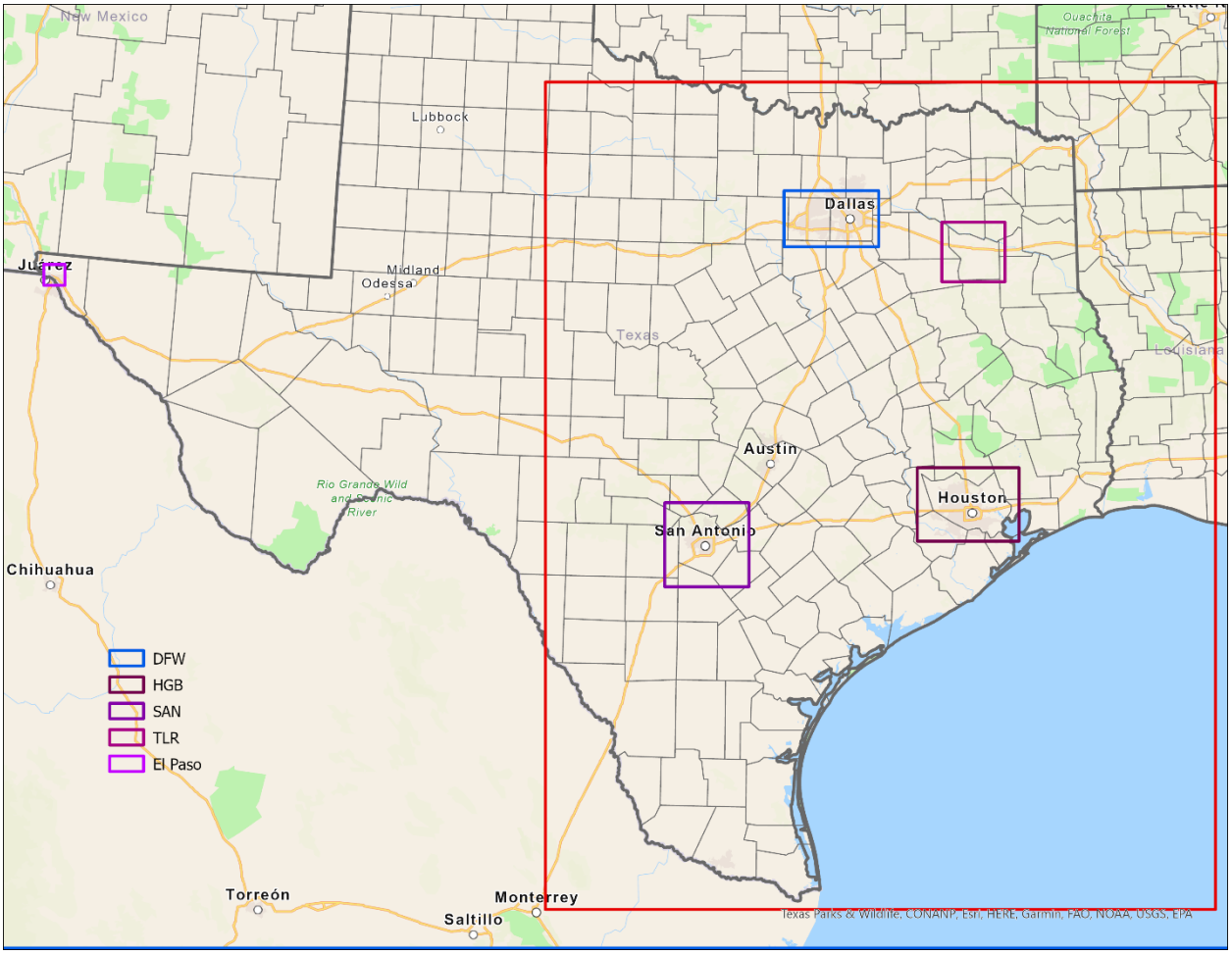

Figure 1. Modeling regions for each of the five Texas locations. DFW, HGB, SAN, and TYL are in the CAMx 4 km modeling domain (outlined in red) and ELP is in the 12 km domain.

Modeling periods for each location are provided in Table 5 and were chosen considering the following factors.

1. Since CAMx input data are extracted from the TCEQ 2019 modeling platform, dates must be between April and October 2019.

2. A multi-day period (4-5 days) with higher 8-hour ozone concentrations near the 2019 design value (DV) was preferred. Data from TCEQ monitoring sites (https://www.tceq.texas.gov/cgi-bin/compliance/monops/8hr_monthly.pl) was used to identify high ozone days and the range of MDA8 ozone values for the selected modeling dates for each location are shown in Table 5. These are not necessarily the same days considered in the 2019 DV. The first 1-2 days in the period are used for model spin-up so that initial conditions have minimal importance and emissions have maximum importance in the model runs.

3. The period also needed to occur under representative ozone conducive conditions. High ozone days occurring at unusual times of year were not considered.

4. Dates were excluded if TCEQ's model performance evaluation (MPE) found poor performance, including issues with either TCEQ's modeling platform or with Weather Research and Forecasting Model (WRF), which is used to specify CAMx box model meteorology including temperature, humidity and PBL depth. There is no MPE for ELP so this factor was not considered for the selection of ELP dates.

5. Dates were excluded if there were known exceptional events which caused high ozone concentrations (i.e., wildfires).

Table 5. Locations and dates for box model scenarios and corresponding range of MDA8 ozone values from TCEQ monitoring stations at each location

Location	Dates	Range of MDA8 ozone values over listed dates
HGB	September 3-7, 2019	22 – 93 ppb
DFW	September 3-7, 2019	41 – 88 ppb
SAN	July 23-27, 2019	41 – 76 ppb
TYL	September 12-16, 2019	39 – 61 ppb
ELP	August 4-8, 2019	57 – 83 ppb

Notes: MDA8 values from https://www.tceq.texas.gov/cgi-bin/compliance/monops/8hr_attainment.pl

4.0 Base Case Model Runs and Emission Sensitivity Tests

4.1 Base Case Simulations

Base case simulations were performed to compare chemical species concentrations at each location between four different mechanisms: CB7r1, RACM2, GEOS-Chem, and SAPRC07. Figure 2 through Figure 11 show diurnal profiles of hourly average concentrations for several species over the five-day simulations for each mechanism and location. Within each subplot, many of the lines overlap, highlighting the similarities between the mechanisms. Divergent mechanisms are also obvious in these figures. More quantitative information is provided in Table 9 through

Table 13. These tables present the average concentrations over days 2 through 5 of the simulations; the first day of each simulation is considered model spin up and is not included in the average. An average for the entire four-day period and for daytime hours only (7:00 am – 7:00 pm) are provided. In some cases the daytime average is lower than the full day average, likely due to O_3 suppression in the morning from rush hour emissions. Species that are explicitly defined in the mechanisms are focused on in the tables to identify chemistry differences in the mechanisms rather than differences caused by species lumping schemes.

8-hour average O_3 concentrations were calculated from hourly model results for comparison to the measured MDA8 values (Table 5). The daily maximum 8-hour average values for each location and mechanism are presented in Table 6 for days 2 through 5 of the simulations. In general, the modeled 8-hour average daily maximums agree well with the top end of the measured MDA8 values, except for ELP. There is considerable spatial variation in the observations at regional monitors which cannot be captured due to the limitations of a box model. The purpose of this study however is to identify chemistry differences between mechanisms rather than perform regulatory modeling that should more precisely match observations. The comparison to monitored values ensures the model is reasonably representing the conditions at HGB, DFW, SAN, and TYL.

The modeled 8-hour average O_3 values at ELP are significantly higher than the observations which is likely due to the complex terrain in the area. Since data is averaged over several CAMx 12 km grid cells to derive the box model input, it is difficult to account for the impact of terrain on emissions, meteorology, and air quality. For example, mountains in the ELP region create barriers between emission sources and localized wind flow patterns that can strongly influence how emissions are dispersed and transported within the ELP airshed. It is likely that 3-D modeling using fine grid resolution (4 km or finer) is needed to adequately describe air quality in ELP.

Table 6. Daily maximum 8-hour average (MDA8) modeled O_3 concentrations (ppb) on days 2 through 5 of the base case simulations for each location and mechanism.

Location and Mechanism	Day 2 MDA8 O_3 (ppb)	Day 3 MDA8 O_3 (ppb)	Day 4 MDA8 O_3 (ppb)	Day 5 MDA8 O_3 (ppb)
HGB				
GEOS-Chem	89.41	90.55	91.10	92.37
RACM2	94.29	95.45	96.12	97.24

Location and Mechanism	Day 2 MDA8 O_3 (ppb)	Day 3 MDA8 O_3 (ppb)	Day 4 MDA8 O_3 (ppb)	Day 5 MDA8 O_3 (ppb)
SAPRC07	93.94	95.28	96.09	97.21
CB7r1	89.14	90.42	91.05	92.24
DFW				
GEOS-Chem	94.74	94.74	94.74	94.74
RACM2	94.74	94.74	94.74	94.74
SAPRC07	94.74	94.74	94.74	94.74
CB7r1	94.74	94.74	94.74	94.74
SAN				
GEOS-Chem	72.88	75.15	75.15	74.27
RACM2	75.59	78.02	78.15	77.19
SAPRC07	74.86	77.42	77.60	76.65
CB7r1	74.45	76.93	76.98	76.06
TYL				
GEOS-Chem	61.21	62.00	60.89	62.28
RACM2	60.27	60.90	59.68	61.33
SAPRC07	58.61	59.26	57.93	59.24
CB7r1	58.81	59.48	58.37	59.67
ELP				
GEOS-Chem	125.76	130.82	131.05	128.21
RACM2	136.36	141.75	142.19	139.26
SAPRC07	137.73	143.24	143.69	140.89
CB7r1	129.25	134.60	134.94	131.93

The modeled hourly average O_3 concentrations for each mechanism over the 5-day simulations are presented in Figure 2. At each location, there is a similar diurnal profile with O_3 concentrations rising in the early morning, peaking in the mid to late afternoon, and then declining throughout the evening and night. Modeled hourly O_3 on days 2 through 5 peaks around 90-100 ppb at HGB, 95-105 ppb at DFW, 72-80 ppb at SAN, 58-63 ppb at TYL, and 130-150 ppb at ELP. All mechanisms show similar O_3 diurnal trends. At HGB, DFW, and ELP the RACM2 and SAPRC07 chemical mechanisms show peak concentrations about 5-10 ppb higher than CB7r1 and GEOS-Chem. These locations also have the highest NO_x concentrations, indicating that the RACM2 and SAPRC07 mechanisms may more efficiently produce O_3 in high NOx environments. RACM2, SAPRC07, and CB7r1 O_3 concentrations agree well at SAN, with slightly lower concentrations in the GEOS-Chem simulation.

TYL is the only location where GEOS-Chem forms the most O_3. NO_2, OH, and HO_2 are also highest in the GEOS-Chem simulation at TYL, consistent with greater O_3 production. Across all locations, OH and HO_2 are generally highest in the GEOS-Chem runs but this is most pronounced at TYL, potentially due to the relatively higher biogenic versus anthropogenic emissions at TYL (see isoprene and terpene concentrations in Figure 10 and Figure 11). Differences in the GEOS-Chem biogenic VOC chemistry compared to the other mechanisms leads to lower daytime isoprene concentrations, causing higher OH levels. Higher terpene concentrations, particularly at night and in the early morning, are also seen with GEOS-Chem on most days, which may be linked to lower NO_3. The impacts of GEOS-Chem's biogenic VOC chemistry on OH and O_3 levels might be particularly enhanced at lower NOx concentrations, as seen at TYL.

There is very little difference in NO_2 levels between mechanisms (Figure 3). Concentrations at each location peak in the early morning due to emissions and shallow boundary layers. As the boundary layer grows throughout the morning, concentrations decrease. NO (Figure 4) similarly shows little difference between mechanisms. While NOx emissions vary based on day of the week (primarily between weekdays and weekends), concentration changes from day to day are also an indication of meteorological conditions, with higher NO_2 caused by stagnant air. For example, the first three days of the SAN model run are weekdays (Tuesday – Thursday) and therefore have similar NOx emissions. The increase in NO_2 levels over these days however indicate conditions likely become more stagnant and daytime boundary layer heights decrease. This information is useful when interpreting results for other species as well and can aid in determining whether O_3 chemistry is NOx or VOC-limited.

Peroxyacyl nitrates (PANs) and organic nitrate (ON) concentrations vary quite significantly between mechanisms (Figure 8 and Figure 9, respectively). Each mechanism has different PANs and ON species, listed in Table 7 and Table 8, which may explain some of the differences in total ON concentration. PANs concentrations can differ by more than a factor of 2 at some times, seen most clearly during the day at TYL and in the early morning at SAN. CB7r1 often has the highest PANs concentration overnight and RACM2 is generally on the higher end as well, particularly during the day at TYL. GEOS-Chem typically shows PANs concentrations lower than or similar to the other mechanisms. GEOS-Chem shows the lowest average ON concentrations (except overnight at TYL) and SAPRC07 shows the highest, with concentrations 2 to 4 times higher than the lowest values. Although ONs act as a NOx sink, the higher concentrations in the SAPRC07 simulations do not seem to impact the NOx concentrations, which are similar among all mechanisms. On a regional scale, however, the difference in ON chemistry between mechanisms may lead to differences in O_3 production if increased ON levels allow NOy to be transported away local emission sources and returned as NOx via photochemical reactions. A similar impact would likely occur with PANs differences as well. A future study focused on nitrogen cycling would be beneficial to further investigate how differences in the nitrogen chemistry among mechanisms impact regional O_3 production.

Table 7. Peroxyacyl nitrate species in each mechanism.

Mechanism	Peroxyacyl nitrate (PAN) species
GEOS-Chem	Peroxyacetyl nitrate (PAN); Peroxymethacroyl nitrate (MPAN); Peroxypropionyl and higher peroxyacyl nitrates (PPN)
RACM2	Peroxyacetyl nitrate (PAN); Peroxymethacroyl nitrate (MPAN); Peroxypropionyl and higher peroxyacyl nitrates (PPN)
SAPRC07	Peroxyacetyl nitrate (PAN); Peroxymethacroyl nitrate (MPAN); Peroxybenzoyl nitrate (PBZN); Peroxypropionyl and higher peroxyacyl nitrates (PAN2)
CB7r1	Peroxyacetyl nitrate (PAN); Peroxymethacroyl nitrate and analogues (OPAN); Peroxypropionyl and higher peroxyacyl nitrates (PANX)

Table 8. Organic nitrate species in each mechanism.

Mechanism	Organic nitrate (ON) species
GEOS-Chem	Isoprene-d-4-hydroxy-nitrates (IHN1, IHN2, IHN3, IHN4); Lumped isoprene delta/beta-hydroperoxy nitrates (INPB, INPD); Organic nitrate from isoprene precursors (INTR); Isopropyl nitrate (IPRN); Lumped tetrafunctional isoprene carbonyl-nitrates and hydroxy-nitrates (ITCN, ITHN); Hydroxynitrates from methacrolein (MCHN, MCNB); Methyl nitrate (MENT); Methyl peroxy nitrate (MPN); Saturated and unsaturated 1st gen monoterpene organic nitrate (MTNS, MTNU); Hydroxynitrate from methyl vinyl ketone (MVKN); Nitrophenols (NPHN); n-Propyl nitrate (NPRN); Organic nitrate peroxides (PNPX); Propanone nitrate (PPNN); >= C4 alkylnitrates (R4N); 2nd generation monoterpene organic nitrate (TNTR)
RACM2	Organic nitrate (ONIT); First-generation isoprene nitrates (ISON); Nitrooxyaldehydes (NALD)
SAPRC07	Lumped organic nitrates (RNO3); Lost nitrogen or nitrogen in unreactive products (XN)
CB7r1	Simpler organic nitrates (NTR1); Multi-functional organic nitrates (NTR2); First-generation isoprene nitrates (INTR); Nitro-cresols (CRON)

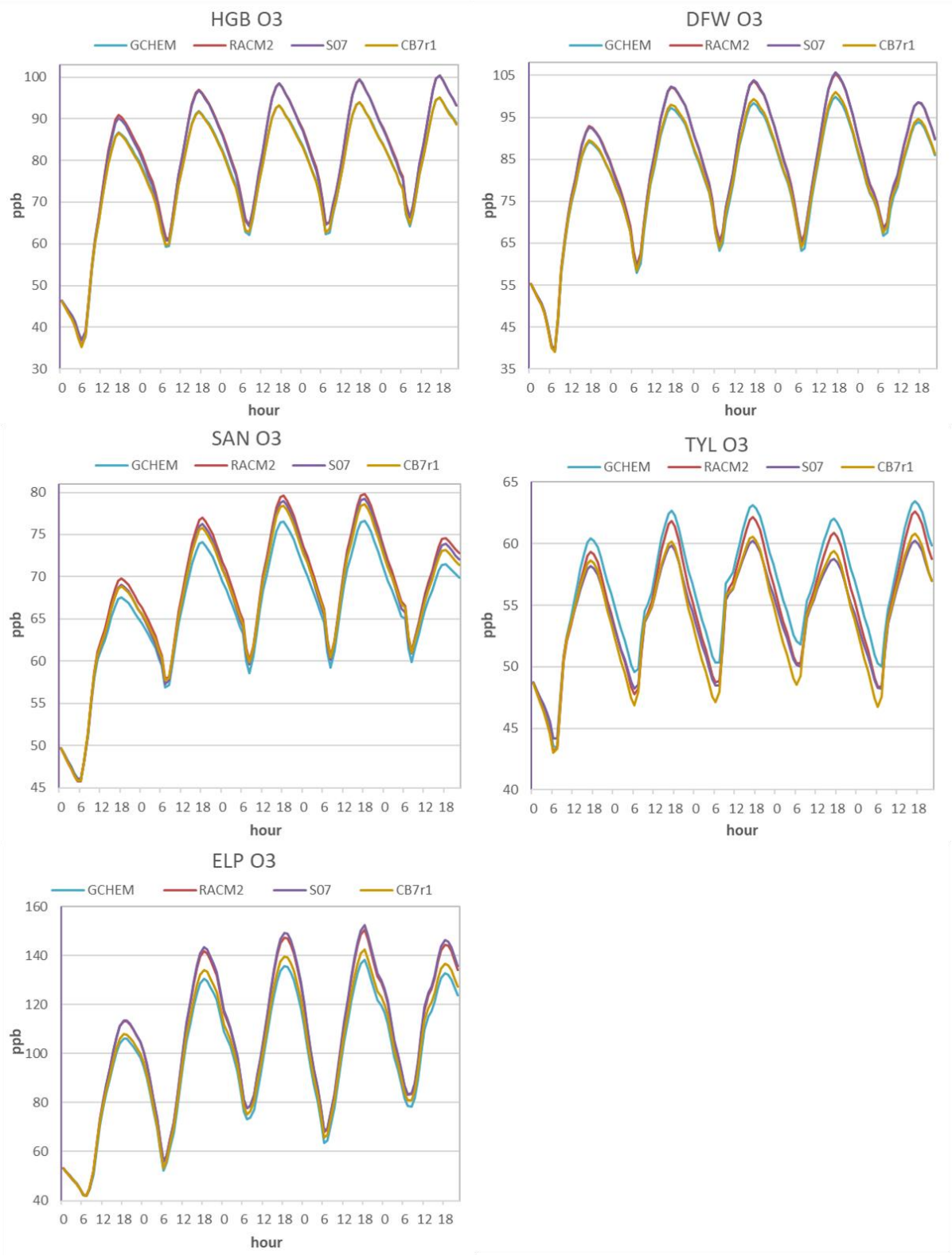

Figure 2. Diurnal profiles of ozone (ppb) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

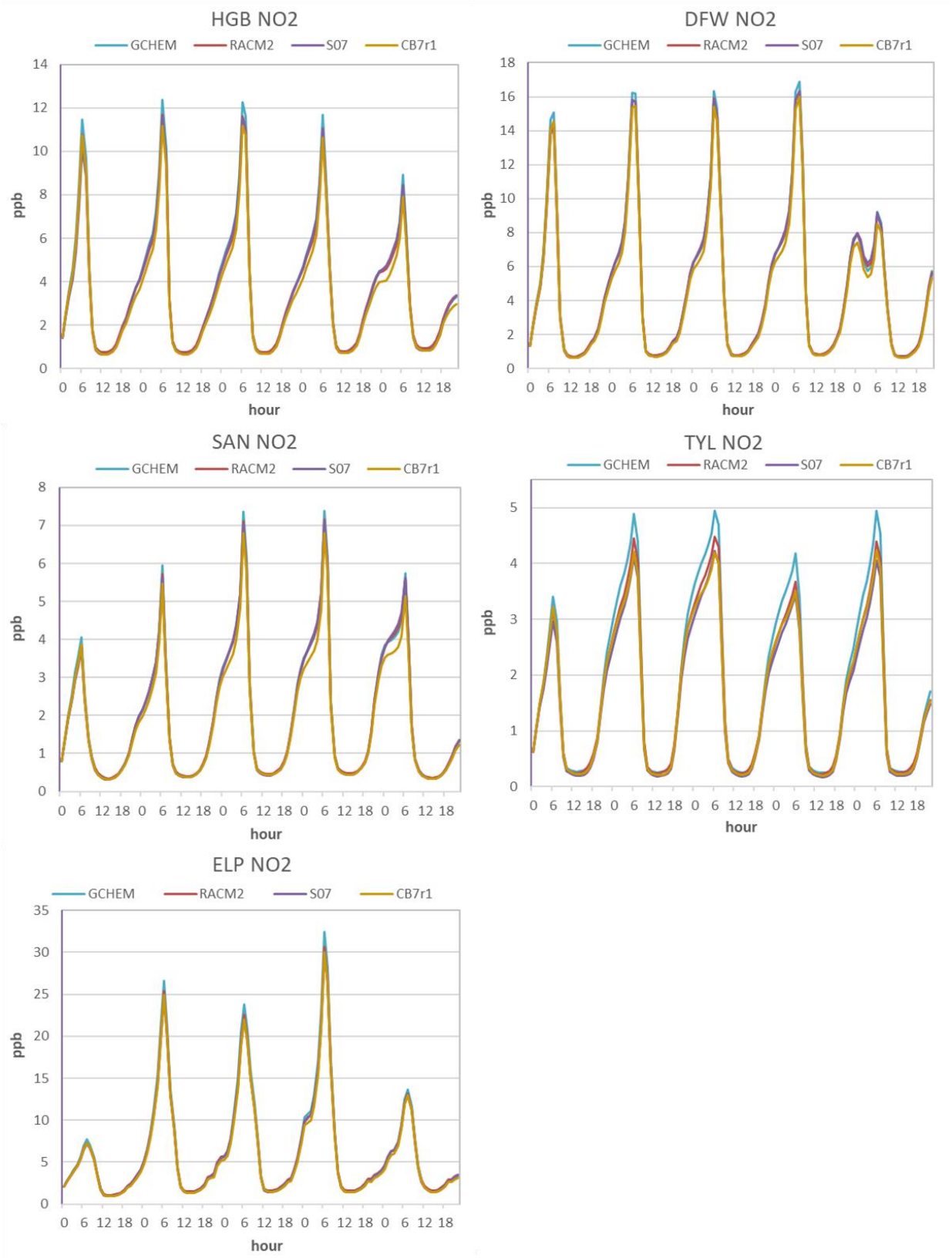

Figure 3. Diurnal profiles of nitrogen dioxide (ppb) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

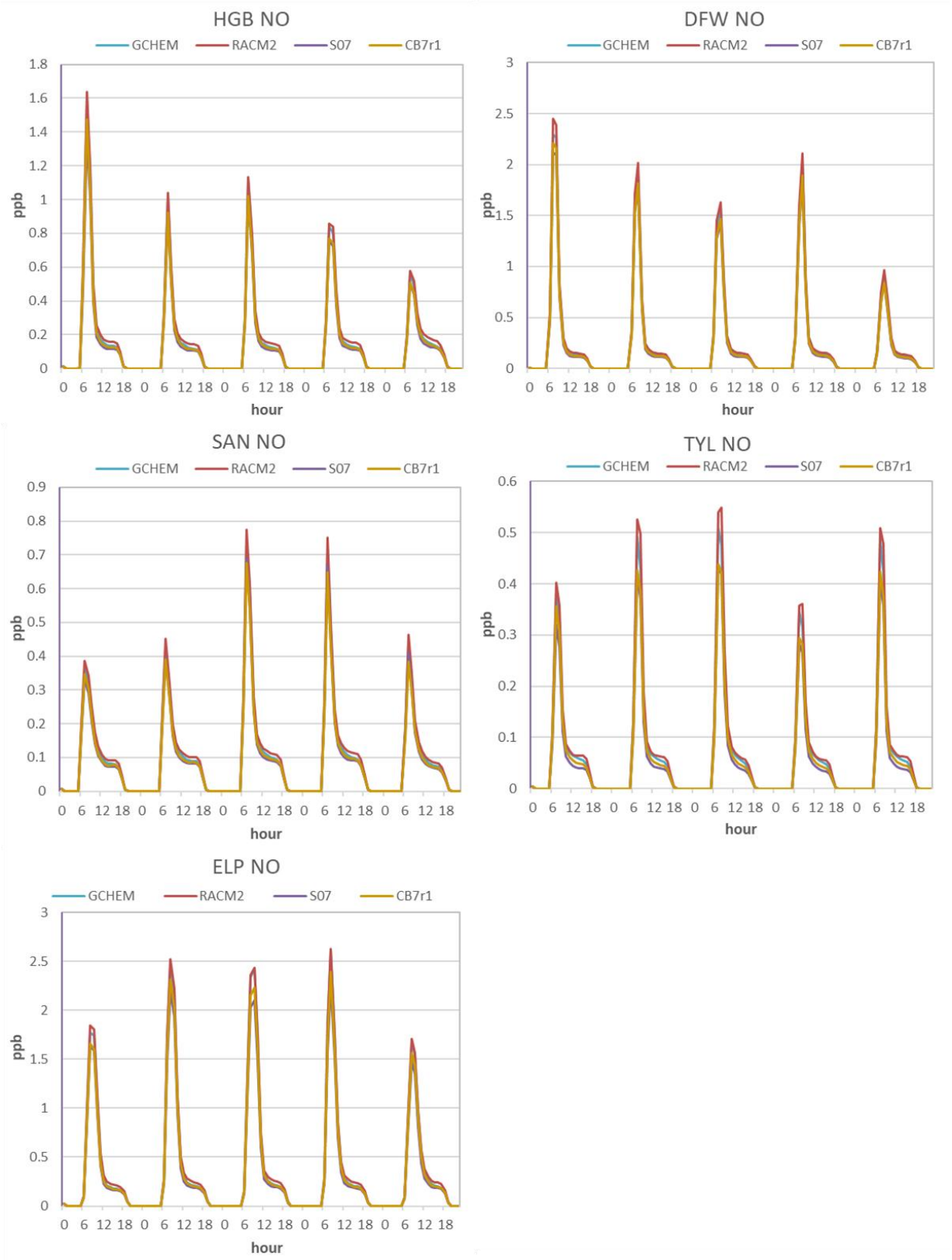

Figure 4. Diurnal profiles of nitrogen oxide (ppb) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

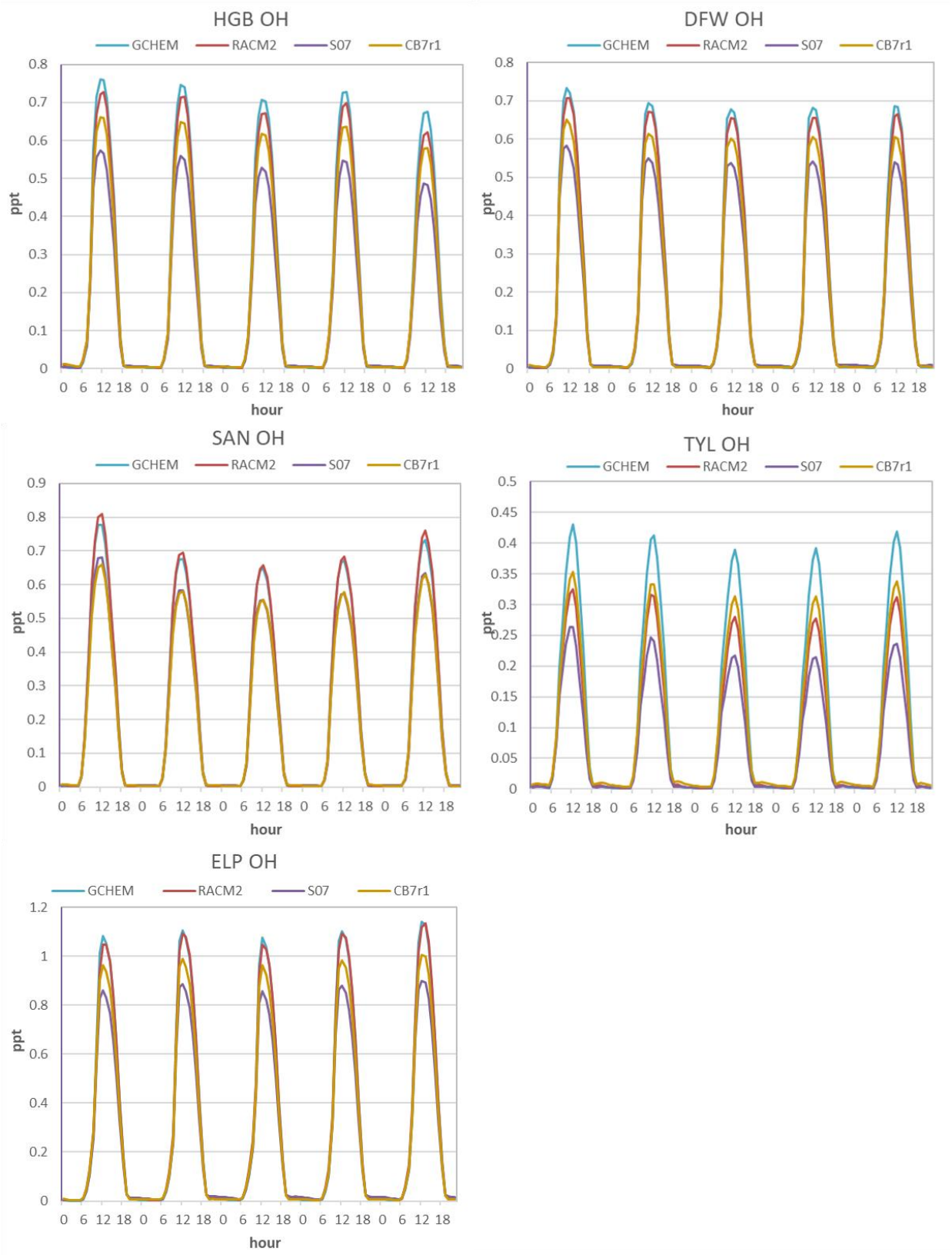

Figure 5. Diurnal profiles of hydroxyl radical (ppt) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

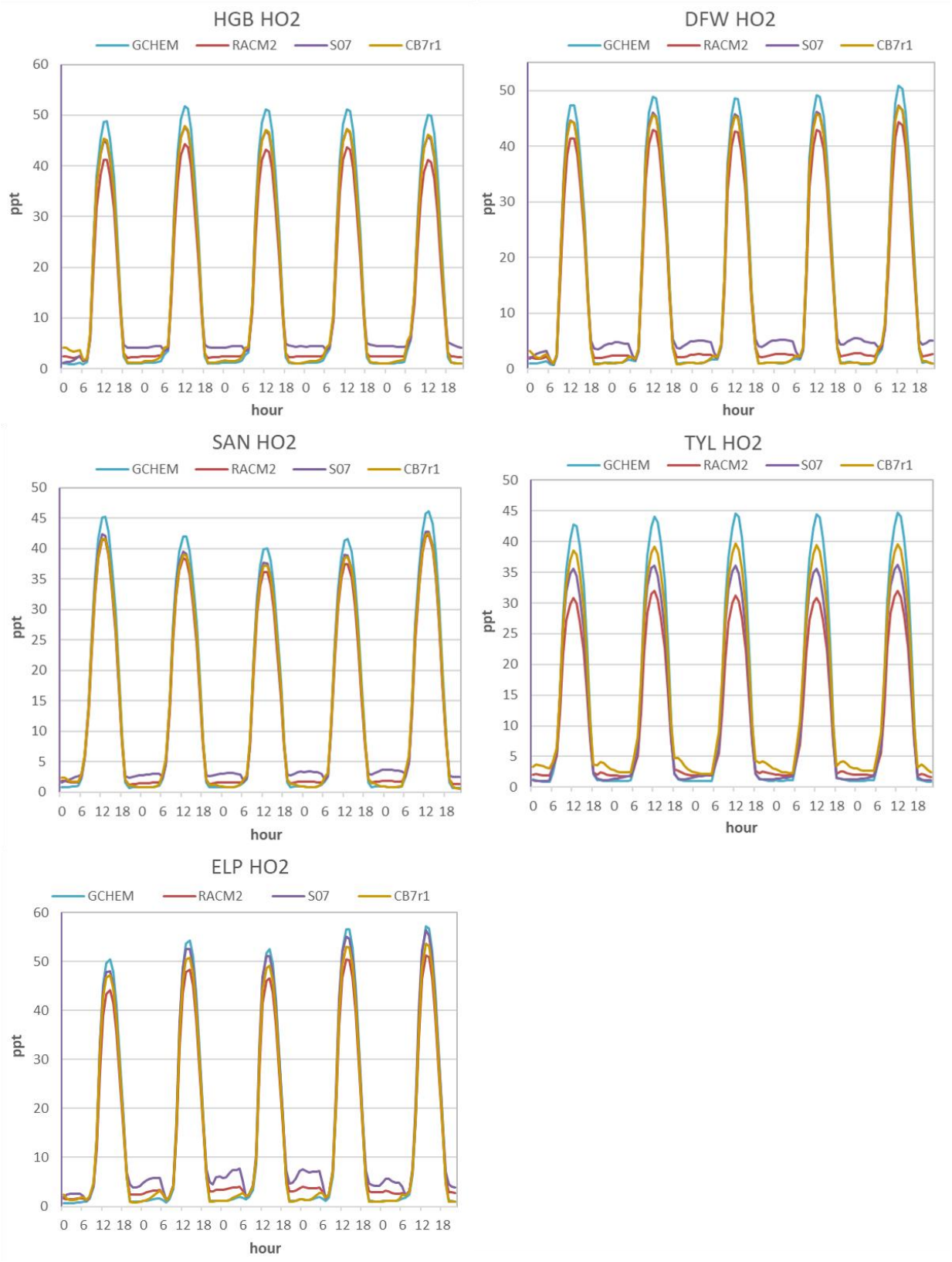

Figure 6. Diurnal profiles of hydroperoxyl radical (ppt) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

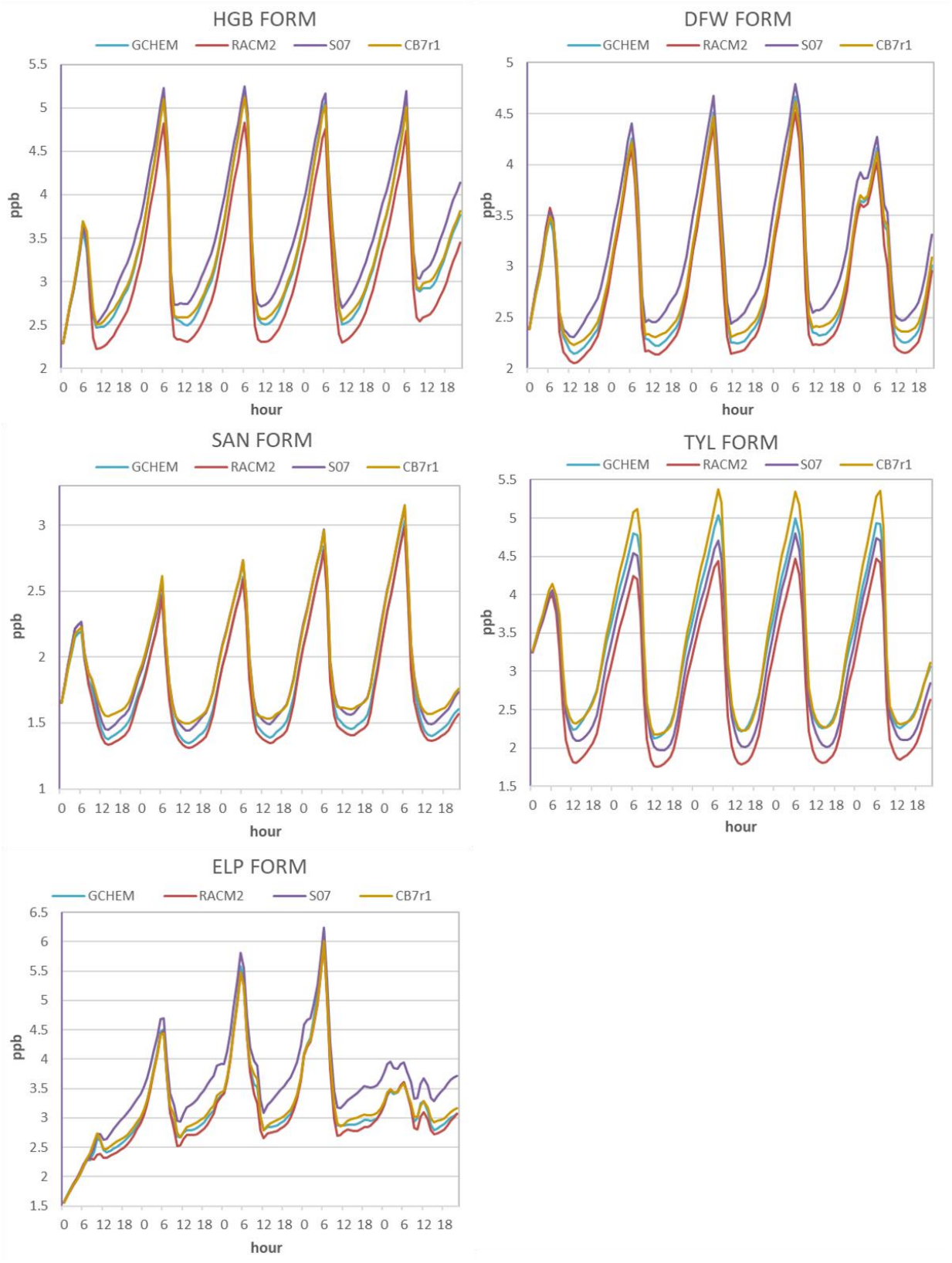

Figure 7. Diurnal profiles of formaldehyde (ppb) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

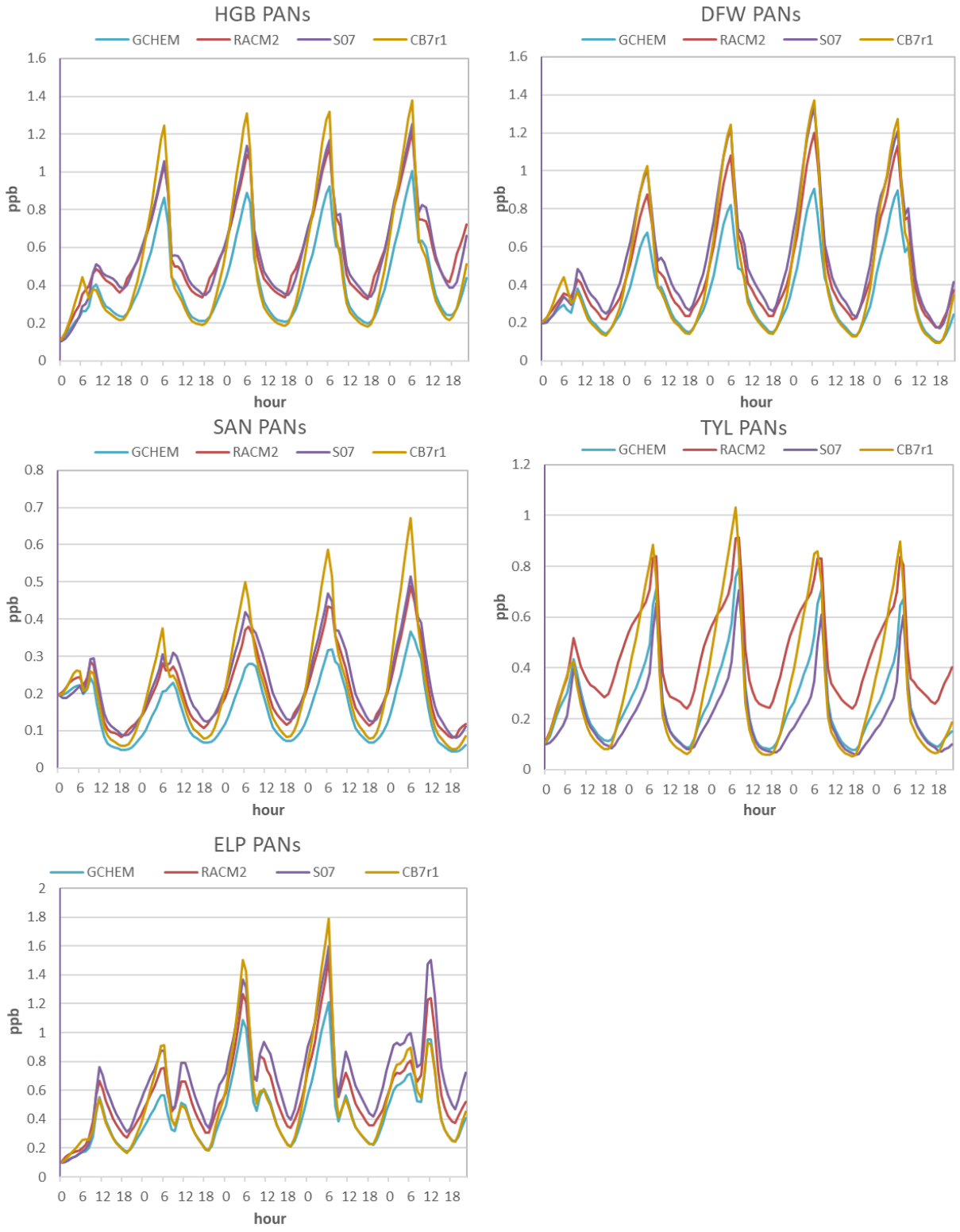

Figure 8. Diurnal profiles of the sum of peroxyacetyl nitrate (PAN) and higher order peroxyacyl nitrates (ppb) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

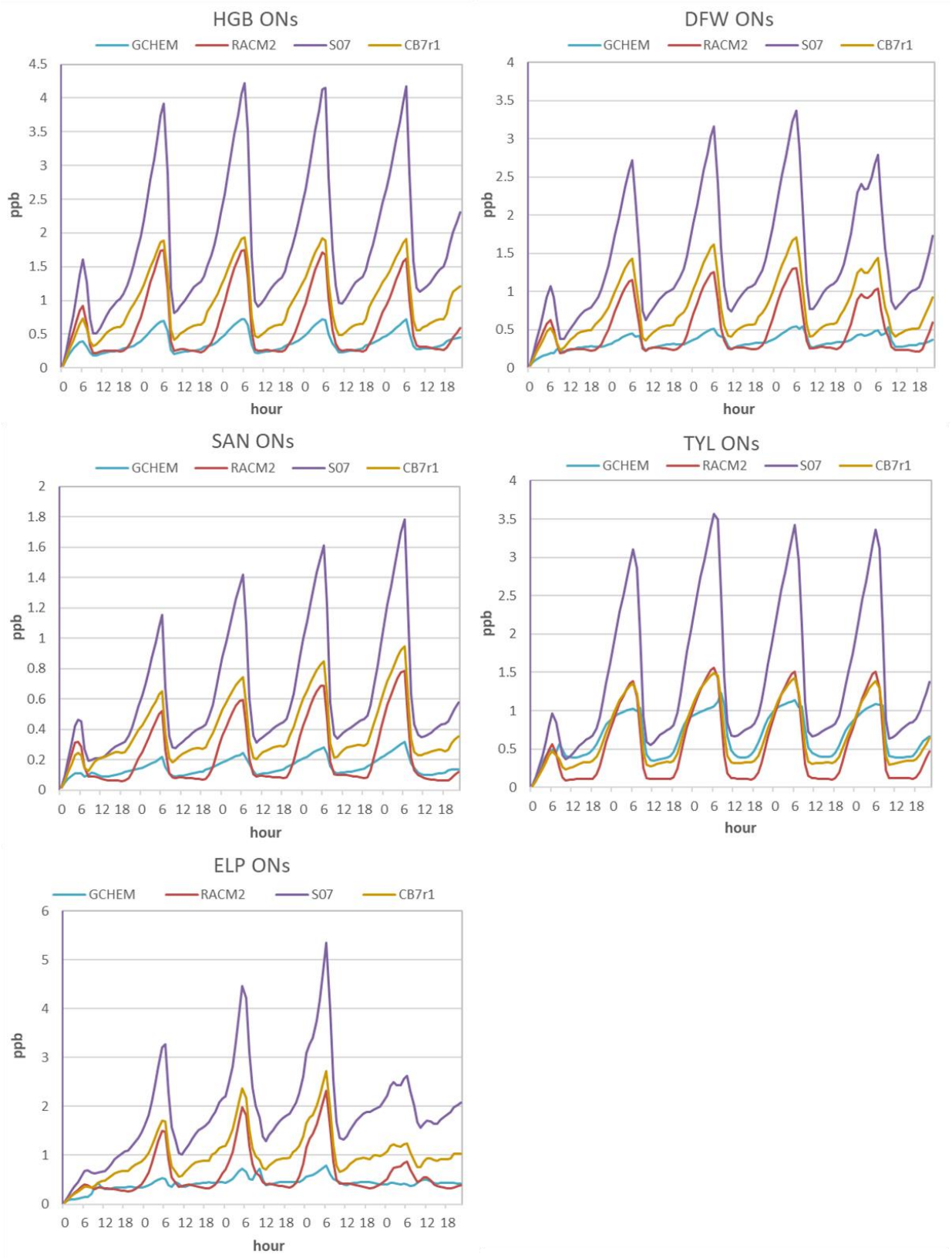

Figure 9. Diurnal profiles of organic nitrates (ppb) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

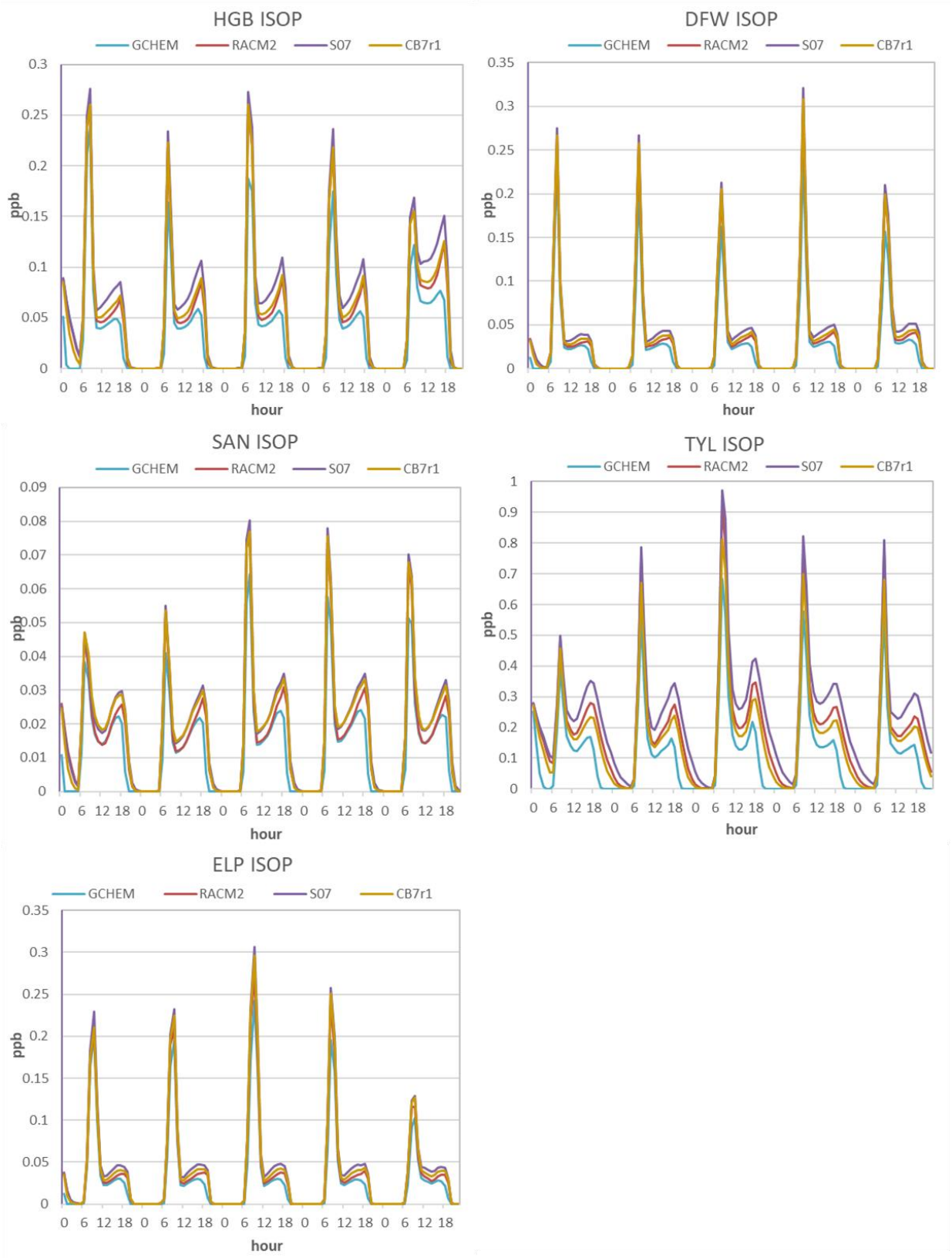

Figure 10. Diurnal profiles of isoprene (ppb) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

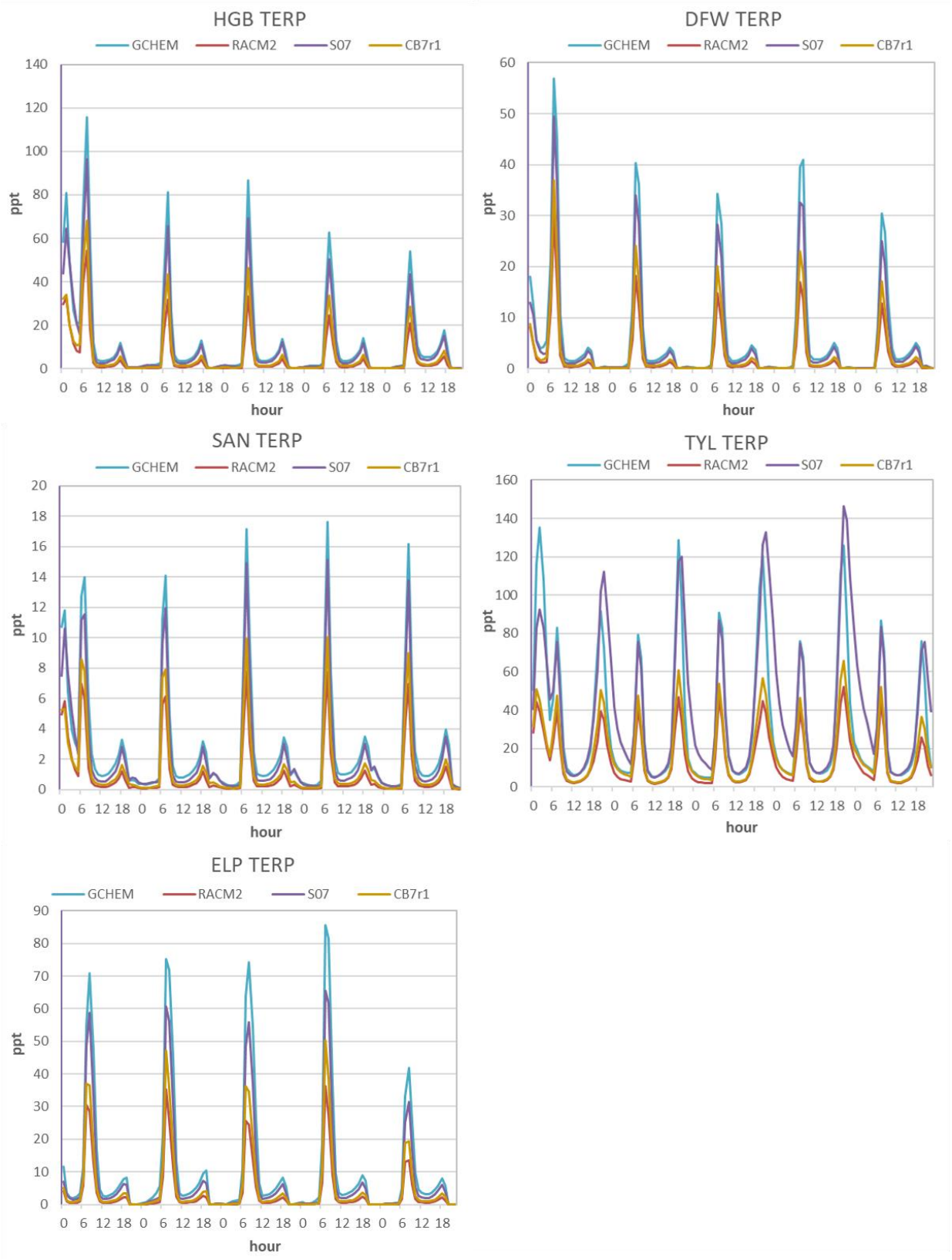

Figure 11. Diurnal profiles of terpene (ppt) from the 5-day box model base simulations at HGB, DFW, SAN, TYL and ELP.

Table 9. HGB average concentrations (ppb) for select species over days 2 through 5 of base model simulations for each chemical mechanism. The average over all hours and over daytime hours only (7am – 7pm) are provided.

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
O_3	80.21	78.76	83.95	82.09	80.32	78.68	83.69	82.00
OH	1.83E-04	3.35E-04	1.96E-04	3.58E-04	2.08E-04	3.82E-04	1.57E-04	2.85E-04
HO_2	1.51E-02	2.66E-02	1.41E-02	2.41E-02	1.59E-02	2.84E-02	1.64E-02	2.65E-02
Acetic acid	0.44	0.37	0.21	0.18	0.25	0.22	0.33	0.29
Acetone	4.72	4.27	3.97	3.61	4.89	4.45	4.63	4.17
Acetaldehyde	1.10	0.92	0.90	0.85	0.82	0.74	1.55	1.35
Benzene	0.19	0.16	0.19	0.16	0.18	0.15	0.19	0.16
CO	247.23	230.67	245.12	228.88	246.36	229.91	245.87	229.48
Ethene	0.57	0.38	0.57	0.37	0.57	0.37	0.58	0.39
Ethane	1.22	0.97	1.22	0.97	1.21	0.96	1.22	0.97
Ethyne	0.27	0.26	0.26	0.25	0.27	0.26	0.28	0.26
Ethanol	1.61	1.16	1.60	1.14	1.57	1.11	1.66	1.20
Formic acid	0.12	0.10	0.10	0.08	0.46	0.40	0.14	0.11
Formaldehyde	3.47	3.14	3.18	2.83	3.44	3.09	3.68	3.31
Glyoxal	0.13	0.10	0.05	0.05	0.06	0.06	0.03	0.03
H_2O_2	4.76	4.49	4.10	3.92	5.07	4.76	5.01	4.71
HNO_3	6.86	5.90	6.83	5.90	6.94	6.02	5.22	4.62
HONO	3.30E-02	2.26E-02	3.24E-02	2.23E-02	3.30E-02	2.27E-02	2.90E-02	1.74E-02
Isoprene	4.88E-02	8.93E-02	4.64E-02	8.51E-02	3.34E-02	6.17E-02	5.62E-02	1.03E-01
Methanol	2.35	2.28	2.30	2.24	2.34	2.27	2.43	2.35
Methyl glyoxal	0.12	0.12	0.06	0.05	0.05	0.04	0.08	0.06
N_2O_5	0.10	0.01	0.12	0.01	0.15	0.01	0.08	0.01
NO	0.12	0.23	0.15	0.27	0.13	0.25	0.12	0.22
NO_2	3.35	2.53	3.63	2.69	3.70	2.73	3.61	2.61

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
NO_3	4.26E-02	3.24E-03	3.56E-02	3.83E-03	4.36E-02	4.28E-03	2.87E-02	2.90E-03
Organic nitrates	1.04	0.77	0.70	0.46	0.41	0.33	2.08	1.58
PANs	0.56	0.44	0.63	0.56	0.46	0.41	0.64	0.58

Notes: PANs include peroxyacetyl nitrate (PAN) and higher order peroxyacyl nitrates, defined in Table 7. Organic nitrate species defined in Table 8

Table 10. DFW average concentrations (ppb) for select species over days 2 through 5 of base model simulations for each chemical mechanism. The average over all hours and over daytime hours only (7am – 7pm) are provided.

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
O_3	83.82	82.77	86.48	85.21	83.14	81.92	86.45	85.30
OH	1.73E-04	3.17E-04	1.88E-04	3.44E-04	1.94E-04	3.56E-04	1.57E-04	2.83E-04
HO_2	1.39E-02	2.46E-02	1.35E-02	2.29E-02	1.46E-02	2.61E-02	1.57E-02	2.49E-02
Acetic acid	0.39	0.34	0.19	0.17	0.22	0.19	0.30	0.26
Acetone	5.12	4.63	4.36	3.95	5.34	4.84	5.07	4.58
Acetaldehyde	1.11	0.97	0.90	0.87	0.87	0.81	1.46	1.31
Benzene	0.22	0.19	0.22	0.19	0.21	0.19	0.22	0.19
CO	289.15	273.87	288.65	273.46	288.20	273.03	288.88	273.61
Ethene	0.56	0.41	0.56	0.40	0.56	0.41	0.56	0.41
Ethane	2.71	2.14	2.71	2.14	2.70	2.13	2.71	2.15
Ethyne	0.38	0.37	0.37	0.36	0.38	0.37	0.38	0.38
Ethanol	1.98	1.50	1.96	1.48	1.93	1.45	2.01	1.53
Formic acid	9.48E-02	7.95E-02	8.41E-02	7.20E-02	0.37	0.32	0.11	9.36E-02
Formaldehyde	3.05	2.82	2.90	2.64	2.99	2.76	3.25	2.99
Glyoxal	0.10	9.00E-02	4.70E-02	5.06E-02	5.42E-02	5.51E-02	3.09E-02	3.32E-02
H_2O_2	4.24	4.06	3.79	3.65	4.47	4.26	4.46	4.25
HNO_3	6.85	6.02	6.85	6.04	6.94	6.13	5.63	5.03

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
HONO	4.74E-02	3.14E-02	4.70E-02	3.16E-02	4.72E-02	3.13E-02	4.33E-02	2.59E-02
Isoprene	3.51E-02	6.45E-02	3.32E-02	6.11E-02	2.56E-02	4.73E-02	3.80E-02	6.96E-02
Methanol	2.64	2.64	2.57	2.57	2.61	2.61	2.70	2.69
Methyl glyoxal	0.08	0.08	0.04	0.04	0.03	0.03	0.05	0.04
N_2O_5	0.20	0.02	0.21	0.02	0.26	0.03	0.16	0.02
NO	0.20	0.37	0.23	0.42	0.21	0.39	0.19	0.36
NO_2	4.62	3.74	4.90	3.89	4.92	3.94	4.87	3.83
NO_3	6.40E-02	4.38E-03	4.89E-02	4.34E-03	6.06E-02	4.80E-03	4.48E-02	4.06E-03
Organic nitrates	0.85	0.67	0.55	0.40	0.36	0.34	1.59	1.27
PANs	0.49	0.40	0.52	0.47	0.38	0.35	0.59	0.52

Notes: PANs include peroxyacetyl nitrate (PAN) and higher order peroxyacyl nitrates, defined in Table 7. Organic nitrate species defined in Table 8

Table 11. SAN average concentrations (ppb) for select species over days 2 through 5 of base model simulations for each chemical mechanism. The average over all hours and over daytime hours only (7am – 7pm) are provided.

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
O_3	69.54	68.47	70.32	69.17	68.17	67.18	69.69	68.61
OH	1.87E-04	3.42E-04	2.17E-04	3.98E-04	2.15E-04	3.95E-04	1.86E-04	3.40E-04
HO_2	1.36E-02	2.41E-02	1.33E-02	2.32E-02	1.43E-02	2.57E-02	1.45E-02	2.42E-02
Acetic acid	0.22	0.19	9.49E-02	8.15E-02	0.11	9.28E-02	0.16	0.14
Acetone	2.75	2.50	2.15	1.97	2.47	2.27	2.37	2.16
Acetaldehyde	0.61	0.49	0.40	0.35	0.37	0.32	0.64	0.52
Benzene	0.11	9.17E-02	0.10	8.96E-02	0.10	8.85E-02	0.10	9.12E-02
CO	178.00	169.42	176.31	167.99	176.29	167.94	176.34	167.99
Ethene	0.32	0.19	0.31	0.19	0.32	0.19	0.32	0.19
Ethane	0.97	0.72	0.97	0.71	0.97	0.71	0.97	0.71

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
Ethyne	0.13	0.13	0.13	0.12	0.13	0.12	0.13	0.12
Ethanol	0.85	0.59	0.82	0.57	0.82	0.56	0.85	0.59
Formic acid	4.44E-02	3.53E-02	3.62E-02	2.98E-02	0.18	0.15	5.30E-02	4.13E-02
Formaldehyde	1.95	1.78	1.79	1.61	1.82	1.66	1.94	1.77
Glyoxal	5.76E-02	4.31E-02	1.89E-02	1.91E-02	2.35E-02	2.35E-02	1.22E-02	1.30E-02
H_2O_2	3.06	2.89	2.83	2.70	3.24	3.04	3.11	2.94
HNO_3	3.73	3.38	3.77	3.44	3.82	3.49	3.24	3.00
HONO	1.80E-02	1.24E-02	1.81E-02	1.28E-02	1.81E-02	1.26E-02	1.63E-02	1.02E-02
Isoprene	1.73E-02	2.94E-02	1.56E-02	2.64E-02	1.24E-02	2.24E-02	1.78E-02	2.99E-02
Methanol	1.60	1.57	1.52	1.50	1.60	1.56	1.59	1.56
Methyl glyoxal	4.44E-02	3.95E-02	1.73E-02	1.58E-02	1.46E-02	1.37E-02	2.24E-02	1.91E-02
N_2O_5	8.22E-02	4.65E-03	8.13E-02	5.24E-03	0.11	6.12E-03	5.97E-02	4.26E-03
NO	8.87E-02	0.16	0.10	0.19	9.64E-02	0.18	8.78E-02	0.16
NO_2	1.98	1.37	2.12	1.44	2.13	1.47	2.10	1.41
NO_3	2.82E-02	8.46E-04	2.05E-02	7.22E-04	2.75E-02	3.57E-04	1.83E-02	7.41E-04
Organic nitrates	0.42	0.32	0.25	0.16	0.16	0.14	0.71	0.53
PANs	0.23	0.22	0.22	0.23	0.15	0.17	0.24	0.26

Notes: PANs include peroxyacetyl nitrate (PAN) and higher order peroxyacyl nitrates, defined in Table 7. Organic nitrate species defined in Table 8

Table 12. TYL average concentrations (ppb) for select species over days 2 through 5 of base model simulations for each chemical mechanism. The average over all hours and over daytime hours only (7am – 7pm) are provided.

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
O_3	54.64	55.76	55.85	56.65	57.13	57.75	54.91	55.66
OH	9.66E-05	1.73E-04	8.41E-05	1.53E-04	1.15E-04	2.11E-04	6.58E-05	1.19E-04
HO_2	1.42E-02	2.38E-02	1.09E-02	1.84E-02	1.45E-02	2.58E-02	1.21E-02	2.12E-02

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
Acetic acid	0.55	0.47	0.24	0.21	0.26	0.23	0.27	0.24
Acetone	3.63	3.35	3.11	2.89	3.64	3.39	3.53	3.24
Acetaldehyde	1.27	1.06	1.05	0.92	0.90	0.80	1.57	1.37
Benzene	0.10	8.80E-02	0.11	9.46E-02	9.81E-02	8.58E-02	0.10	9.17E-02
CO	182.24	175.39	179.11	172.59	181.73	174.96	179.29	172.75
Ethene	0.62	0.40	0.63	0.41	0.62	0.39	0.65	0.42
Ethane	2.11	1.65	2.12	1.66	2.10	1.64	2.12	1.66
Ethyne	0.29	0.29	0.29	0.29	0.29	0.28	0.30	0.30
Ethanol	1.07	0.79	1.09	0.81	1.03	0.76	1.13	0.84
Formic acid	0.18	0.15	0.13	0.11	0.25	0.22	0.20	0.15
Formaldehyde	3.46	3.11	2.85	2.51	3.33	3.01	3.11	2.80
Glyoxal	1.52E-01	0.10	2.57E-02	2.58E-02	4.27E-02	3.98E-02	1.88E-02	1.94E-02
H_2O_2	4.69	4.42	3.70	3.57	5.14	4.85	4.39	4.20
HNO_3	2.22	2.05	2.11	1.98	2.14	2.01	1.34	1.31
HONO	1.29E-02	7.39E-03	1.25E-02	6.95E-03	1.31E-02	7.72E-03	1.16E-02	5.54E-03
Isoprene	0.16	0.26	0.19	0.30	0.11	0.20	0.24	0.35
Methanol	3.04	3.01	3.08	3.04	3.00	2.97	3.18	3.13
Methyl glyoxal	0.16	0.14	6.11E-02	3.78E-02	5.88E-02	4.75E-02	8.43E-02	6.17E-02
N_2O_5	1.38E-02	2.35E-03	1.56E-02	2.80E-03	3.03E-02	4.43E-03	6.55E-03	1.55E-03
NO	5.84E-02	1.08E-01	7.37E-02	1.36E-01	6.61E-02	1.22E-01	5.39E-02	9.95E-02
NO_2	1.73	1.02	1.80	1.10	1.96	1.17	1.66	0.98
NO_3	6.21E-03	8.79E-04	5.16E-03	8.01E-04	9.08E-03	6.99E-04	2.85E-03	5.98E-04
Organic nitrates	0.74	0.55	0.61	0.38	0.73	0.60	1.62	1.26
PANs	0.35	0.30	0.47	0.44	0.27	0.28	0.21	0.24

Notes: PANs include peroxyacetyl nitrate (PAN) and higher order peroxyacyl nitrates, defined in Table 7. Organic nitrate species defined in Table 8

Table 13. ELP average concentrations (ppb) for select species over days 2 through 5 of base model simulations for each chemical mechanism. The average over all hours and over daytime hours only (7am – 7pm) are provided.

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
O_3	107.19	103.82	111.93	108.14	104.18	100.77	112.88	109.07
OH	2.83E-04	5.16E-04	3.15E-04	5.72E-04	3.12E-04	5.71E-04	2.60E-04	4.67E-04
HO_2	1.53E-02	2.69E-02	1.54E-02	2.55E-02	1.60E-02	2.82E-02	1.80E-02	2.83E-02
Acetic acid	0.40	0.35	0.19	0.16	0.23	0.21	0.31	0.27
Acetone	5.44	5.05	4.29	4.02	5.71	5.32	5.20	4.84
Acetaldehyde	1.07	1.03	0.94	0.98	0.83	0.84	1.49	1.43
Benzene	0.18	0.16	0.18	0.16	0.17	0.16	0.18	0.17
CO	247.63	240.90	246.92	240.37	246.91	240.28	247.20	240.51
Ethene	0.47	0.37	0.46	0.36	0.47	0.37	0.47	0.37
Ethane	0.86	0.77	0.86	0.77	0.85	0.76	0.86	0.77
Ethyne	0.18	0.17	0.17	0.17	0.18	0.17	0.18	0.18
Ethanol	1.80	1.57	1.77	1.53	1.75	1.52	1.84	1.60
Formic acid	9.15E-02	8.03E-02	8.33E-02	7.40E-02	0.53	0.47	0.11	0.10
Formaldehyde	3.45	3.28	3.33	3.12	3.40	3.22	3.84	3.62
Glyoxal	0.11	0.11	5.29E-02	6.09E-02	5.65E-02	6.08E-02	3.49E-02	3.98E-02
H_2O_2	2.59	2.41	2.29	2.14	2.73	2.52	2.88	2.66
HNO_3	11.38	10.51	11.41	10.50	11.33	10.48	9.45	8.76
HONO	6.16E-02	5.48E-02	6.17E-02	5.58E-02	6.13E-02	5.43E-02	5.33E-02	4.42E-02
Isoprene	3.83E-02	6.81E-02	3.52E-02	6.26E-02	2.85E-02	5.21E-02	4.07E-02	7.23E-02
Methanol	2.01	2.01	1.93	1.94	2.01	2.01	2.05	2.04
Methyl glyoxal	9.63E-02	1.05E-01	5.55E-02	6.10E-02	3.21E-02	3.64E-02	5.97E-02	5.96E-02
N_2O_5	0.19	4.15E-02	0.21	4.71E-02	0.24	4.97E-02	0.15	3.87E-02
NO	0.35	0.65	0.40	0.73	0.38	0.70	0.33	0.61
NO_2	6.69	6.43	6.98	6.61	7.16	6.80	6.85	6.45

	CB7r1 Avg – all hours	CB7r1 Avg - daytime only	RACM2 Avg – all hours	RACM2 Avg - daytime only	GEOS-Chem Avg – all hours	GEOS-Chem Avg - daytime only	SAPRC07 Avg – all hours	SAPRC07 Avg - daytime only
NO_3	0.10	5.70E-03	7.84E-02	4.90E-03	9.09E-02	3.97E-03	6.95E-02	5.32E-03
Organic nitrates	1.13	0.98	0.69	0.58	0.47	0.46	2.17	1.89
PANs	0.60	0.54	0.65	0.66	0.50	0.49	0.78	0.77

Notes: PANs include peroxyacetyl nitrate (PAN) and higher order peroxyacyl nitrates, defined in Table 7. Organic nitrate species defined in Table 8

4.2 Ozone Response Surface

The response of O_3 concentrations to varying anthropogenic VOC and NOx emissions was investigated by performing a matrix of 100 box simulations for each location and mechanism. The matrix simulations were based on weekday anthropogenic emission rates for all dates and date-specific biogenic emission rates. The scaling factors applied to the base run emissions are provided in Table 14. Ozone response surface plots for daily maximum 1-h (MDA1) O_3, shown in Figure 12 through Figure 16, were constructed using results from the scaled emissions model runs for each location. Ozone response surfaces for each location were similar in shape for each simulation day and so only the fourth simulation day is shown in the Figures. The base case simulations (VOC and NOx scaling factors of 1) are in a NOx-limited regime where O_3 is much more responsive to NOx emission reductions than anthropogenic VOC emission reductions. This is evident in Figure 12 through Figure 16. When starting from the base case (VOC and NOx scaling factors of 1), O_3 concentrations change significantly as NOx varies, whereas O_3 is nearly unaffected by varying VOC.

Because a box model cannot resolve spatial variations in NOx/VOC sensitivity within an urban region, the results are expected to be indicative of locations with higher MDA8 O_3 in each area. Although the high modeled O_3 concentrations at ELP indicate that actual conditions are not accurately captured by the box model, matrix simulations were still performed to compare the mechanisms. The matrix simulations are also a necessary step to computing the VOC reactivity in the next section. ELP was less NOx-limited than the other locations, requiring lower NOx emission scaling factors to transition into a VOC-limited regime. TYL was still under NOx-limited conditions at a NOx scaling factor of 9.0 as shown in Figure 16.

Table 14. VOC and NOx anthropogenic emission scaling factors used to generate ozone response surfaces.

Species	Anthropogenic emission scaling factor									
VOC (all locations)	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8	2.0
NOx (ELP)	0.2	0.6	1.0	1.4	1.8	2.2	2.6	3.0	3.4	3.8
NOx (HGB, DFW, SAN, TYL)	0.0	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0

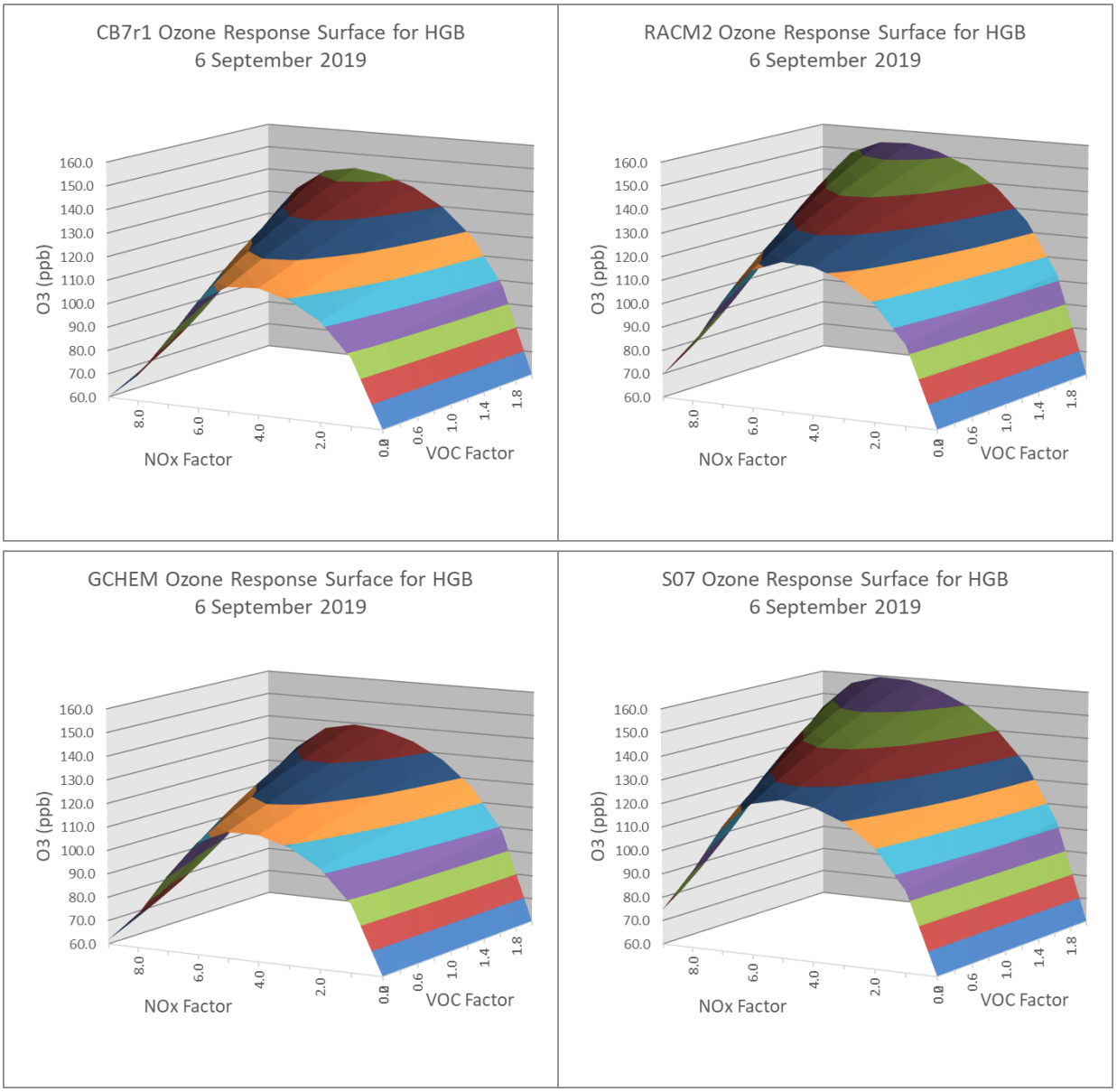

Figure 12. Ozone response surface (MDA1, ppb) to varying anthropogenic NOx and VOC emissions for HGB with the four chemical mechanisms. NOx and VOC scaling factors of 1 are the base case simulation.

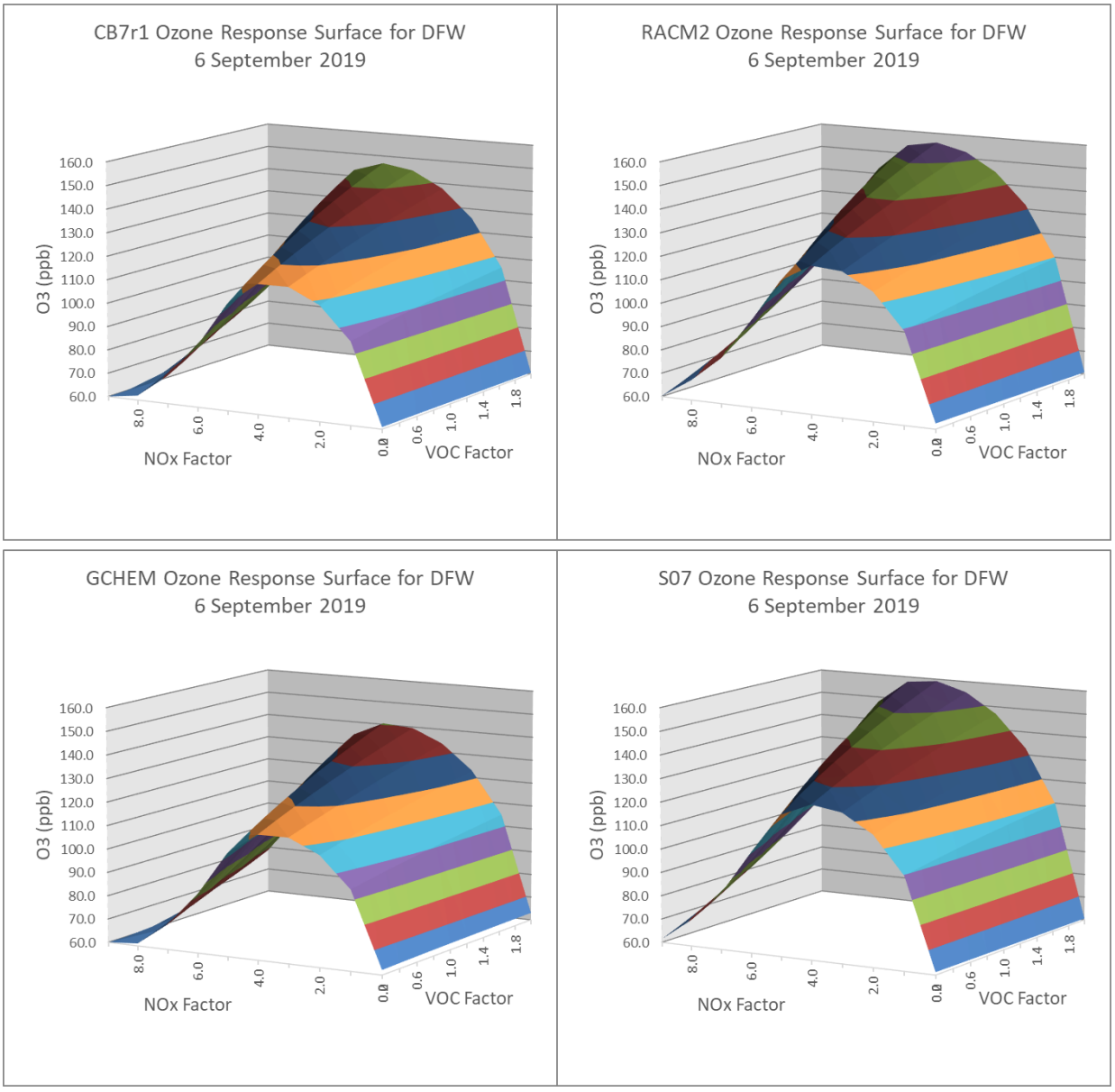

Figure 13. Ozone response surface (MDA1, ppb) to varying anthropogenic NOx and VOC emissions for DFW with the four chemical mechanisms. NOx and VOC scaling factors of 1 are the base case simulation.

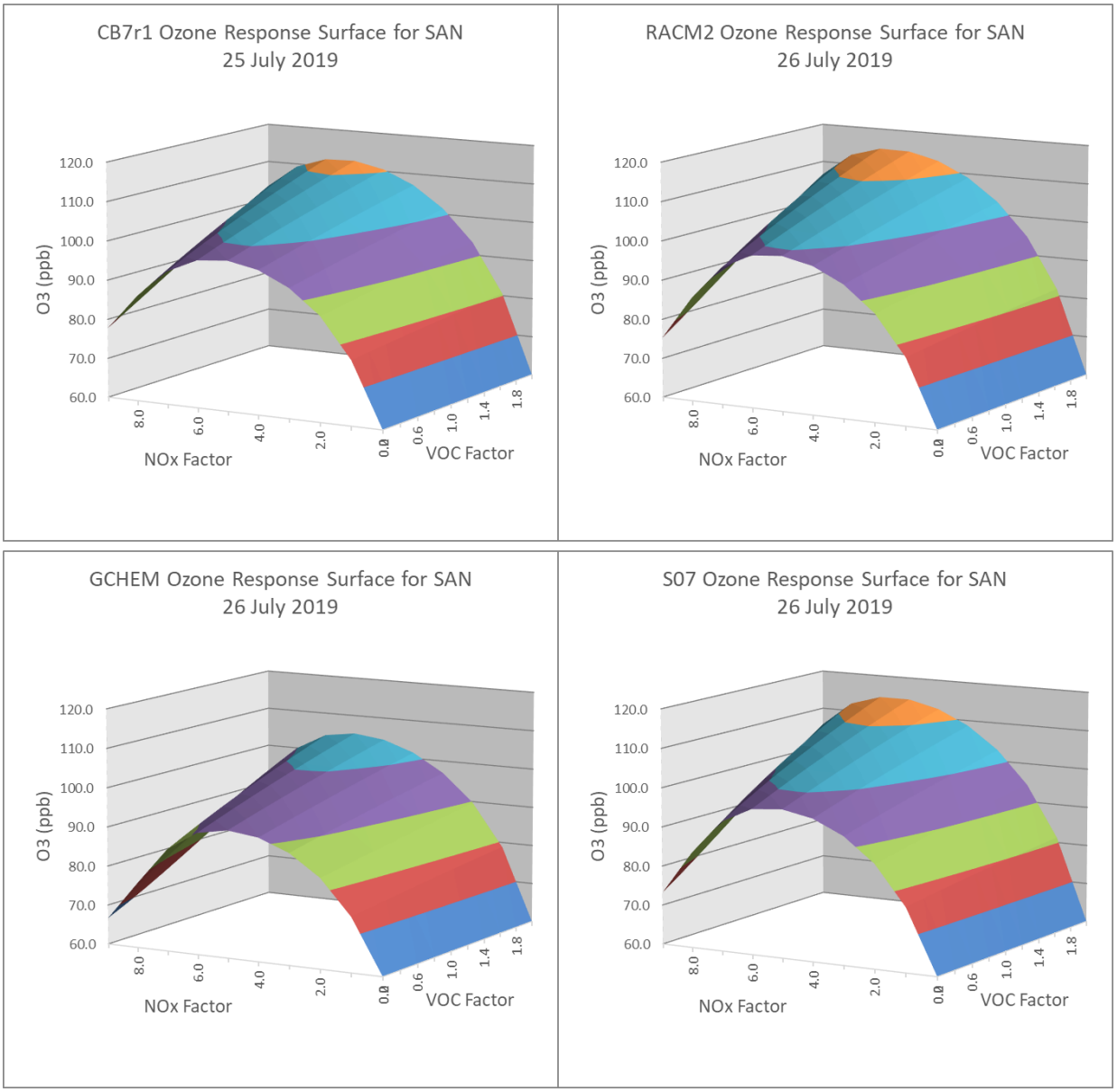

Figure 14. Ozone response surface (MDA1, ppb) to varying anthropogenic NOx and VOC emissions for SAN with the four chemical mechanisms. NOx and VOC scaling factors of 1 are the base case simulation.

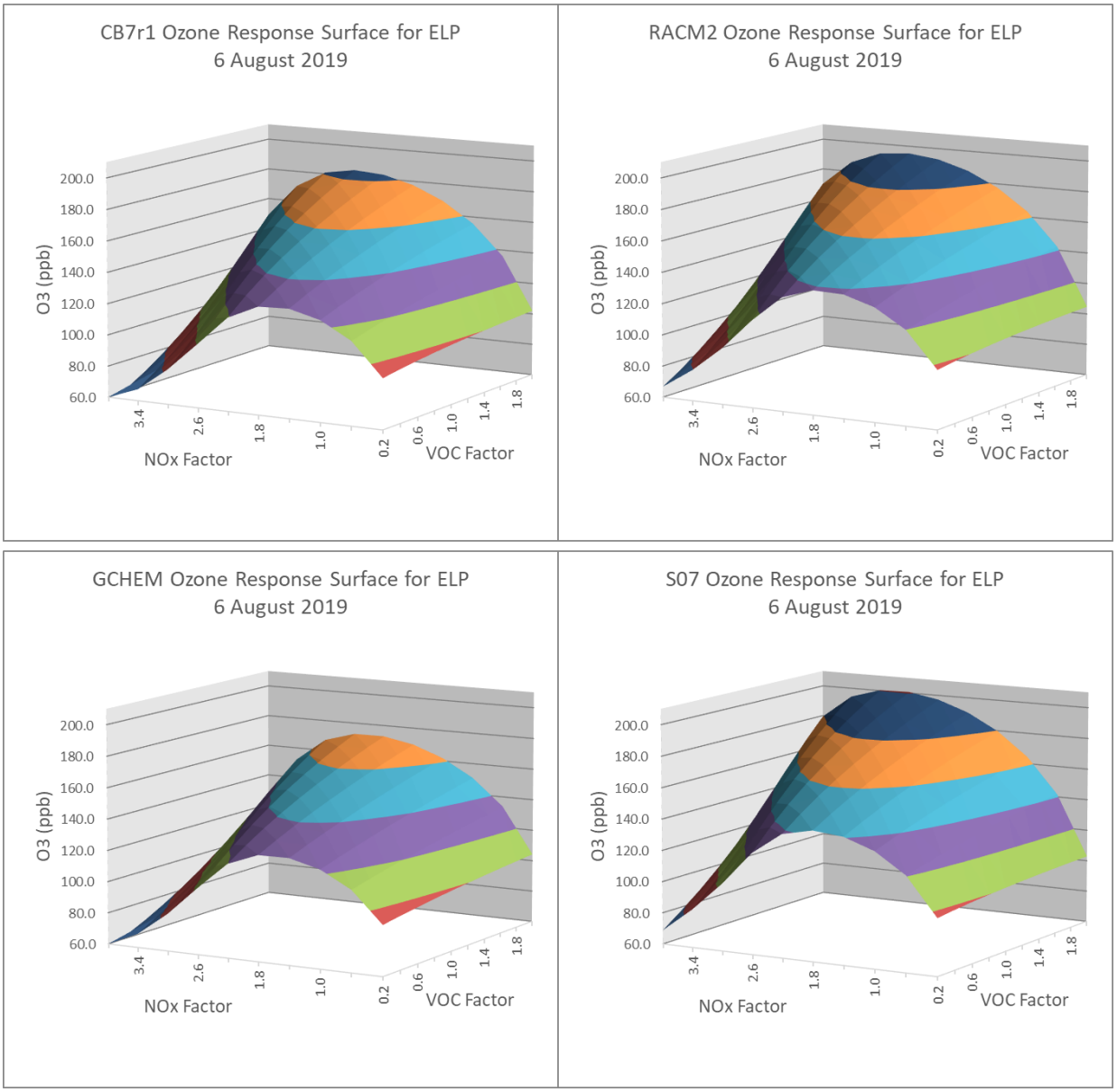

Figure 15. Ozone response surface (MDA1, ppb) to varying anthropogenic NOx and VOC emissions for ELP with the four chemical mechanisms. NOx and VOC scaling factors of 1 are the base case simulation.

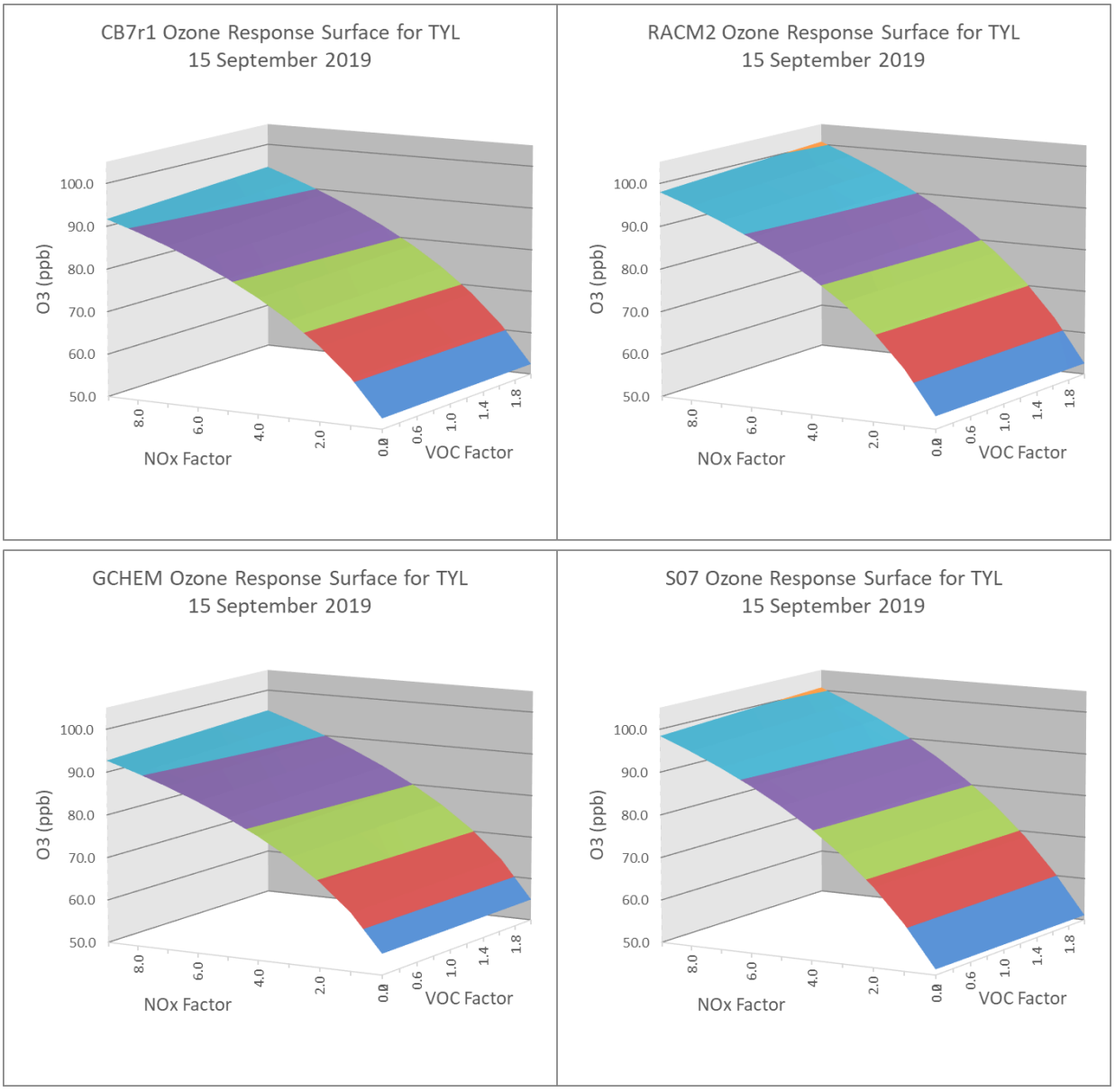

Figure 16. Ozone response surface (MDA1, ppb) to varying anthropogenic NOx and VOC emissions for TYL with the four chemical mechanisms. NOx and VOC scaling factors of 1 are the base case simulation.

4.3 VOC Reactivity (MIR) Factors

VOC reactivity factors (MIR values) characterize the O_3 forming potential of individual VOCs under atmospheric conditions where adding VOC emission yields the highest incremental increase in O_3 concentration (Carter and Atkinson, 1989). By definition, this occurs under VOC-limited O_3 formation regimes where adding VOC has the greatest incremental impact on the O_3 production rate. MIR values for VOC species in each mechanism were computed for HGB, DFW, SAN, and ELP using the Decoupled Direct Method (DDM) probing tool in CAMx (Dunker, 1984; Dunker et al., 2002). We configured DDM to compute the sensitivity of the O_3 concentration to emissions of an individual VOC ($d[O_3]/d[VOC]$) which is

proportional to the MIR. As mentioned above, a VOC-limited scenario was not identified for TYL so an MIR analysis was unable to be performed.

DDM model runs were conducted for three VOC-limited emissions scaling cases (Table 15), which were identified using the O_3 concentration results from the matrix of 100 box simulations described in the previous section. We selected three emission cases to obtain some averaging over representative emission scenarios. The three cases had VOC scaling factors set at 0.5, 1.0, and 1.5 to span conditions of the base case. For each VOC scaling factor, the change in O_3 per change in NOx ($d[O_3]/d[NOx]$) was calculated from the matrix emission run results and the NOx factor that provides the most negative $d[O_3]/d[NOx]$ was chosen for the MIR analysis because negative $d[O_3]/d[NOx]$ is characteristic of VOC-limited conditions. For SAN, the NOx scaling factors are all 9.0, which is the highest value used in the matrix emissions simulations. It is possible that a larger NOx scaling is needed to determine the most negative $d[O_3]/d[NOx]$ for SAN and that the results presented here do not represent the optimal MIR conditions for SAN.

Table 15. VOC and NOx emission scaling factors used to compute VOC reactivity factors.

	HGB			DFW			SAN			ELP		
VOC	0.5	1.0	1.5	0.5	1.0	1.5	0.5	1.0	1.5	0.5	1.0	1.5
NOx	7.0	8.0	8.0	6.0	6.0	7.0	9.0	9.0	9.0	2.6	3.0	3.5

The DDM model results provide the sensitivity of O_3 to emissions of a single chemical species, e.g., to an individual VOC or NO. The MIR analysis was performed using DDM simulation results from days 2 through 5 only since the first day is considered model spin up. On each day, the hour where O_3 is most sensitive to NO was determined from the results. The corresponding sensitivities of O_3 to individual VOCs at this hour are the date-specific VOC MIR values. Daily VOC MIR values were identified for each of the three emissions cases (Table 15) and the average MIR values (averaged over 4 dates and 3 emission scenarios) are presented in Figure 17 and Figure 18 for multiple VOCs. The MIR values have units of moles O_3 per mole VOC can be interpreted as the number of moles of O_3 formed per mole of VOC added ($d[O_3]/d[VOC]$).

Xylenes and larger aromatics have the largest MIR values, meaning that O_3 is most sensitive to these species. The MIR values for xylenes and large aromatics are greatest for the RACM2 mechanism, followed by CB7r1 and SAPRC07, and finally GEOS-Chem. Internal alkenes, isoprene, alpha-pinene, and terpenes have similar MIR values but there can be considerable variation between mechanisms and locations. O_3 is least sensitive to alkanes (including ethane and propane), acetone, methanol, and ethyne, which have the lowest MIR values. Control strategies targeting species with high MIR values (i.e., xylenes and large aromatics) would be an efficient method to reduce O_3, however emissions also need to be considered. The MIR values can be used to determine reactivity-weighted emissions which is a better metric to use in O_3 reduction planning.

The VOC reactivity trend is fairly similar between the four locations (Figure 19 and Figure 20) indicating that MIR is an appropriate measure to compare VOC chemistry. There is also overall good agreement for many VOC MIR values among the mechanisms (Figure 17 and Figure 18). The correlation coefficient and the slope of the linear regression line was calculated for the MIR values from each mechanism against SAPRC07 (Table 16). Since

SAPRC07 MIR values have been evaluated against observations (Carter, 2010b), it is used as the standard reference for this analysis. Across all locations, GEOS-Chem shows the highest correlation with SAPRC07. GEOS-Chem was implemented into CAMx for this project and these high correlation coefficients provide confidence in the implementation. RACM2 has the lowest correlation but all values are above 0.9. The slope shows a different trend, with CB7r1 or RACM2 values closest to SAPRC07. GEOS-Chem slopes are consistently low and RACM2 slopes are consistently high. Certain VOCs show significant MIR variation between mechanisms and are at least partially responsible for the trends in the slope values. These species are discussed below.

Table 16. Correlation coefficient and linear regression slope calculated for VOC MIR values for each mechanism against SAPRC07.

Location and Statistical Paramter	GEOS-Chem	SAPRC07	CB7r1	RACM2
Correlation Coefficient				
HGB	0.98	1.00	0.97	0.95
DFW	0.98	1.00	0.97	0.95
SAN	0.98	1.00	0.95	0.93
ELP	0.97	1.00	0.96	0.92
Linear regression slope				
HGB	0.82	1.00	0.89	1.09
DFW	0.86	1.00	0.93	1.11
SAN	0.83	1.00	0.86	1.05
ELP	0.90	1.00	1.01	1.14

Notes: Correlation coefficient and slope calculated against SAPRC07.

Some of the VOCs with the largest MIR differences between mechanisms include xylenes, large aromatics, isoprene, alpha-pinene, and alkanes (especially propane). The impact of these VOCs on O_3 will therefore differ considerably depending on the choice of chemical mechanism. Some of the differences are likely due to how the different mechanisms handle complex chemistry. For example, aromatics chemistry is uncertain and oxidation products get complicated very quickly. These products are handled slightly differently in each mechanism and these changes obviously affect the MIR values and the overall impact on O_3 formation. The MIR values for large aromatics and xylenes are high for the RACM2 and low for GEOS-Chem compared to SAPRC07 which influences the slope values in Table 16. The MIR differences would have the largest impact on O_3 in areas with high aromatics emissions and concentrations.

Although the MIR values are relatively low for propane and larger alkanes, high emissions make them important species for O_3 production. GEOS-Chem consistently has low alkane MIR values and RACM2 has the highest value at all locations except ELP. RACM2's propane MIR value is also more than two times higher than the other mechanisms. These trends are likely due to how hydrocarbon species are lumped in each mechanism. For example, the

RACM2 species HC3 lumps propane and isobutane together. Isobutane is considerably more reactive than propane leading to a larger propane MIR value reported here (https://ww2.arb.ca.gov/sites/default/files/2020-12/cp_reg_mir-tables.pdf). The MIR differences for propane and alkanes may be particularly important to consider in areas that produce a large amount of oil and gas where emissions are greater. The low alkane and aromatics MIR values for GEOS-Chem are contributing to the generally low O_3 concentrations seen from GEOS-Chem in the base case simulations (except at TYL). Conversely, the high propane and aromatics MIR values for RACM2 lead to the O_3 concentrations on the higher end of all the mechanisms.

Isoprene is another species that has significant MIR differences between mechanisms, with the GEOS-Chem and SAPRC07 MIR values about 2-4 times higher than RACM2. The impact of biogenic VOC chemistry on O_3 levels for GEOS-Chem versus the other mechanisms was discussed in the base case simulation section above. The high GEOS-Chem isoprene MIR value likely contributes to the higher O_3 trends seen at TYL in the GEOS-Chem model run and indicates that GEOS-Chem may be able to make more O_3 from biogenics. It is interesting however that SAPRC07, which has high isoprene MIR values similar to GEOS-Chem, shows much lower O_3 concentrations at TYL. This may indicate that the biogenic chemistry in the mechanisms behave differently under varying NOx conditions. Since MIR values were unable to be calculated at TYL, it is unclear if the isoprene reactivity is responsible for these differing O_3 trends.

While MIR values are useful when interpreting chemistry differences between mechanisms, they do have certain limitations which are highlighted in the isoprene and TYL results. The MIR analysis was unable to be conducted at TYL since it was much more NOx-limited than the other locations and a VOC-limited condition was not identified at relatively high NOx scaling factors. MIR values may not be the most appropriate metric to compare differences in biogenic chemistry in locations with high biogenic emissions. Further model runs to investigate how O_3 production in the chemical mechanisms vary under NOx-limited regimes would be beneficial to understand the mechanism differences under a wider variety of conditions.

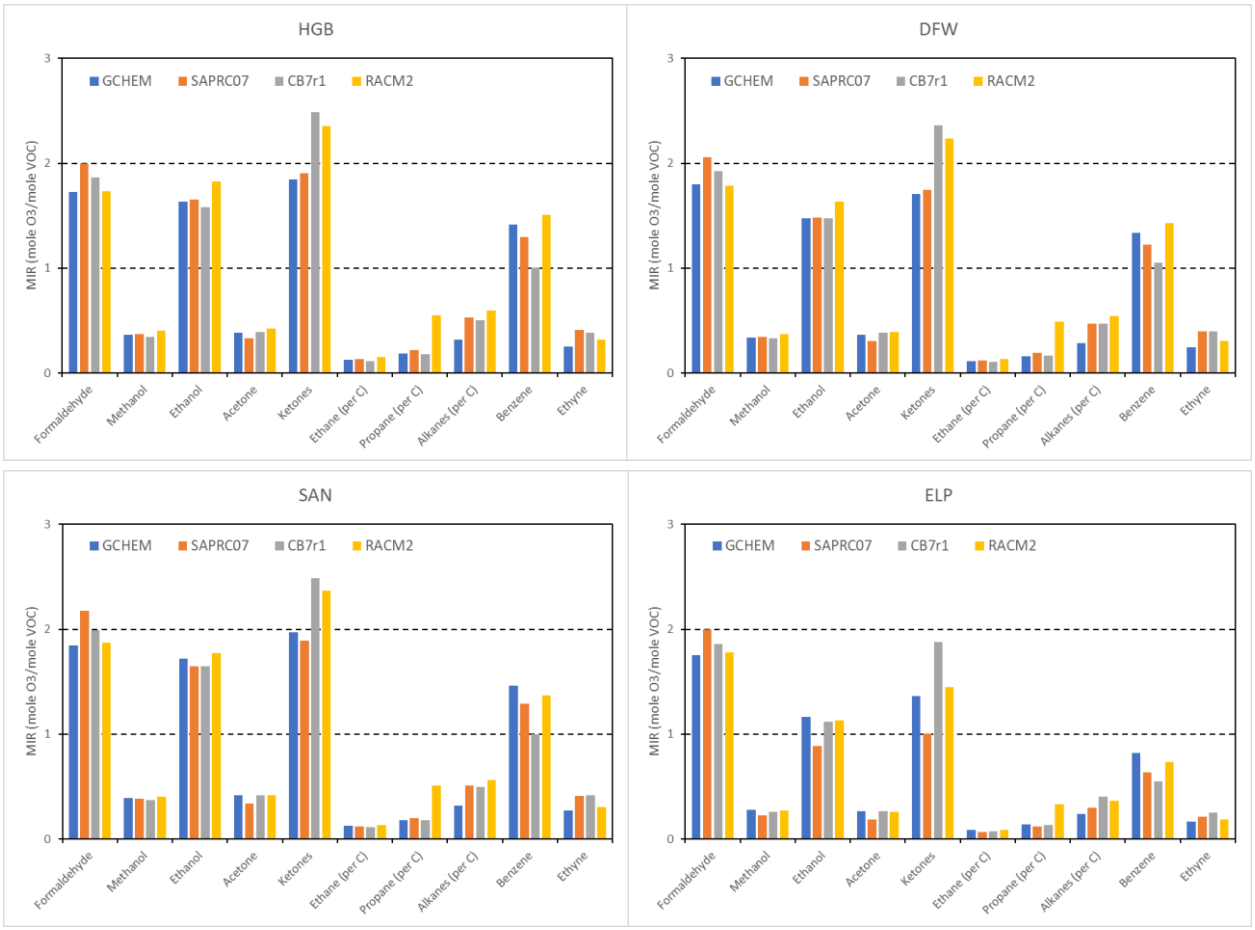

Figure 17. Calculated MIR values (mole O_3/mole VOC) for each location and mechanism.

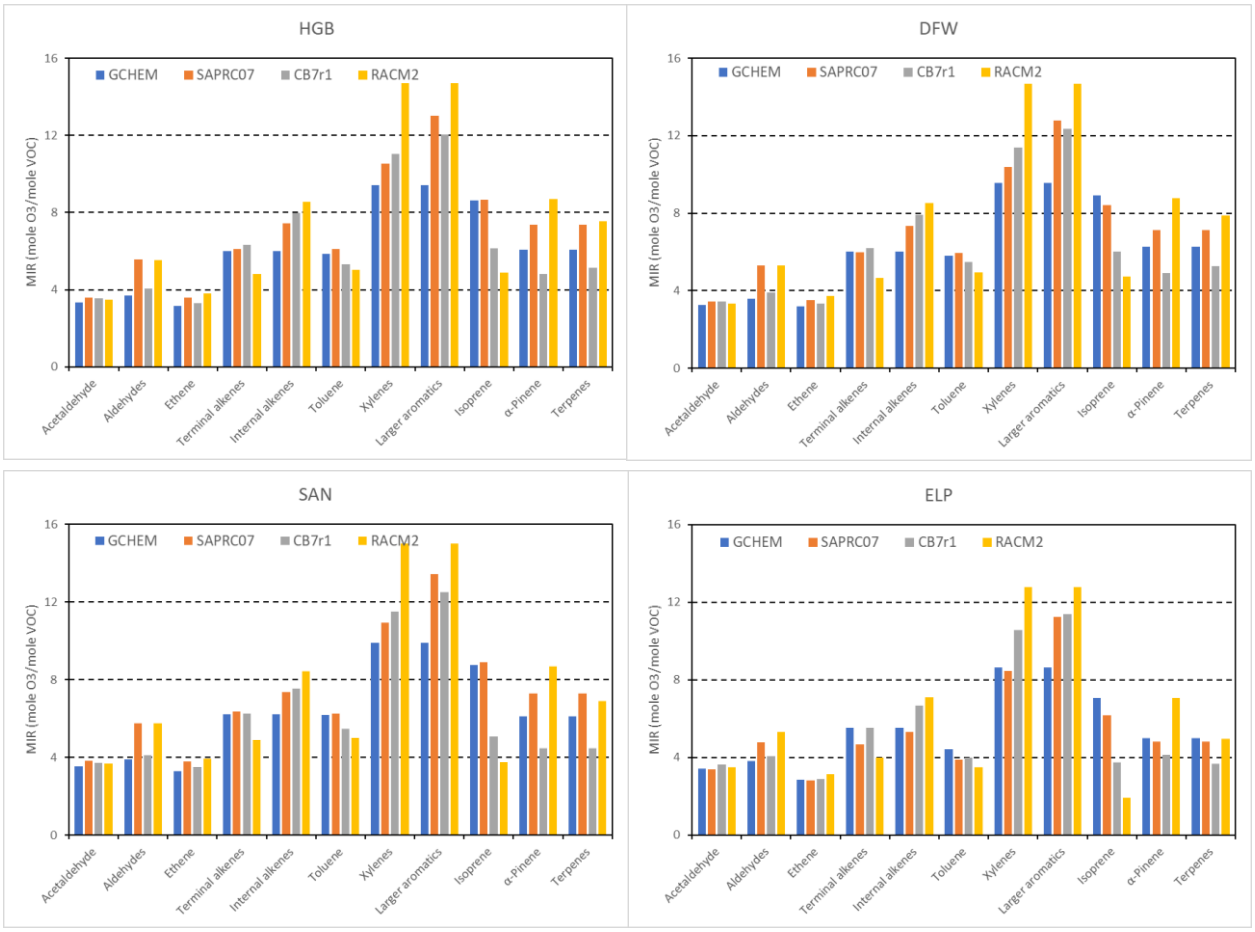

Figure 18. Calculated MIR values (mole O_3/mole VOC) for each location and mechanism.

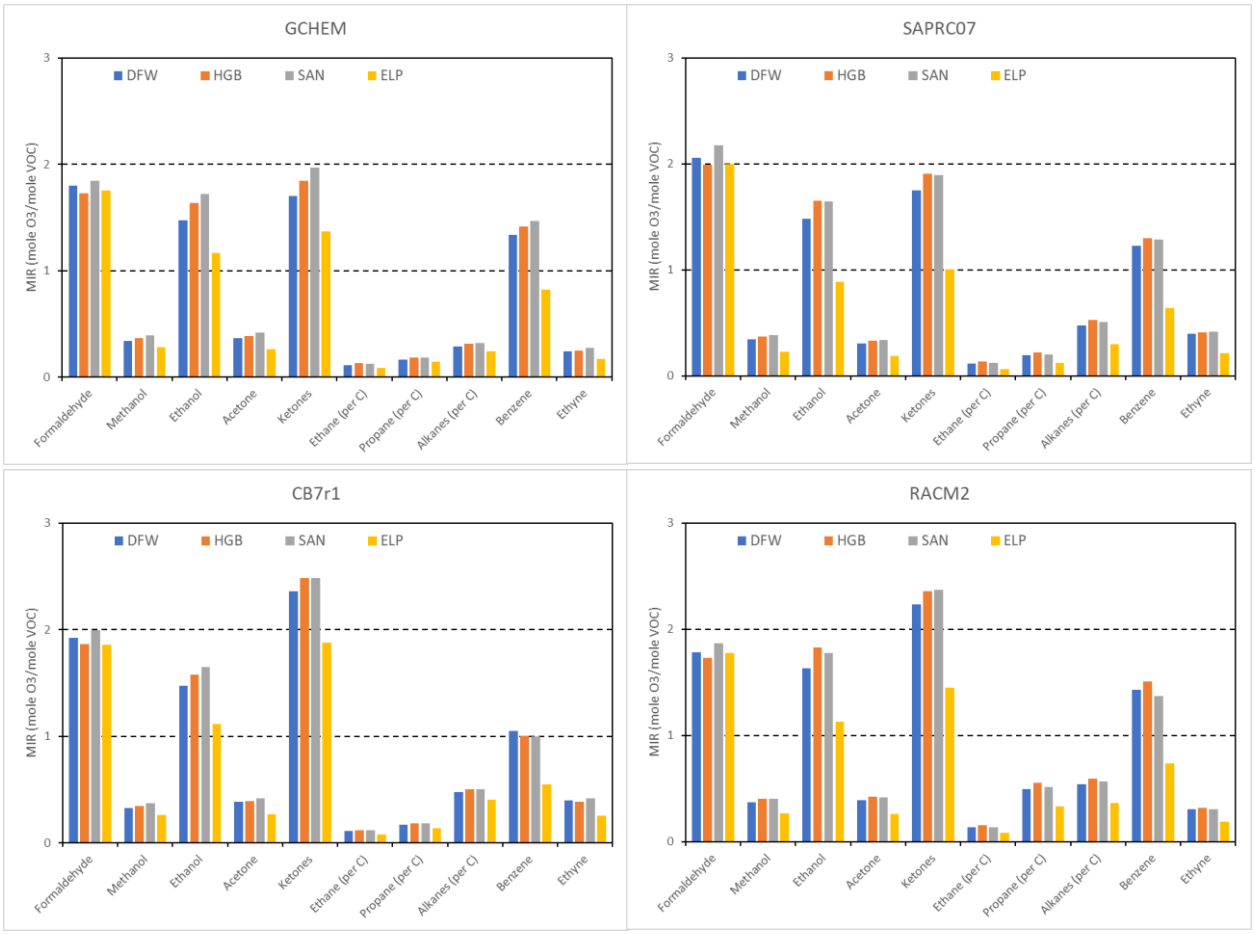

Figure 19. Calculated MIR values (mole O_3/mole VOC) for each location and mechanism.

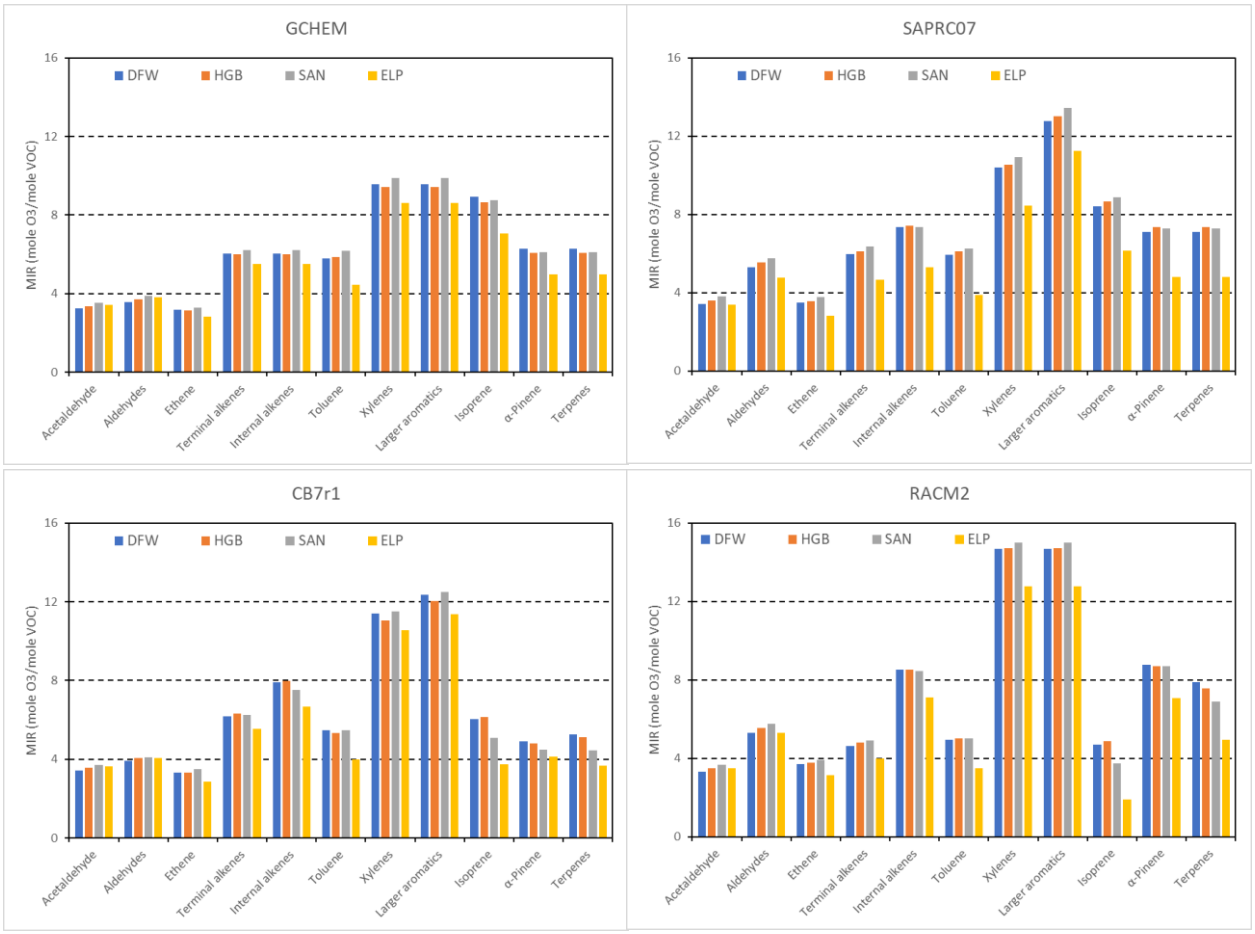

Figure 20. Calculated MIR values (mole O_3/mole VOC) for each location and mechanism.

5.0 Summary and Conclusions

CAMx box model runs were performed to compare four chemical mechanisms commonly used in air quality modeling: CB7r1, SAPRC07, RACM2, and GEOS-Chem. CB7r1, SAPRC07 and RACM2 were already implemented in CAMx, and GEOS-Chem was implemented in CAMx as part of this project. A box model setup (i.e., 1-D CAMx simulations) was chosen because it is an efficient method to investigate atmospheric chemistry and the response of O_3 to NOx and VOC changes. Simulations were performed for five Texas locations (Houston-Galveston-Brazoria (HGB), Dallas-Fort Worth (DFW), San Antonio (SAN), Tyler (TYL), and El Paso (ELP)) and results were used to compare ozone's response to changes in precursor emissions (i.e., NOx and VOC) between the various mechanisms. The VOC reactivity, or Maximum Incremental Reactivity (MIR) factors, were also computed and compared. Results from this study will help TCEQ evaluate chemical mechanism performance and better understand the impacts of mechanism choice on ozone State Implementation Plan (SIP) modeling.

This study focused solely on the O_3 response to anthropogenic emissions changes. While all mechanisms showed a fairly similar O_3 response to varying emissions (Figure 12 through Figure 15), there were slight differences. RACM2 had a higher O_3 response, indicating that it forms O_3 more efficiently, whereas GEOS-Chem had a lower O_3 response and forms O_3 less efficiently. Differences in biogenic VOC chemistry between the mechanisms also appear to play a role in O_3 concentrations, which is most evident in the TYL results. Further sensitivity studies adjusting biogenic emissions would provide more information on how these chemistry differences impact O_3 concentrations.

Overall, the four mechanisms evaluated in this study have similar VOC reactivities, as seen in the MIR value comparisons. The consistency between locations indicate that MIR is an appropriate method to compare VOC chemistry. Impacts to O_3 formation due to VOC chemistry will consequently be similar between the mechanisms as well, particularly under VOC-limited conditions where MIR values are most relevant. Correlation coefficients comparing CB7r1, RACM2, and GEOS-Chem against SAPRC07 at all locations are consistently above 0.9, with GEOS-Chem having the best agreement. The slope of the linear regression line for each mechanism shows that CB7r1 and RACM2 are closest to SAPRC07 and that GEOS-Chem is consistently lower and RACM2 is consistently higher. Since SAPRC07 MIR values have been evaluated against observations (Carter, 2010b), it is used as the standard reference for this analysis.

The MIR differences discussed in the previous section are responsible for the correlation coefficient and slope variations. Some of the most important species that may impact modeling in Texas include aromatics, propane, and larger alkanes. Xylenes and larger aromatics had the greatest MIR values at all locations and mechanisms, however there was significant difference between mechanisms. RACM2 MIR values were much higher than the others and GEOS-Chem values were low. Aromatics chemistry is complex and uncertain, leading to variation in how it is implemented in each mechanism. Future research to better understand oxidation products and reaction rates would help constrain the impact aromatics have on O_3 formation in air quality modeling.

Propane and larger alkanes are also important because of their relatively high emissions. They can make up more than half of the mass of VOC emissions in some regions and play a particularly important role in oil and gas producing areas. While the overall propane and alkane MIR values are lower than many other VOCs, the large emissions make them

important in O_3 formation. The GEOS-Chem MIR values for alkanes were consistently lower than the other mechanisms at all locations. The low MIR values for both alkanes and aromatics indicate that O_3 production in GEOS-Chem is less efficient under VOC-limited conditions. This is evident in the base case simulations where O_3 concentrations are generally lower for GEOS-Chem than the other mechanisms (except at TYL). RACM2 had propane MIR values that were significantly higher than the other mechanisms. This, in addition to the high aromatic MIR values, leads to higher O_3 concentrations.

While VOC reactivity is an important aspect of O_3 formation, other factors, in particular NOx chemistry, also need to be considered. MIR calculations require VOC-limited conditions, so the sensitivity tests performed in this study are most relevant to VOC-limited regions. Many areas in Texas however are strongly NOx-limited and this chemical regime is a large component of the 3-D simulations performed by TCEQ for SIP modeling. The ozone response surface results for TYL (Figure 16) provide a clear example of a NOx-limited region. Results from the base case simulations show significant differences in ONs and PANs concentrations between the mechanisms. Small changes in these species can substantially impact O_3 formation so a better understanding of ON and PAN chemistry in these regions would be beneficial. Using TYL as a representative NOx-limited area, future sensitivity studies could be performed to investigate ON and PAN differences between mechanisms and how they affect O_3 formation.

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