Final Report

UPDATES TO THE CARBON BOND CHEMICAL MECHANISM: CB05

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ABSTRACT

Updated versions of the Carbon Bond mechanism were developed for use in EPA atmospheric modeling studies. The new Carbon Bond mechanism is called CB05 because it was developed in 2005. The CB05 is a condensed mechanism of atmospheric oxidant chemistry that provides a basis for computer modeling studies of ozone, particulate matter (PM), visibility, acid deposition and air toxics issues. Updates in CB05 compared to earlier CB4 mechanisms are:

- Updated rate constants based on recent (2003 – 2005) IUPAC and NASA evaluations.
- An extended inorganic reaction set for urban to remote tropospheric conditions.
- NOx recycling reactions to represent the fate of NOx over multiple days.
- Explicit organic chemistry for methane and ethane.
- Explicit methylperoxy radical, methyl hydroperoxide and formic acid.
- Lumped higher organic peroxides, organic acids and peracids.
- Internal olefin (R-HC=CH-R) species called IOLE.
- Higher aldehyde species ALDX making ALD2 explicitly acetaldehyde.
- Higher peroxyacyl nitrate species from ALDX called PANX.
- Lumped terpene species called TERP.
- Optional mechanism extension for reactive chlorine chemistry.
- Optional extended mechanism with explicit reactions for air-toxics.

The core CB05 mechanism has 51 species and 156 reactions. The CB05 was evaluated against smog chamber data from the Universities of North Carolina and California at Riverside. An updated wall reaction mechanism was developed for the UNC chamber that improved performance in experiments that are sensitive to chamber radical sources. The addition of higher aldehyde (ALDX) and internal olefin (IOLE) species to CB05 improve mechanism performance for simulating these species groups. The addition of organic peroxide species improves the simulation of oxidants that are involved in PM sulfate formation. The addition of explicit methylperoxy radical improves the simulation of hydrogen peroxide under low NOx conditions.

Two CB05 mechanism extensions were developed. The reactive chlorine chemistry mechanism can be used in conjunction with the CB05 core mechanism to model the impact of CL_2 and/or HOCl emissions on oxidant formation and VOC decay rates. The explicit species extension can be used in conjunction with the CB05 (or another) core mechanism to model the following toxic species: primary formaldehyde, primary acetaldehyde, 1,3-butadiene, primary and secondary acrolein. Other explicit species are toluene, o-xylene, m-xylene, p-xylene, apha-pinene and beta-pinene. These include the main precursors to secondary organic aerosol (SOA) and could be used as the basis for refined modeling approach for SOA that is independent of the core mechanism selected (e.g., CB4, CB05 or SAPRC99).

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1. INTRODUCTION

The goals of this study were to develop updated versions of the Carbon Bond mechanism for use in EPA atmospheric modeling studies. The starting point for this study was version 4 of the Carbon Bond mechanism (CB4) developed in the late 1980s (Gery et al., 1989) as updated in the mid 1990s for EPA's "OTAG" study. An overview of the development history of CB4 and related mechanisms is given below.

The new version of the Carbon Bond mechanism is called CB05 because it was developed in 2005. The CB05 is a condensed mechanism of atmospheric oxidant chemistry that provides a basis for computer modeling studies of ozone, particulate matter (PM), visibility, acid deposition and air toxics issues. The CB05 mechanism updates developed for this study are as follows:

1. Incorporating current kinetic and photolysis data in the core mechanism.
2. Extending the chemical mechanism to better support PM modeling needs such as formation of secondary organic aerosols (SOA).
3. Adding extra species and reactions to treat a number of volatile organic compounds (VOCs) explicitly for modeling air toxics.
4. Accounting for the role of reactive chlorine emissions in VOC degradation and oxidant chemistry.

The CB05 mechanism updates are discussed further in Section 2.

HISTORY OF CB4

EPA sponsored the development of version IV of the Carbon Bond (CB4) in the late 1980's for use in urban and regional photochemical modeling and Gery et al., (1989), published the mechanism. The regional models of the late 1980's that utilized CB4 were more limited in domain extent than current regional models (e.g., formulated for the planetary boundary layer and not the upper troposphere) and the original CB4 was more appropriate for urban than regional scale modeling.

EPA made limited updates to the CB4 mechanism in the early 1990s. The three main updates were to PAN chemistry, radical termination reactions and isoprene chemistry and they culminated in the version of CB4 used for the Ozone Transport Assessment Group (OTAG) modeling and EPA's NOx SIP call. Two other versions of CB4 that have appeared since the OTAG version are CBM-Z and CB2002. These mechanisms are reviewed briefly below.

The Urban Airshed Model Version of CB4

The EPA's Urban Airshed Model (UAM-IV; Morris and Myers, 1990) had the first widely used version of the CB4 mechanism. Changes from the Gery et al. (1989) mechanism were the inclusion of explicit chemistry for methanol and ethanol and an update to the PAN chemistry. Dodge (1991) updated the PAN chemistry for CB4 because the Gery et al. (1989) mechanism had incorrect temperature dependencies for PAN formation (Tuazon, Carter and Atkinson, 1991).

The OTAG Version of CB4

The OTAG version of CB4 had two updates were made to better represent regional scale oxidant formation in the eastern US where high isoprene levels occur and rural areas have relatively low NOx concentrations. Yarwood updated the radical-radical termination reactions (among HO_2 and RO_2 radicals) to better represent oxidant formation under conditions of low NOx (Yarwood and Burton, 1994). Whitten updated the isoprene chemistry in the CB4 (Whitten et al., 1996) to reflect newer scientific data on the products and mechanisms of isoprene oxidation (Carter and Atkinson, 1996). The updated isoprene mechanism is a translation from SAPRC to CB4 species of Carter's condensed "1-product" isoprene mechanism (Carter, 1996).

CBM-Z – Pacific Northwest National Laboratory

The Pacific Northwest National Laboratory (PNNL) has developed a mechanism based on the Carbon Bond approach called CBM-Z (Zaveri and Peters, 1999). Changes in CBM-Z were intended to update the mechanism from the published Gery et al., (1989) version and improve performance for regional scale modeling, and included:

- Revised inorganic chemistry.
- Explicit treatment of the lesser reactive alkanes - methane and ethane.
- Revised parameterizations of the reactive paraffin, olefin, and aromatic reactions.
- Inclusion of alkyl and acyl peroxy radical interactions and their reactions with the NO_3 radical.
- Inclusion of organic hydroperoxides.
- Isoprene chemistry based on the condensed one-product mechanism of Carter (1996).

The CBM-Z and CB4 were evaluated against smog chamber data from the TVA chamber and showed improved performance for CBM-Z on these chamber experiments. Sensitivity tests showed larger differences between CBM-Z and CB4 for regional modeling conditions than for urban or smog chamber conditions. One factor that contributed to differences under regional conditions (Zaveri and Peters, 1999) was the inclusion in CBM-Z of reactions for organic nitrates that slowly recycle nitrogen from an inactive form (organic nitrates) to an active form (NOx).

CB2002 – University of North Carolina

In late 1990s, UNC started to update and re-evaluate the CB4 mechanism against smog chamber data. UNC's approach was to retain the overall structure of CB4 but update rate constants and some product yields based on recent data. The first mechanism produced by UNC was called CB99. Unfortunately, the CB99 work was completed just as literature values for a critical rate constant ($OH + NO_2$) changed. UNC repeated the work with the new $OH + NO_2$ rate constant and developed CB2002 to supercede CB99 (Jeffries, Voicu, and Sexton, 2002). The CB2002 was evaluated against UNC smog chamber data as described in detail in Jeffries, Voicu, and Sexton (2002).

The main changes between CB2002 and CB4 were:

- Updated inorganic reaction rate constants with new reactions for NO_3 reacting with OH, HO_2 and itself, and O_3 reacting with $O(^3P)$.
- A new HONO photolysis reaction yielding NO_2 and H-atoms. IUPAC (2004) now recommends setting this reaction to zero for tropospheric conditions.
- New rate constants for N_2O_5 reacting with water (Wahner et al., 1998). This update also includes a reaction of N_2O_5 with water dimers (i.e., $N_2O_5 + H_2O + H_2O$).
- Lower rate constants for radical-radical termination reactions involving XO2 and HO_2.
- New rate constants for all olefin reactions involving ETH, OLE and ISOP.
- New products for reactions of ETH and OLE.

2. MECHANISM UPDATES

The main CB05 mechanism is referred to as the core mechanism. There are two extensions to the core mechanism for modeling explicit species (e.g., toxics) and reactive chlorine chemistry. The core mechanism and extensions are described below. Finally, the process for mapping "real species" to CB05 "model species" is discussed (e.g., for emission inventory modeling).

CB05 CORE MECHANISM

The core CB05 mechanism has 51 chemical species (Table 2-1) and 156 reactions (Table 2-2). The changes in the mechanism from CB4 (Gery et al., 1989) fall into the following categories that are discussed following Tables 2-1 and 2-2.

- Kinetic Updates
- Photolysis Updates
- Extended Inorganic Reaction Set
- Simple Alkanes (Methane and Ethane)
- Higher Aldehydes
- Alkenes with Internal Double Bonds
- Oxygenated Products and Intermediates
- Terpene Chemistry

Table 2-1. Species names for the CB05 core mechanism.

Species Name	Description	Number of Carbons
NO	Nitric oxide	0
NO2	Nitrogen dioxide	0
O3	Ozone	0
O	Oxygen atom in the $O^3(P)$ electronic state	0
O1D	Oxygen atom in the $O^1(D)$ electronic state	0
OH	Hydroxyl radical	0
HO2	Hydroperoxy radical	0
H2O2	Hydrogen peroxide	0
NO3	Nitrate radical	0
N2O5	Dinitrogen pentoxide	0
HONO	Nitrous acid	0
HNO3	Nitric acid	0
PNA	Peroxynitric acid (HNO_4)	0
CO	Carbon monoxide	1
FORM	Formaldehyde	1
ALD2	Acetaldehyde	2
C2O3	Acetylperoxy radical	2
PAN	Peroxyacetyl nitrate	2
ALDX	Propionaldehyde and higher aldehydes	2
CXO3	C3 and higher acylperoxy radicals	2
PANX	C3 and higher peroxyacyl nitrates	2
XO2	NO to NO2 conversion from alkylperoxy (RO_2) radical	0
XO2N	NO to organic nitrate conversion from alkylperoxy (RO_2) radical	0
NTR	Organic nitrate (RNO_3)	1
ETOH	Ethanol	2

Species Name	Description	Number of Carbons
CH4	Methane	1
MEO2	Methylperoxy radical	1
MEOH	Methanol	1
MEPX	Methylhydroperoxide	1
FACD	Formic acid	1
ETHA	Ethane	2
ROOH	Higher organic peroxide	1
AACD	Acetic and higher carboxylic acids	2
PACD	Peroxyacetic and higher peroxycarboxylic acids	2
PAR	Paraffin carbon bond (C-C)	1
ROR	Secondary alkoxy radical	0
ETH	Ethene	2
OLE	Terminal olefin carbon bond (R-C=C)	2
IOLE	Internal olefin carbon bond (R-C=C-R)	4
ISOP	Isoprene	5
ISPD	Isoprene product (lumped methacrolein, methyl vinyl ketone, etc.)	4
TERP	Terpene	10
TOL	Toluene and other monoalkyl aromatics	7
XYL	Xylene and other polyalkyl aromatics	8
CRES	Cresol and higher molecular weight phenols	8
TO2	Toluene-hydroxyl radical adduct	7
OPEN	Aromatic ring opening product	4
CRO	Methylphenoxy radical	7
MGLY	Methylglyoxal and other aromatic products	3
SO2	Sulfur dioxide	0
SULF	Sulfuric acid (gaseous)	0

Table 2-2. Reactions in the CB05 core mechanism.

Label	Reactants	Products	Rate Expression	Notes
R1	NO2	NO + O	1.0 x <NO2_SAPRC99>	20
R2	O+O2+M	O3 + M	6.0E–34^–2.4	1
R3	O3+NO	NO2	3.0E–12 @ 1500	1
R4	O+NO2	NO	5.6E–12 @ –180	1
R5	O+NO2	NO3	2.5E–31^–1.8 & 2.2E–11^–0.7	1
R6	O+NO	NO2	9.0E–32^–1.5 & 3.0E–11	1
R7	NO2+O3	NO3	1.2E–13 @ 2450	1
R8	O3	O	1.0 x <O3_O3P_IUPAC05>	2
R9	O3	O1D	1.0 x <O3_O1D_IUPAC05>	2
R10	O1D+M	O + M	2.1E–11 @ –102	1
R11	O1D+H2O	2*OH	2.20E–10	1
R12	O3+OH	HO2	1.7E–12 @ 940	1
R13	O3+HO2	OH	1.0E–14 @ 490	1
R14	NO3	NO2 + O	1.0 x <NO3NO2_SAPRC99>	20
R15	NO3	NO	1.0 x <NO3NO_SAPRC99>	20
R16	NO3+NO	2*NO2	1.5E–11 @ –170	1
R17	NO3+NO2	NO + NO2	4.5E–14 @ 1260	1
R18	NO3+NO2	N2O5	2.0E–30^–4.4 &	1

Label	Reactants	Products	Rate Expression	Notes
			1.4E–12^–0.7	
R19	N2O5+H2O	2*HNO3	2.50E–22	2
R20	N2O5+H2O+H2O	2*HNO3	1.80E–39	2
R21	N2O5	NO3 + NO2	1E–03^–3.5 @ 11000 & 9.7E14^0.1 @ 11080 & 0.45 & 1.0	2
R22	NO+NO+O2	2*NO2	3.3E–39 @ –530	2
R23	NO+NO2+H2O	2*HONO	5.00E–40	3
R24	NO+OH	HONO	7.0E–31^–2.6 & 3.6E–11^–0.1	1
R25	HONO	NO + OH	1.0 x <HONO_IUPAC05>	2
R26	OH+HONO	NO2	1.8E–11 @ 390	1
R27	HONO+HONO	NO + NO2	1.00E–20	4
R28	NO2+OH	HNO3	2.0E–30^–3.0 & 2.5E–11	1
R29	OH+HNO3	NO3	%2 2.4E–14 @ –460 & 2.7E–17 @ –2199 & 6.5E–34 @ –1335	1
R30	HO2+NO	OH + NO2	3.5E–12 @ –250	1
R31	HO2+NO2	PNA	1.8E–31^–3.2 & 4.7E–12 & 0.6	2
R32	PNA	HO2 + NO2	4.1E–5 @ 10650 & 4.8E15 @ 11170 & 0.6	2
R33	OH+PNA	NO2	1.3E–12 @ –380	1
R34	HO2+HO2	H2O2	%3 2.3E–13 @ –600 & 1.7E–33 @ –1000	1
R35	HO2+HO2+H2O	H2O2	%3 3.22E–34 @ –2800 & 2.38E–54 @ –3200	1
R36	H2O2	2*OH	1.0 x <H2O2_SAPRC99>	20
R37	OH+H2O2	HO2	2.9E–12 @ 160	1
R38	O1D+H2	OH + HO2	1.10E–10	1
R39	OH+H2	HO2	5.5E–12 @ 2000	1
R40	OH+O	HO2	2.2E–11 @ –120	1
R41	OH+OH	O	4.2E–12 @ 240	1
R42	OH+OH	H2O2	6.9E–31^–1.0 & 2.6E–11^0	1
R43	OH+HO2		4.8E–11 @ –250	1
R44	HO2+O	OH	3.0E–11 @ –200	1
R45	H2O2+O	OH + HO2	1.4E–12 @ 2000	1
R46	NO3+O	NO2	1.00E–11	1
R47	NO3+OH	HO2 + NO2	2.20E–11	1
R48	NO3+HO2	HNO3	3.50E–12	1
R49	NO3+O3	NO2	1.00E–17	5
R50	NO3+NO3	2*NO2	8.5E–13 @ 2450	1
R51	PNA	0.610*HO2 + 0.610*NO2 + 0.390*OH + 0.390*NO3	1.0 x <HO2NO2_IUPAC05>	2
R52	HNO3	OH + NO2	1.0 x <HNO3_IUPAC05>	2
R53	N2O5	NO2 + NO3	1.0 x <N2O5_IUPAC05>	2
R54	XO2+NO	NO2	2.6E–12 @ –365	6

Label	Reactants	Products	Rate Expression	Notes
R55	XO2N+NO	NTR	2.6E–12 @ –365	6
R56	XO2+HO2	ROOH	7.5E–13 @ –700	7
R57	XO2N+HO2	ROOH	7.5E–13 @ –700	7
R58	XO2+XO2		6.80E–14	8
R59	XO2N+XO2N		6.80E–14	8
R60	XO2+XO2N		6.80E–14	8
R61	NTR+OH	HNO3 + HO2 + 0.330*FORM + 0.330*ALD2 + 0.330*ALDX – 0.660*PAR	5.9E–13 @ 360	9
R62	NTR	NO2 + HO2 + 0.330*FORM + 0.330*ALD2 + 0.330*ALDX – 0.660*PAR	1.0 x <NTR_IUPAC05>	28
R63	ROOH+OH	XO2 + 0.500*ALD2 + 0.500*ALDX	3.01E–12 @ –190	1
R64	ROOH	OH + HO2 + 0.500*ALD2 + 0.500*ALDX	1.0 x <COOH_SAPRC99>	20
R65	OH+CO	HO2	%3 1.44E–13 @ 0.0 & 3.43E–33 @ 0.0	2
R66	OH+CH4	MEO2	2.45E–12 @ 1775	1
R67	MEO2+NO	FORM + HO2 + NO2	2.8E–12 @ –300	1
R68	MEO2+HO2	MEPX	4.1E–13 @ –750	1
R69	MEO2+MEO2	1.370*FORM + 0.740*HO2 + 0.630*MEOH	9.5E–14 @ –390	1
R70	MEPX+OH	0.700*MEO2 + 0.300*XO2 + 0.300*HO2	3.8E–12 @ –200	1
R71	MEPX	FORM + HO2 + OH	1.0 x <COOH_SAPRC99>	20
R72	MEOH+OH	FORM + HO2	7.3E–12 @ 620	1
R73	FORM+OH	HO2 + CO	9.00E–12	1
R74	FORM	2*HO2 + CO	1.0 x <HCHO_R_SAPRC99>	20
R75	FORM	CO	1.0 x <HCHO_M_SAPRC99>	20
R76	FORM+O	OH + HO2 + CO	3.4E–11 @ 1600	1
R77	FORM+NO3	HNO3 + HO2 + CO	5.80E–16	1
R78	FORM+HO2	HCO3	9.7E–15 @ –625	2
R79	HCO3	FORM + HO2	2.4E+12 @ 7000	1
R80	HCO3+NO	FACD + NO2 + HO2	5.60E–12	1
R81	HCO3+HO2	MEPX	5.6E–15 @ –2300	1
R82	FACD+OH	HO2	4.00E–13	1
R83	ALD2+O	C2O3 + OH	1.8E–11 @ 1100	1
R84	ALD2+OH	C2O3	5.6E–12 @ –270	1
R85	ALD2+NO3	C2O3 + HNO3	1.4E–12 @ 1900	1
R86	ALD2	MEO2 + CO + HO2	1.0 x <CCHO_R_SAPRC99>	20
R87	C2O3+NO	MEO2 + NO2	8.1E–12 @ –270	1
R88	C2O3+NO2	PAN	2.7E–28^–7.1 & 1.2E–11^–0.9 & 0.3	2
R89	PAN	C2O3 + NO2	4.9E–3 @ 12100 & 5.4E16 @ 13830 & 0.3	2
R90	PAN	C2O3 + NO2	1.0 x <PAN_IUPAC05>	2
R91	C2O3+HO2	0.800*PACD + 0.200*AACD + 0.200*O3	4.3E–13 @ –1040	1
R92	C2O3+MEO2	0.900*MEO2 + 0.900*HO2 + FORM + 0.100*AACD	2.0E–12 @ –500	1
R93	C2O3+XO2	0.900*MEO2 + 0.100*AACD	4.4E–13 @ –1070	2

Label	Reactants	Products	Rate Expression	Notes
R94	C2O3+C2O3	2*MEO2	2.9E–12 @ –500	1
R95	PACD+OH	C2O3	4.0E–13 @ –200	10
R96	PACD	MEO2 + OH	0.0 x <COOH_SAPRC99>	20
R97	AACD+OH	MEO2	4.0E–13 @ –200	1
R98	ALDX+O	CXO3 + OH	1.3E–11 @ 870	11
R99	ALDX+OH	CXO3	5.1E–12 @ –405	2
R100	ALDX+NO3	CXO3 + HNO3	6.50E–15	2
R101	ALDX	MEO2 + CO + HO2	1.0 x <C2CHO_SAPRC99>	20
R102	CXO3+NO	ALD2 + NO2 + HO2 + XO2	6.7E–12 @ –340	2
R103	CXO3+NO2	PANX	2.7E–28^–7.1 & 1.2E–11^–0.9 & 0.3	12
R104	PANX	CXO3 + NO2	4.9E–3 @ 12100 & 5.4E16 @ 13830 & 0.3	12
R105	PANX	CXO3 + NO2	1.0 x <PAN_IUPAC05>	2
R106	PANX+OH	ALD2 + NO2	3.00E–13	13
R107	CXO3+HO2	0.800*PACD + 0.200*AACD + 0.200*O3	4.3E–13 @ –1040	14
R108	CXO3+MEO2	0.900*ALD2 + 0.900*XO2 + HO2 + 0.100*AACD + 0.100*FORM	2.0E–12 @ –500	15
R109	CXO3+XO2	0.900*ALD2 + 0.100*AACD	4.4E–13 @ –1070	16
R110	CXO3+CXO3	2*ALD2 + 2*XO2 + 2*HO2	2.9E–12 @ –500	1
R111	CXO3+C2O3	MEO2 + XO2 + HO2 + ALD2	2.9E–12 @ –500	1
R112	PAR+OH	0.870*XO2 + 0.130*XO2N + 0.110*HO2 + 0.060*ALD2 – 0.110*PAR + 0.760*ROR + 0.050*ALDX	8.10E–13	17
R113	ROR	0.960*XO2 + 0.600*ALD2 + 0.940*HO2 – 2.100*PAR + 0.040*XO2N + 0.020*ROR + 0.500*ALDX	1.0E+15 @ 8000	17
R114	ROR	HO2	1.60E+03	17
R115	ROR+NO2	NTR	1.50E–11	17
R116	O+OLE	0.200*ALD2 + 0.300*ALDX + 0.300*HO2 + 0.200*XO2 + 0.200*CO + 0.200*FORM + 0.010*XO2N + 0.200*PAR + 0.100*OH	1.E–11 @ 280	18
R117	OH+OLE	0.800*FORM + 0.330*ALD2 + 0.620*ALDX + 0.800*XO2 + 0.950*HO2 – 0.700*PAR	3.20E–11	21
R118	O3+OLE	0.180*ALD2 + 0.740*FORM + 0.320*ALDX + 0.220*XO2 + 0.100*OH + 0.330*CO + 0.440*HO2 – PAR	6.5E–15 @ 1900	22
R119	NO3+OLE	NO2 + FORM + 0.910*XO2 + 0.090*XO2N + 0.560*ALDX + 0.350*ALD2 – PAR	7E–13 @ 2160	23
R120	O+ETH	FORM + 1.700*HO2 + CO + 0.700*XO2 + 0.300*OH	1.04E–11 @ 792	4
R121	OH+ETH	XO2 + 1.560*FORM + 0.220*ALDX + HO2	1.0E–28^–0.8 & 8.8E–12	1
R122	O3+ETH	FORM + 0.630*CO + 0.130*HO2 + 0.130*OH + 0.370*FACD	1.2E–14 @ 2630	1
R123	NO3+ETH	NO2 + XO2 + 2.0*FORM	3.3E–12 @ 2880	2
R124	IOLE+O	1.240*ALD2 + 0.660*ALDX + 0.100*HO2 + 0.100*XO2 + 0.100*CO + 0.100*PAR	2.3E–11	26
R125	IOLE+OH	1.300*ALD2 + 0.700*ALDX + HO2 + XO2	1.0E–11 @ –550	26
R126	IOLE+O3	0.650*ALD2 + 0.350*ALDX + 0.250*FORM + 0.250*CO + 0.500*O + 0.500*OH + 0.500*HO2	8.4E–15 @ 1100	26

Label	Reactants	Products	Rate Expression	Notes
R127	IOLE+NO3	1.180*ALD2 + 0.640*ALDX + HO2 + NO2	9.6E–13 @ 270	26
R128	TOL+OH	0.440*HO2 + 0.080*XO2 + 0.360*CRES + 0.560*TO2	1.8E–12 @ –355	24
R129	TO2+NO	0.900*NO2 + 0.900*HO2 + 0.900*OPEN + 0.100*NTR	8.10E–12	17
R130	TO2	CRES + HO2	4.2	17
R131	OH+CRES	0.400*CRO + 0.600*XO2 + 0.600*HO2 + 0.300*OPEN	4.10E–11	17
R132	CRES+NO3	CRO + HNO3	2.20E–11	17
R133	CRO+NO2	NTR	1.40E–11	17
R134	CRO+HO2	CRES	5.50E–12	25
R135	OPEN	C2O3 + HO2 + CO	9.0 x <HCHO_R_SAPRC99>	20
R137	OPEN+O3	0.030*ALDX + 0.620*C2O3 + 0.700*FORM + 0.030*XO2 + 0.690*CO + 0.080*OH + 0.760*HO2 + 0.200*MGLY	5.4E–17 @ 500	17
R138	OH+XYL	0.700*HO2 + 0.500*XO2 + 0.200*CRES + 0.800*MGLY + 1.100*PAR + 0.300*TO2	1.7E–11 @ –116	17
R139	OH+MGLY	XO2 + C2O3	1.7E–11	17
R140	MGLY	C2O3 + HO2 + CO	1.0 x <MGLY_IUPAC05>	2
R141	O+ISOP	0.750*ISPD + 0.500*FORM + 0.250*XO2 + 0.250*HO2 + 0.250*CXO3 + 0.250*PAR	3.60E–11	19
R142	OH+ISOP	0.912*ISPD + 0.629*FORM + 0.991*XO2 + 0.912*HO2 + 0.088*XO2N	2.54E–11 @ –407.6	19
R143	O3+ISOP	0.650*ISPD + 0.600*FORM + 0.200*XO2 + 0.066*HO2 + 0.266*OH + 0.200*CXO3 + 0.150*ALDX + 0.350*PAR + 0.066*CO	7.86E–15 @ 1912	19
R144	NO3+ISOP	0.200*ISPD + 0.800*NTR + XO2 + 0.800*HO2 + 0.200*NO2 + 0.800*ALDX + 2.400*PAR	3.03E–12 @ 448	19
R145	OH+ISPD	1.565*PAR + 0.167*FORM + 0.713*XO2 + 0.503*HO2 + 0.334*CO + 0.168*MGLY + 0.252*ALD2 + 0.210*C2O3 + 0.250*CXO3 + 0.120*ALDX	3.36E–11	19
R146	O3+ISPD	0.114*C2O3 + 0.150*FORM + 0.850*MGLY + 0.154*HO2 + 0.268*OH + 0.064*XO2 + 0.020*ALD2 + 0.360*PAR + 0.225*CO	7.10E–18	19
R147	NO3+ISPD	0.357*ALDX + 0.282*FORM + 1.282*PAR + 0.925*HO2 + 0.643*CO + 0.850*NTR + 0.075*CXO3 + 0.075*XO2 + 0.150*HNO3	1.00E–15	19
R148	ISPD	0.333*CO + 0.067*ALD2 + 0.900*FORM + 0.832*PAR + 1.033*HO2 + 0.700*XO2 + 0.967*C2O3	0.0036 x <ACROLEIN_SAPRC99>	20
R149	TERP+O	0.150*ALDX + 5.12*PAR	3.60E–11	20
R150	TERP+OH	0.750*HO2 + 1.250*XO2 + 0.250*XO2N + 0.280*FORM + 1.66*PAR + 0.470*ALDX	1.5E–11 @ –449	20
R151	TERP+O3	0.570*OH + 0.070*HO2 + 0.760*XO2 + 0.180*XO2N + 0.240*FORM + 0.001*CO + 7.000*PAR + 0.210*ALDX + 0.390*CXO3	1.2E–15 @ 821	20
R152	TERP+NO3	0.470*NO2 + 0.280*HO2 + 1.030*XO2 + 0.250*XO2N + 0.470*ALDX + 0.530*NTR	3.7E–12 @ –175	20
R153	SO2+OH	SULF + HO2	3.0E–31^–3.3 & 1.5E–12	1
R154	OH+ETOH	HO2 + 0.900*ALD2 + 0.050*ALDX + 0.100*FORM + 0.100*XO2	6.9E–12 @ 230	1
R155	OH+ETHA	0.991*ALD2 + 0.991*XO2 + 0.009*XO2N + HO2	8.7E–12 @ 1070	1

Label	Reactants	Products	Rate Expression	Notes
R156	NO2+ISOP	0.200*ISPD + 0.800*NTR + XO2 + 0.800*HO2 + 0.200*NO + 0.800*ALDX + 2.400*PAR	1.50E–19	19

Table Notes:

Rate constants are in units of molecules cm^{-3} and $seconds^{-1}$

Read rate expressions as follows:

A / <J_label>	k = A x j
A @ E	k = A x exp(–E/T)
A ^ B @ E	k = A x $(T/300)^B$ x exp(–E/T)
A^o ^ B^o @ E^o & A^∞ ^ B^∞ @ E^∞ & F & n	$k = \left[\frac{k^o[M]}{1+k^o[M]/k^\infty}\right]F^G$ where $G = \left[1+\left(\frac{\log(k^o[M]/k^\infty)}{n}\right)^{-2}\right]^{-1}$
%2 A^o @ E^o & A_2 @ E_2 & A_3 @ E_3	$k = k^o + \frac{k_3[M]}{1+k_3[M]/k_2}$
%3 A_1 @ E_1 & A_2 @ E_2	$k = k_1 + k_2$ [M]

1 Rate constant from NASA/JPL (2003)
2 Rate constant from IUPAC (2005)
3 Kaiser and Wu (1977)
4 Jeffries et al. (2002)
5 Hjorth (1992)
6 Based on NASA/JPL (2003) C2H5O2 + NO
7 Based on NASA/JPL (2003) C2H5O2 + HO2
8 Based on NASA/JPL (2003) C2H5O2 + C2H5O2
9 Average based on NASA/JPL (2003) CH3/C2H5 nitrates
10 Same as AACD+OH
11 Herron (1988)
12 Same as for PAN
13 Average based on NASA/JPL (2003) CH3/C2H5 nitrate ratio and IUPAC (2005) PAN+OH
14 NASA/JPL (2003) for CH3C(O)OO + HO2
15 NASA/JPL (2003) for CH3C(O)OO + CH3O2
16 IUPAC (2005) for CH3C(O)OO
17 Gery et al. (1989)
18 Cvetanovic (1987)
19 Atkinson and Carter (1994) single lumped product mechanism for isoprene.
20 SAPRC99
21 Consistent with IUPAC (2005) high-pressure limit for OH + propene. Falloff from the high-pressure limit isn't significant in the troposphere. Stoichiometric coefficients consistent with Atkinson (1997) and those developed and tested by Adelmann (1999).
22 Rate constant consistent with IUPAC (2005) for O3 + propene. Products based on Gery et al. (1989) assuming a 2 to 1 product ratio of higher aldehydes (ALDX) to acetaldehyde (ALD2).
23 Rate constant from Canosa-Mas et al. (1991) for minor pathway. May need future adjustment.
24 Rate constant from Le Bras (1997), products from Gery et al. (1989).
25 Adelmann (1999).
26 Ligocki, et al. (2002).
27 Homogeneous gas-phase reactions of N2O5 with water measured by Wahner, Mentel and Sohn (1998) and selected by IUPAC (2005). Rate contributions from heterogeneous reactions (see IUPAC 2005) may be added to the homogeneous rate.
28 IUPAC (2005) photolysis data for isopropyl nitrate.

Kinetic Data

Kinetic data for rate constant expressions were updated from the most recent evaluations by the IUPAC and NASA/JPL review panels, as detailed in the notes to Table 2-2. In general, values from IUPAC (2005) were selected. NASA/JPL (2003) values were used in some cases where IUPAC did not provide evaluated data.

Photolysis Data

Mechanism specific data required to calculate photolysis rates are absorption cross-sections and quantum yields. Photolysis data for CB05 are from the IUPAC (2005) evaluation or the SAPRC99 chemical mechanism (Carter, 2000). In general, data were used from SAPRC99 unless the IUPAC (2005) recommendations were found to be significantly different. Using the same data as SAPRC99 simplifies implementation in air quality models and promotes consistency between two mechanisms that may be compared.

Extended Inorganic Reaction Set

Yarwood, Whitten and Rao (2005) reviewed the inorganic reaction set in the CB4 to identify reactions that should be added to account for conditions of temperature, pressure and chemical environment encountered in annual simulations at scales ranging from urban to continental. Seventeen reactions were added as discussed below. The extended inorganic reactions are summarized briefly here and discussed in more detail below.

Reactions of molecular hydrogen (38 and 39) are somewhat important to odd-hydrogen (OH and HO_2) for very dry conditions in the upper troposphere. Including hydrogen will allow the air quality impacts of hydrogen as an alternative fuel to be evaluated. Hydrogen has a tropospheric background concentration of about 0.6 ppm (Novelli et al, 1999).

Reactions 40 to 45 involving odd-oxygen and odd-hydrogen species may be important for pristine conditions such as the upper troposphere. Including these reactions provides a more complete description of hydroxyl radical (OH) chemistry in the upper troposphere to improve modeling for persistent air toxics and mercury.

Additional NO_3 radical reactions (46 to 50) improve nighttime chemistry. NO_3 radical is the main driver for atmospheric chemistry at night and including additional NO_3 removal reactions improves the calculation of nighttime destruction rates for several types of reactive hydrocarbons (e.g., aldehydes, olefins) and for NOx (via NO_3 and N_2O_5 reactions).

Additional NOx recycling reactions (51 to 53 and 61 to 62) improve the representation of the fate of NOx over multi-day timescales by slowly recycling nitrogen from inactive forms of NOz to NOx. Reactions 51 and 53 are potentially important for very cold conditions such as the upper troposphere. Reactions 52, 61 and 62 of nitric acid and organic nitrates are potentially important to regional ozone and oxidant chemistry in the lower troposphere (Zaveri and Peters, 1999).

Simple Alkanes (Methane and Ethane)

Explicit reactions were added for OH with methane (CH4) and ethane (ETHA) to better describe the chemistry in remote atmospheres.

Higher Aldehydes

A new higher aldehyde species (ALDX) was added based on propionaldehyde chemistry (Ligocki and Whitten, 1992). Note that ALDX and related species contain two carbon atoms, not three, because this simplifies. Species related to ALDX are the corresponding peroxyacyl radicals (CXO3), peroxynitrates (PANX), carboxylic acids (AACD) and peroxycarboxylic acids (PACD). The species ALD2 and related species (C2O3 and PAN) now explicitly represent the chemistry of acetaldehyde. In important difference between higher aldehydes and acetaldehyde is that they photolyse more rapidly because higher aldehydes have larger quantum yields than acetaldehyde. The benefits of including the lumped higher aldehyde (ALDX) in CB05 are that acetaldehyde becomes explicit for air toxics modeling, faster photolysis rates for higher aldehydes are better represented, and the degradation sequence for higher aldehydes becomes deeper (ALDX to ALD2 to FORM). ALDX also improves the representation of internal olefins, as discussed next.

Alkenes with Internal Double Bonds

A new species (IOLE) was added to represent alkenes with internal double bonds (internal olefins) such as 2-butenes. IOLE is four carbon species. Internal olefins react very rapidly to produce photolytic products (aldehydes). Internal olefins were represented by their aldehyde products (e.g., 2-butene was represented as 2 ALD2) in the CB4. Including the explicit species IOLE in CB05 better describes the rate (kinetics) of internal olefin reactions than the CB4 approach. The IOLE chemistry is improved by having both acetaldehyde (ALD2) and lumped higher aldehydes (ALDX) as reaction products (Ligocki and Whitten, 1992).

Oxygenated Products and Intermediates

Several oxygenated species were added in conjunction with methane. Methylperoxy radicals were added as an explicit species (MEO2) rather than representing them by XO2. This change allows explicit representation of the products of the methylperoxy self-reaction (formaldehyde and methanol) and the reaction between methylperoxy and hydroperoxy radicals (methyl hydroperoxide). This change is expected to improve the representation of peroxide products that are important in sulfate production.

Other organic peroxides also were added as products of peroxy radical reactions. Higher organic peroxides (ROOH) were added as products of XO2 reacting with HO2 with chemistry based on ethyl hydroperoxide reactions. Peroxycarboxylic acids were added based on peroxyacetic acid (PACD) as products of the reactions of peroxyacetyl (C2O3) and higher peroxyacyl (CXO3) radicals with HO2.

Two carboxylic acids were added as products of peroxy radical reactions. Formic acid (FACD) is produced by reactions of HO2 with formaldehyde. Higher carboxylic acids were added based on acetic acid (AACD) as products of the reactions of peroxyacetyl (C2O3) and higher peroxyacyl (CXO3) radicals with HO2.

Terpene Chemistry

A new species TERP was added to CB05 to represent terpenes. The CB05 TERP chemistry is based on the SAPRC99 lumped terpene chemistry (Carter, 2000) translated to CB05 species.

EXTENDED MECHANISM WITH EXPLICIT SPECIES

An extended version of CB05 was developed by adding explicit reactions for several organic compounds. Explicit chemistry was added for organic compounds that are air toxics and/or precursors to secondary organic aerosol. The explicit compounds were added as tracer species that are decayed by oxidants (OH, etc.) without perturbing the oxidant levels. This approach makes the extended mechanism independent of the core mechanism so that the explicit compounds in the extended mechanism could be used in conjunction with any core mechanism (e.g., CB05, CB4, SAPRC99). The reactions for the extended organic mechanism are listed in Table 2-3.

Table 2-3. Reactions in the extended CB05 mechanism that may be added to the core mechanism.

Reaction Label	Reactants	Products	Rate Expression
T01	PFRM + OH	OH	9.0E-12
T02	PFRM + NO3	NO3	5.8E-16
T03	PFRM + O	O	3.4E-11 @ 1600
T04	PFRM		1.0/<HCHO_R_SAPRC99>
T05	PFRM		1.0/<HCHO_M_SAPRC99>
T06	PACT + OH	OH	5.6E-12 @ -270
T07	PACT + NO3	NO3	1.4E-12 @ 1900
T08	PACT + O	O	1.8E-11 @ 1100
T09	PACT		1.0/<CCHO_R_SAPRC99>
T10	BUTD + OH	OH + SACR	1.4E-11 @ -424.
T11	BUTD + O3	O3 + SACR	8.2E-15 @ 2070.
T12	BUTD + NO3	NO3 + SACR	1.79E-13
T13	BUTD + O	O3 + SACR	3.99E-12(T/298)**1.45
T14	PACR + OH	OH	2.0E-11
T15	PACR + O3	O3	2.61E-19
T16	PACR + NO3	NO3	1.7E-11 @ 3131.
T17	PACR		1.0/<ACROLEIN_SAPRC99>
T18	SACR + OH	OH	2.0E-11
T19	SACR + O3	O3	2.61E-19
T20	SACR + NO3	NO3	1.7E-11 @ 3131.
T21	SACR		1.0/<ACROLEIN_SAPRC99>
T22	TOLU + OH	OH	1.8E-12 @ -355.
T23	MXYL + OH	OH	1.7E-11 @ -116.
T24	OXYL + OH	OH	1.22E-11
T25	PXYL + OH	OH	1.3E-11
T26	APIN + O	O	2.79E-11

Reaction Label	Reactants	Products	Rate Expression
T27	APIN + OH	OH	1.2E-11 @ -440.
T28	APIN + O3	O3	6.3E-16 @ 580.
T29	APIN + NO3	NO3	1.2E-12 @ -490.
T30	BPIN + O	O	2.81E-11
T31	BPIN + OH	OH	7.51E-11
T32	BPIN + O3	O3	1.74E-15 @ 1260.
T33	BPIN + NO3	NO3	2.81E-11

Explicit Air Toxics

The following explicit toxic species are included in the extended mechanism:

PFRM = primary formaldehyde
PACT = primary acetaldehyde
BUTD = 1,3-butadiene
PACR = primary acrolein
SACR = secondary acrolein from 1,3-butadiene

The primary formaldehyde and acetaldehyde species allow the contributions of these primary aldehydes to be quantified. For example, the species FORM in CB05 is the sum of primary and secondary formaldehyde. If PFRM is included in the mechanism, primary formaldehyde is given directly by PFRM and secondary formaldehyde is the difference FORM – PFRM. For this approach to work, emissions of formaldehyde must be mapped to both PFRM and FORM. This does not double count the oxidant formation potential of formaldehyde emissions because the PFRM species is oxidant neutral. In this approach, PFRM is a "tracer" species whereas FORM is an "active" species.

The same approach works for distinguishing primary from secondary acetaldehyde by using the tracer species PACT and the active species ALD2.

Acrolein is explicitly apportioned as primary and secondary by the tracer species PACR and SACR. SACR is formed in CB05 only by reaction of the BUTD tracer (1,3-butadiene), which is expected to be the dominant source of secondary acrolein in the atmosphere.

The mapping of real compounds to model species for tasks such as emissions processing is discussed below.

Explicit Secondary Organic Aerosol Precursors

Secondary organic aerosol (SOA) formation is dominated by aromatics and biogenic terpene and sesquiterpene emissions (Odum et al., 1997). Aerosol yields can be attached to the corresponding lumped species in the CB05 core mechanism (TOL, XYL and TERP) to model SOA production. However, including explicit aromatics and terpene species in the extended mechanism can permit a more refined treatment of SOA production. The following explicit aromatics and terpenes are included in the extended mechanism:

TOLU = toluene
MXYL = m-xylene
OXYL = o-xylene
PXYL = p-xylene
APIN = alpha-pinene
BPIN = beta-pinene

The methodology for using the CB05 explicit species to model SOA formation will depend upon how SOA formation is implemented in the host air quality model. In general, SOA formation is modeled by forming semi-volatile products (SVPs) in VOC reactions. The SVPs are partitioned between the gas and aerosol phase according to the ambient conditions (e.g., temperature, pre-existing aerosols). Yields of SVPs should be added to the CB05 explicit species reactions in a format (i.e., species names and yields) that is compatible with the host air quality model. Data on SVP yields are available from Odum et al., 1997 and other studies.

The explicit aromatic species also may be of interest as air toxics.

Rate Constant Data

The rate constant data sources for species in the extended mechanism that are not also in the CB05 core mechanism are listed below.

OH + BUTD. Liu, A., W.A. Mulac, and C.D. Jonah (1992) "Rate constants for the gas phase reactions of OH radicals with 1,3 butadiene and allene at 1 atmosphere in Ar and over the temperature range 303-1173K" J. Phys. Chem. Vol. 92

O3 + BUTD. Treacy, J., M. ElHag, D. O'Farrell, and H. Sidebottom (1992) "Reactions of ozone with unsaturated organic compounds" Ber. Bunsenges. Phys. Chem., Vol. 96, pp 422-7.

NO3 + BUTD. Ellermann, T., O.J. Nielsen, and H. Skov (1992) "Absolute rate constents for the reactions of NO3 radicals with a series of dienes at 295K" Chem. Phy. Lett., Vol. 200, pp. 224-9.

O3P + BUTD. Adusei, G.Y.; Fontijn, A 1993 "Kinetics of the reaction between O(3P) atoms and 1,3-butadiene between 280 and 1015 K" J. Phys. Chem, Vol. 97, pp 1406 – 1408.

OH + PACR. Orlando, J.J.; Tyndall, G.S. (2002) "Mechanisms for the reactions of OH with two unsaturated aldehydes: Crotonaldehyde and acrolein" J. Phys. Chem. A, Vol. 106, pp 12252 – 12259.

O3 + PACR. Grosjean, D.; Grosjean, E.; Williams, E.L., II (1993) "Rate constants for the gas-phase reactions of ozone with unsaturated alcohols, esters, and carbonyls" Int. J. Chem. Kinet Vol 25, pp 783 – 794.

NO3 + PACR. Cabanas, B.; Salgado, S.; Martin, P.; Baeza, M.T.; Martinez, E. (2001) "Night-time Atmospheric Loss Process for Unsaturated Aldehydes: Reaction with NO3 Radicals" J. Phys. Chem. A: Vol. 105, pp 4440 – 4445.

OH + OXYL and PXYL. Atkinson, R. and Aschmann S.M (1989) "Rate constants for the gas-phase reactions of the OH radical with a series of aromatic hydrocarbons at 296K" Int. J. Chem. Kinet., Vol. 21, pp 355-365.

OH + MXYL. Atkinson, R. (1986) "Kinetics and Mechanisms of the Gas Phase Reactions of the Hydroxyl Radical with Organic Compounds", Chem. Rev., Vol. 86, pp 69-201.

O + APIN and BPIN. Luo, D., J.A. Pierce, I.L. Malkina, and W.P.L. Carter (1996) "Rate constants for the reactions of O(3P) with selected monoterpenes" Int. J. Chem. Kinet., Vol. 28, pp 1-8.

OH, O3 and NO3 + APIN. IUPAC (2005)

OH + BPIN. Foster, P., I. Denis and V. Jacob (1996) "Chap.7: Aerosol surface reactions and photocatalysis" in Vol. 2 of Hetreogeneous and Liquid Phase Processess book, pp 191-196.

O3 + BPIN. Khamaganor, V.G. and R.A. Hites (2001) "Rate Constants for the Gas-Phase Reactions of Ozone with Isoprene, alpha, and beta-Pinene, and Limonene as a Function of Temperature" J. Phys. Chem. A., Vol. 105, pp 815-822.

NO3 + BPIN. Kind, I., T. Berndt and O. Boge (1998) "Gas-phase rate constants for the reaction of NO3 radicals with a series of cyclic alkenes, 2-ethyl-1-butene and 2,3-dimethyl-1,3-butadiene" Chem. Phys. Lett., Vol. 288, pp 111-118.

REACTIVE CHLORINE CHEMISTRY

Tanaka et al. (2003) developed an extension to the CB4 mechanism with chlorine chemistry to evaluate the potential impact of reactive chlorine emissions (i.e., Cl_2 and HOCl) on tropospheric ozone formation. The Tanaka chlorine mechanism was reviewed and updated to be compatible with CB05. The reactions in Table 2-4 should be added to the CB05 core mechanism for modeling reactive chlorine. Table 2-5 identifies the species added for the reactive chlorine mechanism.

Table 2-4. Reactions in the CB05 reactive chlorine mechanism that may be added to the CB05 core mechanism.

Reaction Label	Reactants	Products	Rate Expression
CL1	CL2	2 CL	1.0 x <CL2_CB05>
CL2	HOCL	OH + CL	1.0 x <HOCL_CB05>
CL3	CL + O3	CLO	2.3E-11 @ 200
CL4	CLO + CLO	0.3 CL2 + 1.4 CL	1.63E-14
CL5	CLO + NO	CL + NO2	6.4E-12 @ -290
CL6	CLO + HO2	HOCL	2.7E-12 @ -220
CL7	OH + FMCL	CL + CO	5.0E-13
CL8	FMCL	CL + CO + HO2	1.0 x <FMCL_CB05>
CL9	CL + CH4	HCL + MEO2	6.6E-12 @ 1240
CL10	CL + PAR	HCL + 0.870*XO2 + 0.130*XO2N + 0.110*HO2 + 0.060*ALD2 - 0.110*PAR + 0.760*ROR + 0.050*ALDX	5.0E-11
CL11	CL + ETHA	HCL + 0.991*ALD2 + 0.991*XO2 + 0.009*XO2N +	8.3-11 @ 100

Reaction Label	Reactants	Products	Rate Expression
		HO2	
CL12	CL + ETH	FMCL + 2.000*XO2 + 1.000*HO2 + 1.000*FORM	1.07E-10
CL13	CL + OLE	FMCL + 0.330*ALD2 + 0.670*ALDX + 2.000*XO2 + 1.000*HO2 - 1.000*PAR	2.5E-10
CL14	CL + IOLE	0.300*HCL + 0.700*FMCL + 0.450*ALD2 + 0.550*ALDX + 0.300*OLE + 0.300*PAR + 2.000*XO2 + 1.000*HO2	3.5E-10
CL15	CL + ISOP	0.15HCL + 1.000*XO2 + 1.000*HO2 + 0.850*FMCL + 1.000*ISPD	4.3E-10
CL16	CL + FORM	HCL + 1.000*HO2 + 1.000*CO	8.2E-11 @ 34
CL17	CL + ALD2	HCL + C2O3	7.9-11
CL18	CL + ALDX	HCL + CXO3	1.3E-10
CL19	CL + MEOH	HCL + 1.000*HO2 + 1.000*FORM	5.5-11
CL20	CL + ETOH	HCL + 1.000*HO2 + 1.000*ALD2	8.2-11 @ -45

Table 2-5. Species added to CB05 by the reactive chlorine mechanism.

Species Name	Description
CL2	Molecular chlorine
HOCL	Hypochlorous acid
CL	Chlorine atom
CLO	Chlorine monoxide
FMCL	Formyl chloride (HC(O)Cl)

Considerations in updating the reactive chlorine mechanism for CB05 are:

1. Reaction rate constants were updated from Tanaka et al (2003) using the latest IUPAC (2005) recommendations except as described below.

2. CH4 is added as an explicit species and the Cl + CH4 are products updated to be explicit methylperoxy radical.

3. The Cl + PAR products are updated to be the same as OH + PAR in CB05. The Cl + PAR rate is an average over the absolute rates (on a per carbon atom basis) of the alkanes listed by in Tanaka et al (2003).

4. The Cl + OLE rate is updated to an average over the absolute rates (on a per C=C basis) for the alkenes presented in Tanaka et al (2003). Reaction products assume that reaction with C=C goes by addition and that the Cl atom ends up in a carbonyl compound, represented by formyl chloride (HC(O)Cl) as a surrogate. Other carbonyl products are ALD2 and ALDX by analogy with OH + OLE reaction. Note that in CB05 there is no need to consider H-abstraction from paraffinic carbons adjacent to the C=C group because OLE is a 2 carbon species (C=C).

5. The Cl + IOLE reaction is added. The rate is estimated as the rate for Cl reacting with OLE + 2 PAR because IOLE is a 4 carbon species, whereas OLE is a 2 carbon species. The products assume that reaction goes 70% by Cl-addition and 30% by H-abstraction, consistent with the rate constant assumption. The products for each channel are assumed to be:

C=C addition => FMCL + 0.65 ALD2 + 0.35 ALDX + 2 XO2 + HO2
H-abstraction => HCL + ALDX + OLE + XO2 + HO2

Cl-addition reactions are assumed to form acyl chlorides that are represented by formyl chloride (FMCL) as a surrogate, plus aldehydes that are split between ALD2 and ALDX by analogy with the OH + IOLE reaction. H-abstraction is assumed to form HCl plus unsaturated carbonyls that are represented as ALDX + OLE.

6. The Cl + isoprene chemistry is extensively revised from Tanaka et al. (2003). The goal of Tanaka et al. was to track a unique marker for the CL + ISOP reaction to permit comparison with ambient data. The goal for CB05 is to track the fate of the Cl and the fate of the carbon in isoprene. The HCl and FMCL yields reflect the balance between H-abstraction and addition pathways of 15% and 85% (Personal communication from Dr. Renyi Zhang, Texas A&M University: manuscript submitted). FMCL acts as a surrogate for the fate of all Cl-addition pathways. The lumped isoprene oxidation product from the CB05 mechanism (ISPD) accounts for the carbon containing products.

7. FMCL (formyl chloride) serves as a surrogate for all products where chlorine is incorporated into a chlorocarbonyl after an addition reaction, i.e., for olefins. The purpose is to account for sequestration of Cl in an organic molecule (chlorocarbonyl) allowing for the Cl to return later as a Cl-atom after the chlorocarbonyl reacts with OH or photolyses.

8. Reactions of Cl-atoms with aldehydes (ALD2 and ALDX) are included with rate constants from IUPAC (2005) and products the same as corresponding OH reactions. The organic products of Cl + ALDX are uncertain because there may be H-abstraction at the paraffinic carbon atoms of higher aldehydes.

9. No Cl-atom reactions are included for TOL, XYL or TERP because the products are uncertain. Omitting these reactions may not greatly alter the fate of Cl-atoms because, unlike OH, Cl-atoms react rapidly with all VOCs. For example, the global background for methane of ~1.7 ppm provides a significant "universal" sink for Cl-atoms because Cl-atoms react quite rapidly with methane.

10. The self-reaction of ClO radicals is added to account for situations where intense sources of ClO (e.g., high Cl_2 emissions) exceed the availability of NO or HO2 to act as sinks for ClO. The products of the CLO self-reaction are highly condensed to approximate the final products under tropospheric conditions.

11. No Cl-atom reaction with NO_2 is included because the product $CLNO_2$ photolyses rapidly.

CHEMICAL SPECIES MAPPING FOR CB05 MECHANISMS

An integral part of any condensed chemical mechanism is the assignment from real world organic species to the lumped species of the condensed mechanism. The existing chemical species mapping for CB4 was updated for CB05. The changes were:

1. All assignments to 2 ALD2 representing internal olefins were changed to IOLE. Note that internal olefins substituted at the double bond are different, as described next.

2. All remaining ALD2 assignments were changed to ALDX except for acetaldehyde, 2-methyl-2-butene and 3-substituted alk-2-enes (which remain assigned to n PAR + ALD2). Alkenes that are branched at the double bond are represented as aldehyde + PAR because their dominant reaction products (e.g., acetone plus acetaldehyde from 2-methyl-2-butene) are less reactive than the IOLE.

3. Terpenes were mapped to TERP

A list of mappings from real organic species to CB05 model species is provided in Appendix A.

The following species mapping changes apply specifically to the extended version of the CB05 mechanism:

4. Formaldehyde is mapped to PFRM as well as FORM

5. Acetaldehyde is mapped to PACT as well as ALD2

6. 1,3-Butadiene is mapped to BUTD as well as 2 OLE

7. Acrolein is mapped to PACR as well as 0.5 OLE plus ALDX

8. Toluene is mapped to TOLU as well as TOL

9. p-Xylene is mapped to PXYL as well as XYL

10. o-Xylene is mapped to OXYL as well as XYL

11. m-Xylene is mapped to MXYL as well as XYL

12. α-Pinene is mapped to APIN as well as TERP

13. β- Pinene is mapped to APIN as well as TERP

No changes to species mappings for organic compounds are required for the CB05 reactive chlorine mechanism. However, emission inventory preparation for the CB05 reactive chlorine mechanism should consider sources of reactive chlorine (CL_2 and HOCl).

3. CB05 IMPLEMENTATION TESTING

EPA is implementing the CB05 mechanism into the CMAQ air quality model. Tests were performed to confirm that the CMAQ implementation is correct. Independent rate constant calculations performed by SmogReyes and EPA checked the kinetic rate constant expressions. Independent box model simulations by the same groups checked the complete mechanism implementation, i.e., the reactions, photolysis data and rate constant data. Box model calculations also compared the CB05 mechanism to CB4, and these comparisons are discussed first.

COMPARING CB05 TO CB4

The CB05 mechanism was implemented in the OZIPM box model for comparison with CB4 as shown in Figure 3-1. The version of CB4 compared is the OTAG version of CB4 (discussed in Section 1). The scenario modeled is an MIR (maximum incremental reactivity) condition with an urban emissions mix of VOCs and NOx. The MIR condition has low VOC/NOx ratio where adding VOC has the greatest incremental impact on the ozone production rate. The VOC composition used for CB4 and CB05 is compared in Table 3-1 on a moles carbon basis. The difference from CB4 to CB05 is that ALD2 is disaggregated to ALD2, IOLE and ALDX.

Table 3-1. VOC composition used for the box model comparison of CB4 and CB05.

	Fractional Contribution to Moles Carbon	
CB Species	**CB4**	**CB05**
PAR	0.675	0.675
ETH	0.045	0.045
OLE	0.034	0.034
TOL	0.116	0.116
XYL	0.078	0.078
MEOH	0.001	0.001
ETOH	0.009	0.009
ISOP	0.5	0.5
CRES	0.002	0.002
FORM	0.009	0.009
ALD2	0.027	0.006
IOLE	N/A	0.018
ALDX	N/A	0.003
Total	**1.496**	**1.496**

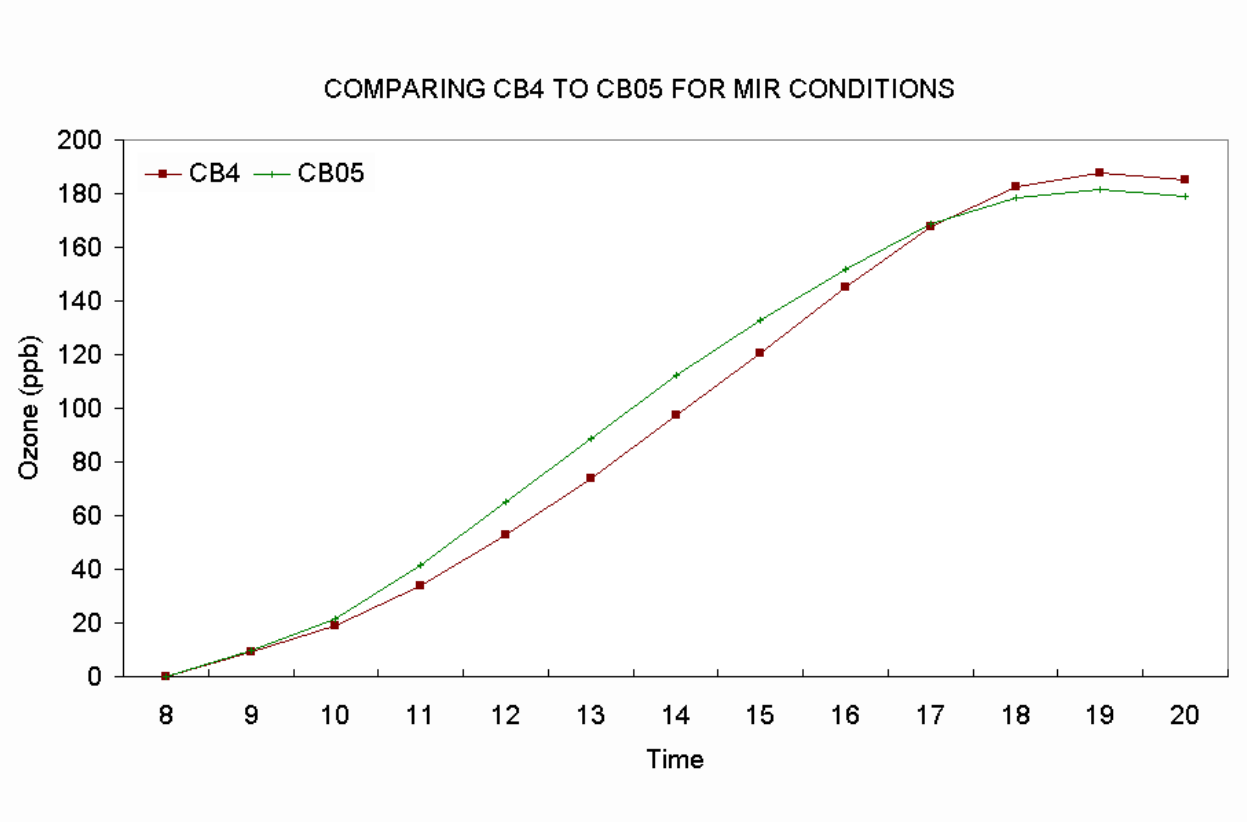

Figure 3-1. Comparison of CB4 and CB05 ozone predictions for urban MIR conditions.

CB05 forms ozone more rapidly than CB4 for the MIR condition compared in Figure 3-1, but ultimately CB4 and CB05 form the same amount of ozone. The faster ozone formation rate in CB05 results from including ALDX (higher aldehydes) and IOLE (internal olefins) in the mechanism that boost radical production in the morning. ALDX boosts radical production because higher aldehydes produce more radicals than acetaldehyde (i.e., have a higher quantum yield for radicals) when they photolyse. IOLE boosts radical production directly via reaction products and indirectly because ALDX is a product of IOLE degradation.

The formation of nitric acid and hydrogen peroxide by CB4 and CB05 is compared in Figures 3-2 and 3-3 for the MIR condition. Nitric acid formation is similar, but hydrogen peroxide production is slower in CB05. However, note that very little hydrogen peroxide is formed by either CB05 or CB4 at MIR conditions. Comparing hydrogen peroxide is more meaningful for MOR than MIR conditions. CB05 and CB4 also were compared under maximum ozone formation (MOIR) box model conditions (Figures 3-4 to 3-6). The VOC compositions for the MOR simulations were the same as for the MIR simulations (Table 3-1). The MOIR condition differs from the MIR condition in having lower NOx levels, resulting in higher ozone. The MOIR VOC/NOx ratio was set for CB4 and not re-adjusted for CB05, so the CB05 result is probably not exactly at the MOIR condition. CB05 produced slightly lower final ozone and nitric acid than CB4, but slightly higher hydrogen peroxide. CB05 had more rapid initial production of ozone, nitric acid and hydrogen peroxide than CB4 due to the ALOX and IOLE changes to CB05.

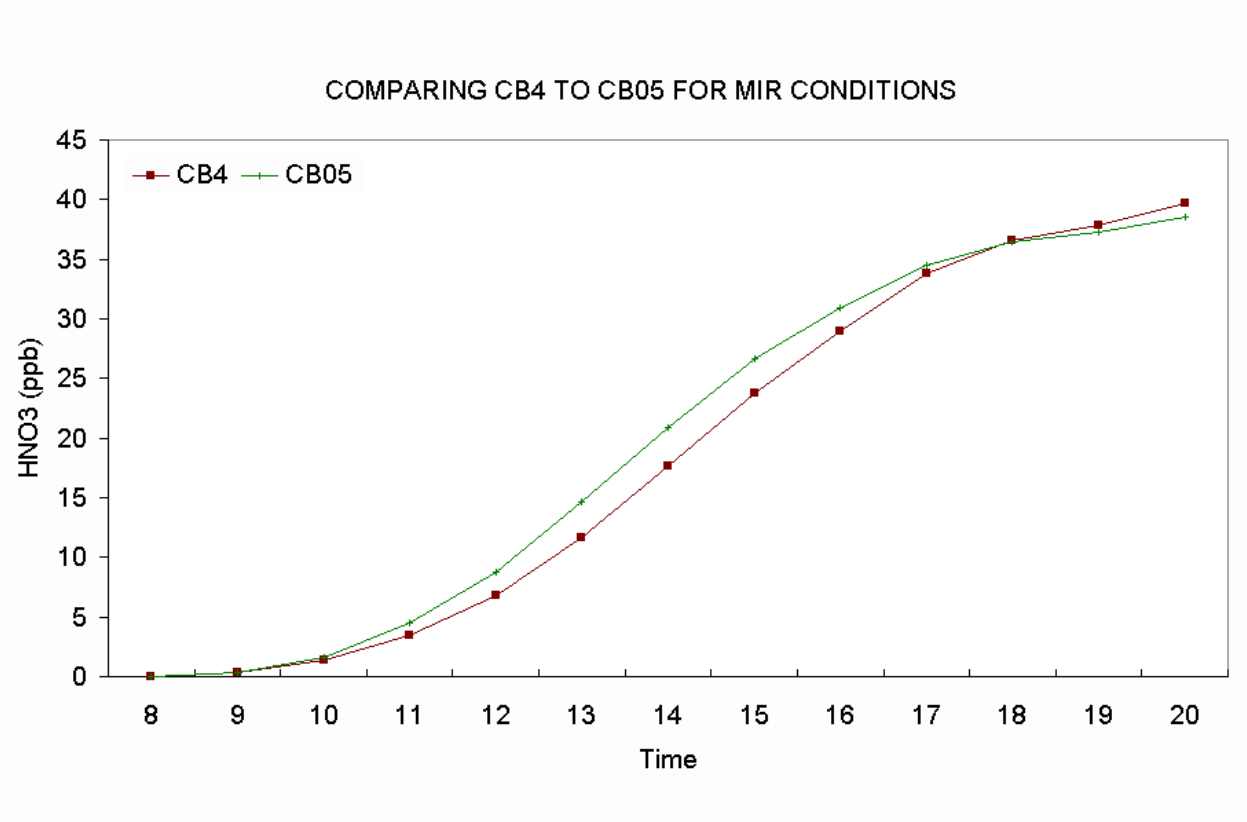

Figure 3-2. Comparison of CB4 and CB05 HNO_3 predictions for urban MIR conditions.

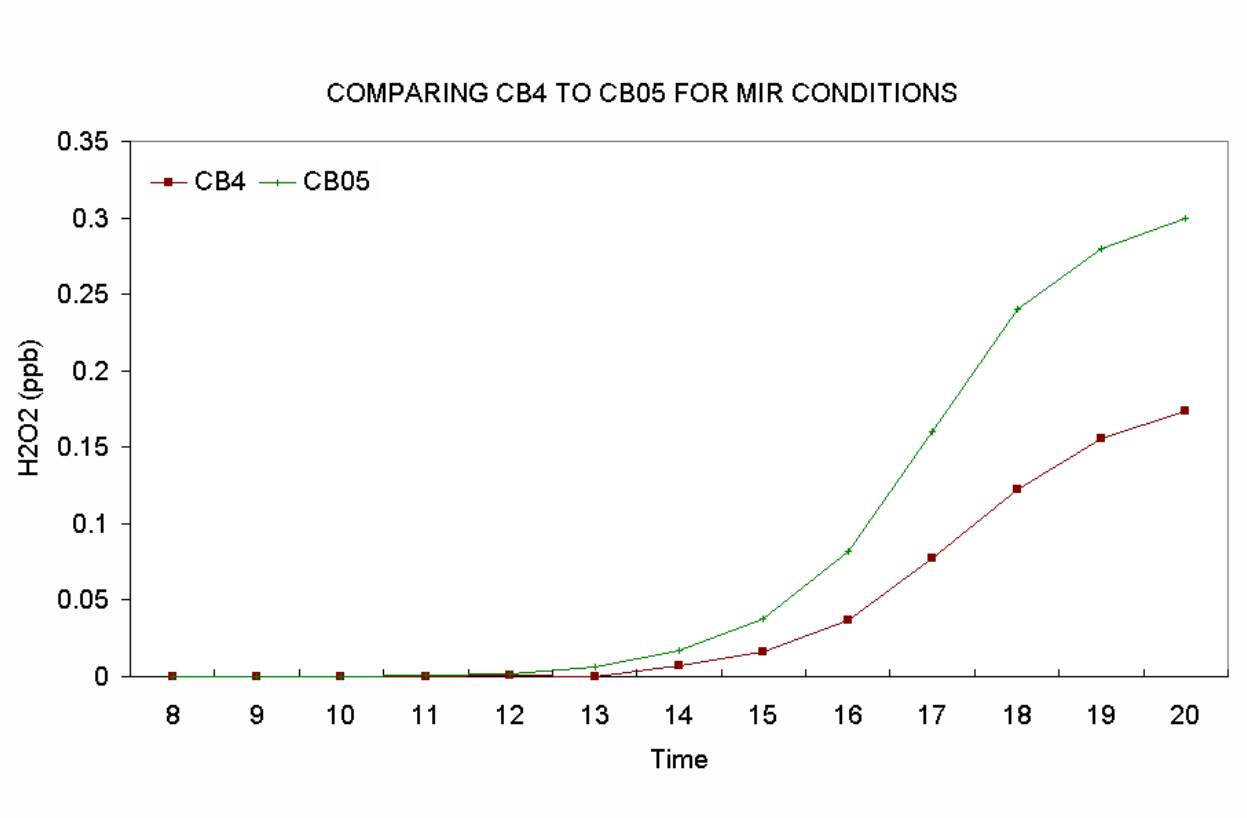

Figure 3-3. Comparison of CB4 and CB05 H_2O_2 predictions for urban MIR conditions.

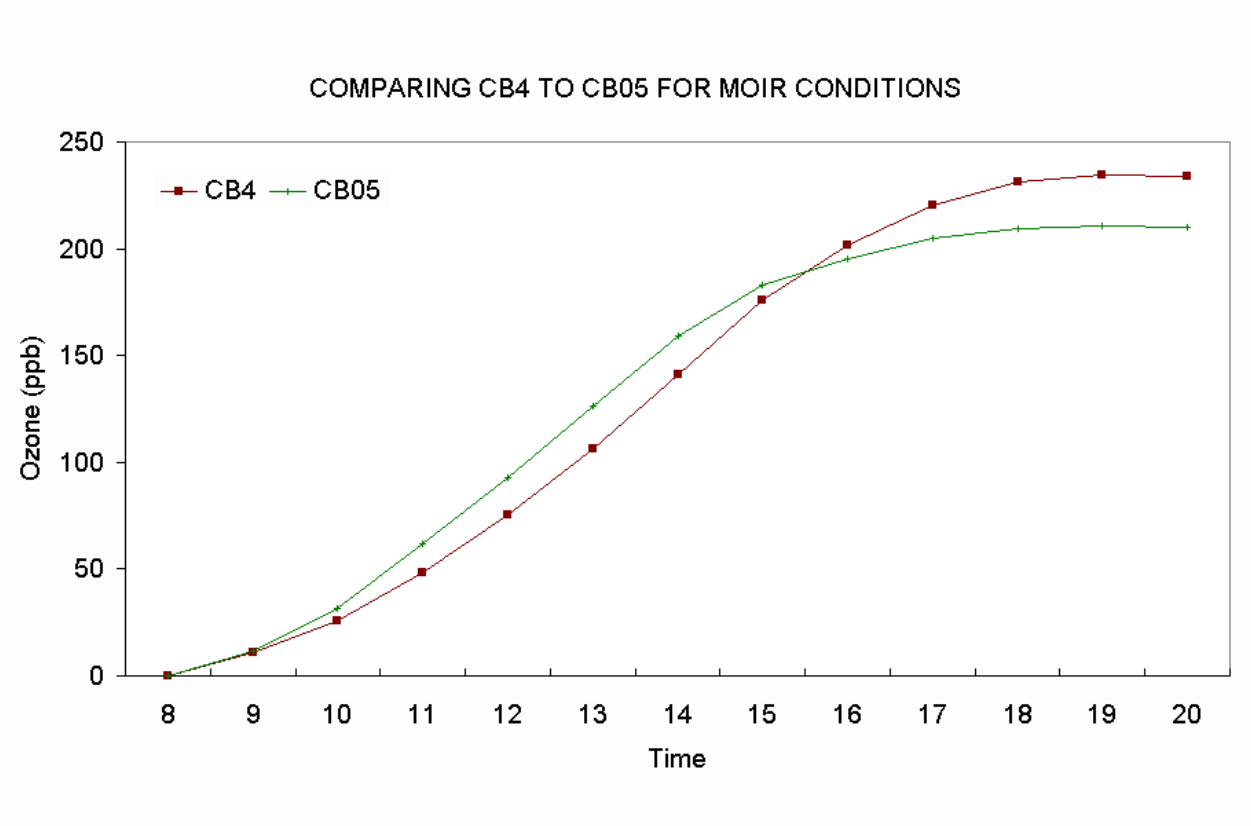

Figure 3-4. Comparison of CB4 and CB05 ozone predictions for urban MOIR conditions.

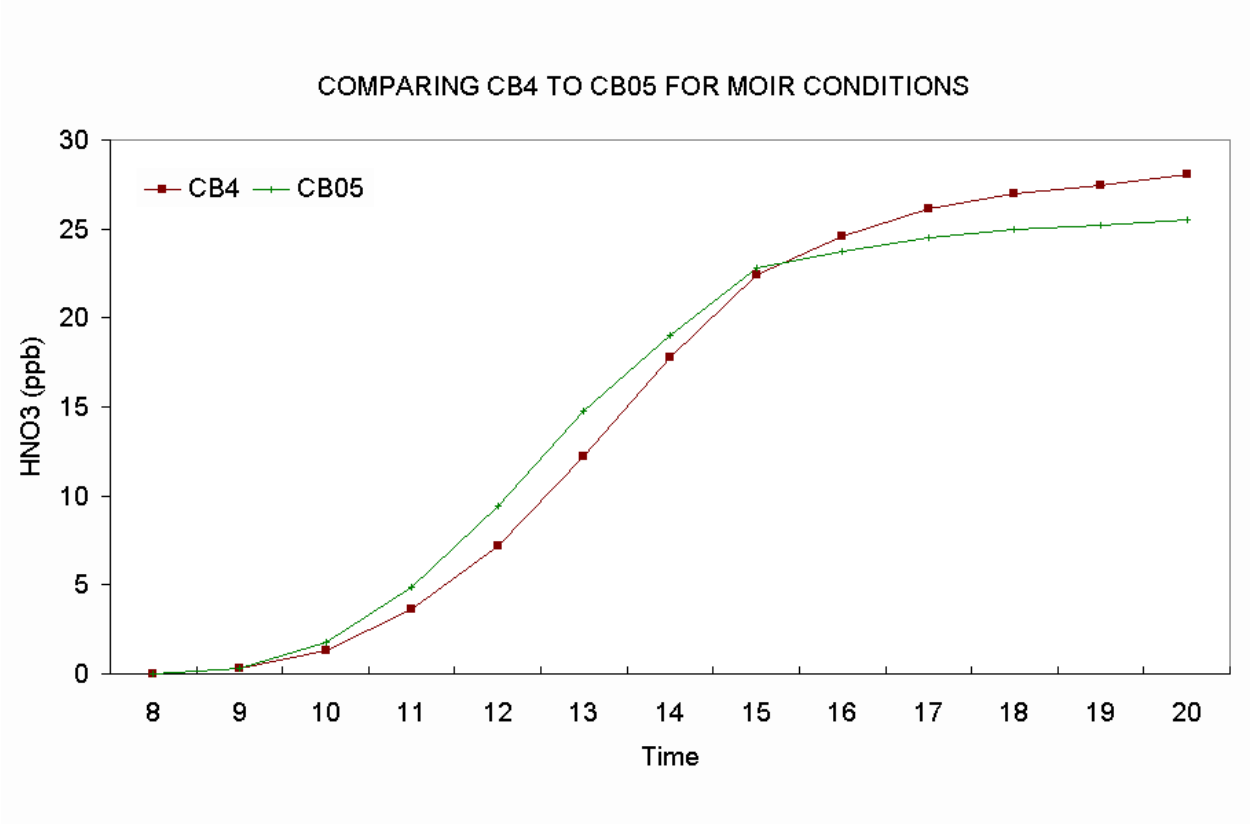

Figure 3-5. Comparison of CB4 and CB05 HNO_3 predictions for urban MOIR conditions.

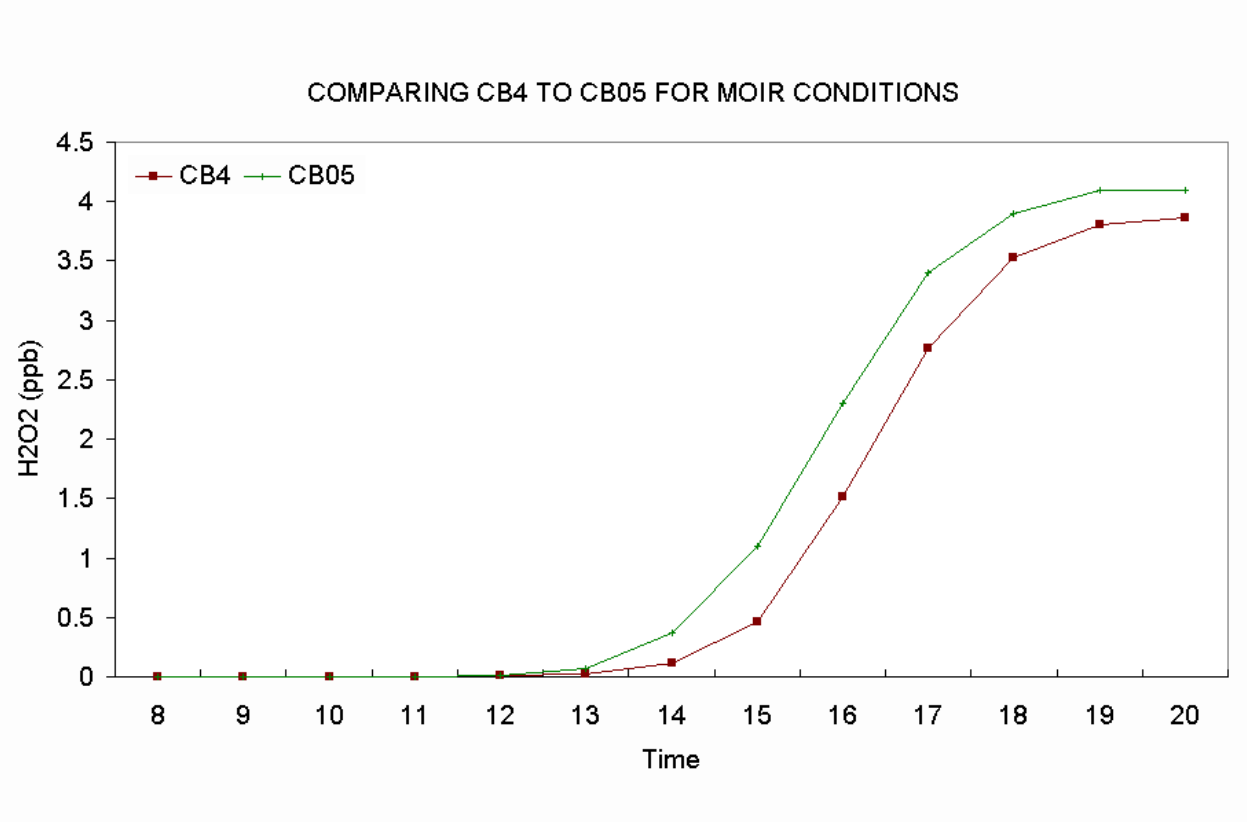

Figure 3-6. Comparison of CB4 and CB05 H_2O_2 predictions for urban MOIR conditions.

RATE CONSTANT COMPARISONS

The CB05 kinetic rate constant expressions were checked by independent calculations for three temperature/pressure conditions:

Pressure	Temperature (K)
1 atm	298
0.5 atm	298
1 atm	310

Both temperature and pressure were varied because some rate expressions depend upon both parameters. Rate constants were compared in units of ppm and minutes, as used within the CMAQ air quality model, such that units conversion from the molecular units (molecules per cm^3 and seconds) of the rate expressions also was tested. The rate constant comparison (Table 3-2) found very good agreement for all reactions. The largest difference of 1.2% was for the reaction of OH with CO that uses a unique rate expression.

Table 3-2. Comparison of CB05 thermal rate constants calculated by SmogReyes and EPA for three different temperature/pressure conditions (units are ppm and minutes).

Reaction		SmogReyes			EPA			Percent Difference [1]		
	Temperature (K)	298	298	310	298	298	310	298	298	310
	Pressure (Atm)	1	0.5	1	1	0.5	1	1	0.5	1
1	NO2 + hv [2]									
2	O + O2 + M	2.22E-05	5.55E-06	1.87E-05	2.22E-05	5.55E-06	1.87E-05	0.0%	0.0%	0.2%
3	O3 + NO	2.89E+01	1.44E+01	3.38E+01	2.89E+01	1.44E+01	3.37E+01	0.0%	0.3%	0.2%
4	O + NO2	1.51E+04	7.54E+03	1.42E+04	1.51E+04	7.57E+03	1.42E+04	0.2%	0.4%	0.1%
5	O + NO2	4.85E+03	1.50E+03	4.30E+03	4.85E+03	1.50E+03	4.30E+03	0.1%	0.0%	0.1%
6	O + NO	2.46E+03	6.74E+02	2.18E+03	2.46E+03	6.74E+02	2.18E+03	0.0%	0.0%	0.2%
7	NO2 + O3	4.76E-02	2.38E-02	6.30E-02	4.77E-02	2.38E-02	6.30E-02	0.2%	0.0%	0.1%
8	O3 + hv [2]									
9	O3 + hv [2]									
10	O1D + M	4.37E+04	2.19E+04	4.15E+04	4.37E+04	2.19E+04	4.15E+04	0.0%	0.2%	0.1%
11	O1D + H2O	3.25E+05	1.63E+05	3.12E+05	3.25E+05	1.63E+05	3.13E+05	0.0%	0.3%	0.2%
12	O3 + OH	1.07E+02	5.36E+01	1.16E+02	1.07E+02	5.36E+01	1.16E+02	0.2%	0.0%	0.2%
13	O3 + HO2	2.85E+00	1.43E+00	2.92E+00	2.85E+00	1.43E+00	2.92E+00	0.1%	0.2%	0.0%
14	NO3 + hv [2]									
15	NO3 + hv [2]									
16	NO3 + NO	3.92E+04	1.96E+04	3.69E+04	3.92E+04	1.96E+04	3.69E+04	0.1%	0.1%	0.1%
17	NO3 + NO2	9.70E-01	4.85E-01	1.10E+00	9.70E-01	4.85E-01	1.10E+00	0.0%	0.0%	0.2%
18	NO3 + NO2	1.74E+03	8.08E+02	1.60E+03	1.74E+03	8.08E+02	1.60E+03	0.1%	0.0%	0.1%
19	N2O5 + H2O	3.70E-07	1.85E-07	3.56E-07	3.69E-07	1.85E-07	3.55E-07	0.1%	0.1%	0.2%
20	N2O5 + H2O + H2O	6.55E-11	1.64E-11	6.06E-11	6.55E-11	1.64E-11	6.05E-11	0.0%	0.1%	0.1%
21	N2O5	3.17E+00	2.85E+00	1.31E+01	3.17E+00	2.85E+00	1.31E+01	0.1%	0.1%	0.1%
22	NO + NO + O2	7.11E-10	1.78E-10	6.13E-10	7.11E-10	1.78E-10	6.14E-10	0.0%	0.1%	0.1%
23	NO + NO2 + H2O	1.82E-11	4.55E-12	1.68E-11	1.82E-11	4.55E-12	1.68E-11	0.0%	0.0%	0.1%
24	NO + OH	1.09E+04	3.60E+03	9.69E+03	1.09E+04	3.60E+03	9.69E+03	0.4%	0.1%	0.1%
25	HONO + hv [2]									
26	OH + HONO	7.19E+03	3.59E+03	7.27E+03	7.19E+03	3.59E+03	7.27E+03	0.0%	0.1%	0.0%
27	HONO + HONO	1.48E-05	7.39E-06	1.42E-05	1.48E-05	7.39E-06	1.42E-05	0.1%	0.0%	0.1%
28	NO2 + OH	1.55E+04	5.56E+03	1.38E+04	1.55E+04	5.56E+03	1.38E+04	0.3%	0.1%	0.2%
29	OH + HNO3	2.28E+02	1.13E+02	1.95E+02	2.28E+02	1.13E+02	1.95E+02	0.0%	0.1%	0.1%
30	HO2 + NO	1.20E+04	5.99E+03	1.11E+04	1.20E+04	5.98E+03	1.11E+04	0.2%	0.1%	0.4%
31	HO2 + NO2	2.05E+03	7.10E+02	1.81E+03	2.05E+03	7.10E+02	1.81E+03	0.2%	0.0%	0.1%
32	PNA	4.99E+00	3.50E+00	2.02E+01	4.99E+00	3.50E+00	2.02E+01	0.1%	0.0%	0.1%
33	OH + PNA	6.88E+03	3.44E+03	6.29E+03	6.88E+03	3.44E+03	6.29E+03	0.0%	0.0%	0.0%
34	HO2 + HO2	4.32E+03	1.72E+03	3.70E+03	4.32E+03	1.72E+03	3.70E+03	0.0%	0.2%	0.1%
35	HO2 + HO2 + H2O	2.39E-01	4.76E-02	1.48E-01	2.39E-01	4.76E-02	1.48E-01	0.2%	0.1%	0.2%
36	H2O2 + hv [2]									
37	OH + H2O2	2.51E+03	1.25E+03	2.46E+03	2.51E+03	1.25E+03	2.46E+03	0.2%	0.2%	0.0%
38	O1D + H2	1.63E+05	8.13E+04	1.56E+05	1.63E+05	8.13E+04	1.56E+05	0.3%	0.0%	0.2%
39	OH + H2	9.89E+00	4.95E+00	1.23E+01	9.89E+00	4.95E+00	1.23E+01	0.0%	0.1%	0.2%
40	OH + O	4.86E+04	2.43E+04	4.60E+04	4.86E+04	2.43E+04	4.60E+04	0.1%	0.1%	0.1%
41	OH + OH	2.77E+03	1.39E+03	2.75E+03	2.77E+03	1.39E+03	2.75E+03	0.2%	0.2%	0.0%
42	OH + OH	9.30E+03	3.14E+03	8.57E+03	9.30E+03	3.14E+03	8.57E+03	0.0%	0.1%	0.0%
43	OH + HO2	1.64E+05	8.20E+04	1.53E+05	1.64E+05	8.21E+04	1.53E+05	0.0%	0.1%	0.1%
44	HO2 + O	8.68E+04	4.34E+04	8.13E+04	8.67E+04	4.34E+04	8.12E+04	0.1%	0.0%	0.1%
45	H2O2 + O	2.51E+00	1.26E+00	3.14E+00	2.52E+00	1.26E+00	3.14E+00	0.3%	0.3%	0.0%
46	NO3 + O	1.48E+04	7.39E+03	1.42E+04	1.48E+04	7.39E+03	1.42E+04	0.1%	0.0%	0.1%
47	NO3 + OH	3.25E+04	1.63E+04	3.13E+04	3.25E+04	1.63E+04	3.13E+04	0.0%	0.3%	0.1%

Reaction		SmogReyes			EPA			Percent Difference [1]		
	Temperature (K)	298	298	310	298	298	310	298	298	310
	Pressure (Atm)	1	0.5	1	1	0.5	1	1	0.5	1
48	NO3 + HO2	5.17E+03	2.59E+03	4.97E+03	5.17E+03	2.59E+03	4.97E+03	0.1%	0.1%	0.0%
49	NO3 + O3	1.48E-02	7.39E-03	1.42E-02	1.48E-02	7.39E-03	1.42E-02	0.1%	0.0%	0.1%
50	NO3 + NO3	3.38E-01	1.69E-01	4.47E-01	3.38E-01	1.69E-01	4.46E-01	0.1%	0.1%	0.2%
51	PNA + hv [2]									
52	HNO3 + hv [2]									
53	N2O5 + hv [2]									
54	XO2 + NO	1.31E+04	6.54E+03	1.20E+04	1.31E+04	6.54E+03	1.20E+04	0.2%	0.0%	0.1%
55	XO2N + NO	1.31E+04	6.54E+03	1.20E+04	1.31E+04	6.54E+03	1.20E+04	0.2%	0.0%	0.1%
56	XO2 + HO2	1.16E+04	5.81E+03	1.02E+04	1.16E+04	5.81E+03	1.02E+04	0.1%	0.1%	0.2%
57	XO2N + HO2	1.16E+04	5.81E+03	1.02E+04	1.16E+04	5.81E+03	1.02E+04	0.1%	0.1%	0.2%
58	XO2 + XO2	1.01E+02	5.03E+01	9.66E+01	1.00E+02	5.02E+01	9.66E+01	0.5%	0.1%	0.0%
59	XO2N + XO2N	1.01E+02	5.03E+01	9.66E+01	1.00E+02	5.02E+01	9.66E+01	0.5%	0.1%	0.0%
60	XO2 + XO2N	1.01E+02	5.03E+01	9.66E+01	1.00E+02	5.02E+01	9.66E+01	0.5%	0.1%	0.0%
61	NTR + OH	2.60E+02	1.30E+02	2.62E+02	2.61E+02	1.30E+02	2.62E+02	0.2%	0.2%	0.1%
62	NTR + hv [2]									
63	ROOH + OH	8.42E+03	4.21E+03	7.89E+03	8.42E+03	4.21E+03	7.89E+03	0.0%	0.0%	0.1%
64	ROOH + hv [2]									
65	OH + CO	3.55E+02	1.44E+02	3.41E+02	3.56E+02	1.44E+02	3.37E+02	0.4%	0.1%	1.2%
66	OH + CH4	9.38E+00	4.69E+00	1.14E+01	9.37E+00	4.69E+00	1.13E+01	0.1%	0.0%	0.5%
67	MEO2 + NO	1.13E+04	5.66E+03	1.05E+04	1.13E+04	5.66E+03	1.05E+04	0.2%	0.0%	0.3%
68	MEO2 + HO2	7.51E+03	3.75E+03	6.55E+03	7.51E+03	3.75E+03	6.55E+03	0.0%	0.1%	0.1%
69	MEO2 + MEO2	5.20E+02	2.60E+02	4.75E+02	5.20E+02	2.60E+02	4.75E+02	0.1%	0.1%	0.0%
70	MEPX + OH	1.10E+04	5.49E+03	1.03E+04	1.10E+04	5.49E+03	1.03E+04	0.1%	0.1%	0.0%
71	MEPX + hv [2]									
72	MEOH + OH	1.35E+03	6.74E+02	1.40E+03	1.35E+03	6.74E+02	1.40E+03	0.2%	0.1%	0.2%
73	FORM + OH	1.33E+04	6.65E+03	1.28E+04	1.33E+04	6.65E+03	1.28E+04	0.0%	0.0%	0.1%
74	FORM + hv [2]									
75	FORM + hv [2]									
76	FORM + O	2.34E+02	1.17E+02	2.77E+02	2.34E+02	1.17E+02	2.77E+02	0.0%	0.0%	0.0%
77	FORM + NO3	8.57E-01	4.29E-01	8.24E-01	8.57E-01	4.29E-01	8.24E-01	0.0%	0.1%	0.0%
78	FORM + HO2	1.17E+02	5.84E+01	1.03E+02	1.17E+02	5.84E+01	1.03E+02	0.2%	0.0%	0.5%
79	HCO3	9.05E+03	9.05E+03	2.25E+04	9.05E+03	9.05E+03	2.25E+04	0.0%	0.0%	0.1%
80	HCO3 + NO	8.28E+03	4.14E+03	7.96E+03	8.28E+03	4.14E+03	7.96E+03	0.0%	0.0%	0.0%
81	HCO3 + HO2	1.86E+04	9.30E+03	1.33E+04	1.86E+04	9.30E+03	1.33E+04	0.0%	0.0%	0.2%
82	FACD + OH	5.91E+02	2.96E+02	5.68E+02	5.91E+02	2.96E+02	5.68E+02	0.0%	0.1%	0.0%
83	ALD2 + O	6.63E+02	3.32E+02	7.35E+02	6.63E+02	3.32E+02	7.36E+02	0.1%	0.1%	0.1%
84	ALD2 + OH	2.05E+04	1.02E+04	1.90E+04	2.05E+04	1.02E+04	1.90E+04	0.1%	0.4%	0.0%
85	ALD2 + NO3	3.52E+00	1.76E+00	4.33E+00	3.52E+00	1.76E+00	4.33E+00	0.1%	0.1%	0.0%
86	ALD2 + hv [2]									
87	C2O3 + NO	2.96E+04	1.48E+04	2.75E+04	2.96E+04	1.48E+04	2.75E+04	0.1%	0.1%	0.1%
88	C2O3 + NO2	1.55E+04	7.50E+03	1.42E+04	1.55E+04	7.49E+03	1.42E+04	0.1%	0.1%	0.0%
89	PAN	1.99E-02	1.93E-02	1.19E-01	1.99E-02	1.93E-02	1.19E-01	0.2%	0.1%	0.4%
90	PAN + hv [2]									
91	C2O3 + HO2	2.08E+04	1.04E+04	1.75E+04	2.08E+04	1.04E+04	1.75E+04	0.2%	0.2%	0.0%
92	C2O3 + MEO2	1.58E+04	7.91E+03	1.43E+04	1.58E+04	7.91E+03	1.43E+04	0.2%	0.1%	0.3%
93	C2O3 + XO2	2.36E+04	1.18E+04	1.97E+04	2.36E+04	1.18E+04	1.97E+04	0.1%	0.1%	0.1%
94	C2O3 + C2O3	2.30E+04	1.15E+04	2.07E+04	2.29E+04	1.15E+04	2.07E+04	0.2%	0.2%	0.1%
95	PACD + OH	1.16E+03	5.78E+02	1.08E+03	1.16E+03	5.78E+02	1.08E+03	0.3%	0.1%	0.3%
96	PACD + hv [2]									

Reaction		SmogReyes			EPA			Percent Difference [1]		
	Temperature (K)	298	298	310	298	298	310	298	298	310
	Pressure (Atm)	1	0.5	1	1	0.5	1	1	0.5	1
97	AACD + OH	1.16E+03	5.78E+02	1.08E+03	1.16E+03	5.78E+02	1.08E+03	0.3%	0.1%	0.3%
98	ALDX + O	1.04E+03	5.18E+02	1.12E+03	1.04E+03	5.18E+02	1.12E+03	0.3%	0.1%	0.1%
99	ALDX + OH	2.93E+04	1.47E+04	2.67E+04	2.93E+04	1.47E+04	2.68E+04	0.1%	0.2%	0.3%
100	ALDX + NO3	9.61E+00	4.80E+00	9.24E+00	9.61E+00	4.80E+00	9.23E+00	0.0%	0.1%	0.1%
101	ALDX + hv [2]									
102	CXO3 + NO	3.10E+04	1.55E+04	2.85E+04	3.10E+04	1.55E+04	2.85E+04	0.0%	0.0%	0.0%
103	CXO3 + NO2	1.55E+04	7.50E+03	1.42E+04	1.55E+04	7.49E+03	1.42E+04	0.1%	0.1%	0.0%
104	PANX	1.99E-02	1.93E-02	1.19E-01	1.99E-02	1.93E-02	1.19E-01	0.2%	0.1%	0.4%
105	PANX + hv [2]									
106	PANX + OH	4.43E+02	2.22E+02	4.26E+02	4.43E+02	2.22E+02	4.26E+02	0.1%	0.1%	0.0%
107	CXO3 + HO2	2.08E+04	1.04E+04	1.75E+04	2.08E+04	1.04E+04	1.75E+04	0.2%	0.2%	0.0%
108	CXO3 + MEO2	1.58E+04	7.91E+03	1.43E+04	1.58E+04	7.91E+03	1.43E+04	0.2%	0.1%	0.3%
109	CXO3 + XO2	2.36E+04	1.18E+04	1.97E+04	2.36E+04	1.18E+04	1.97E+04	0.2%	0.2%	0.2%
110	CXO3 + CXO3	2.30E+04	1.15E+04	2.07E+04	2.29E+04	1.15E+04	2.07E+04	0.2%	0.2%	0.1%
111	CXO3 + C2O3	2.30E+04	1.15E+04	2.07E+04	2.29E+04	1.15E+04	2.07E+04	0.2%	0.2%	0.1%
112	PAR + OH	1.20E+03	5.99E+02	1.15E+03	1.20E+03	5.99E+02	1.15E+03	0.2%	0.1%	0.1%
113	ROR	1.32E+05	1.32E+05	3.72E+05	1.32E+05	1.32E+05	3.72E+05	0.3%	0.3%	0.0%
114	ROR	9.60E+04	9.60E+04	9.60E+04	9.60E+04	9.60E+04	9.60E+04	0.0%	0.0%	0.0%
115	ROR + NO2	2.22E+04	1.11E+04	2.13E+04	2.22E+04	1.11E+04	2.13E+04	0.1%	0.1%	0.1%
116	O + OLE	5.78E+03	2.89E+03	5.76E+03	5.78E+03	2.89E+03	5.76E+03	0.1%	0.1%	0.0%
117	OH + OLE	4.73E+04	2.36E+04	4.55E+04	4.73E+04	2.36E+04	4.55E+04	0.0%	0.2%	0.1%
118	O3 + OLE	1.63E-02	8.13E-03	2.01E-02	1.64E-02	8.18E-03	2.01E-02	0.9%	0.6%	0.2%
119	NO3 + OLE	7.36E-01	3.68E-01	9.37E-01	7.36E-01	3.68E-01	9.37E-01	0.0%	0.0%	0.0%
120	O + ETH	1.08E+03	5.39E+02	1.15E+03	1.08E+03	5.39E+02	1.15E+03	0.2%	0.0%	0.1%
121	OH + ETH	1.20E+04	5.90E+03	1.16E+04	1.20E+04	5.90E+03	1.16E+04	0.4%	0.1%	0.3%
122	O3 + ETH	2.61E-03	1.30E-03	3.53E-03	2.61E-03	1.30E-03	3.52E-03	0.2%	0.2%	0.3%
123	NO3 + ETH	3.10E-01	1.55E-01	4.33E-01	3.10E-01	1.55E-01	4.33E-01	0.1%	0.1%	0.0%
124	IOLE + O	3.40E+04	1.70E+04	3.27E+04	3.40E+04	1.70E+04	3.27E+04	0.0%	0.0%	0.0%
125	IOLE + OH	9.36E+04	4.68E+04	8.38E+04	9.36E+04	4.68E+04	8.38E+04	0.0%	0.0%	0.0%
126	IOLE + O3	3.10E-01	1.55E-01	3.44E-01	3.10E-01	1.55E-01	3.43E-01	0.1%	0.1%	0.2%
127	IOLE + NO3	5.73E+02	2.87E+02	5.71E+02	5.73E+02	2.87E+02	5.71E+02	0.1%	0.1%	0.1%
128	TOL + OH	8.76E+03	4.38E+03	8.04E+03	8.76E+03	4.38E+03	8.04E+03	0.0%	0.0%	0.0%
129	TO2 + NO	1.20E+04	5.99E+03	1.15E+04	1.20E+04	5.99E+03	1.15E+04	0.2%	0.1%	0.3%
130	TO2	2.52E+02	2.52E+02	2.52E+02	2.52E+02	2.52E+02	2.52E+02	0.0%	0.0%	0.0%
131	OH + CRES	6.06E+04	3.03E+04	5.83E+04	6.06E+04	3.03E+04	5.82E+04	0.0%	0.0%	0.1%
132	CRES + NO3	3.25E+04	1.63E+04	3.12E+04	3.25E+04	1.63E+04	3.13E+04	0.0%	0.3%	0.2%
133	CRO + NO2	2.07E+04	1.03E+04	1.99E+04	2.07E+04	1.03E+04	1.99E+04	0.0%	0.4%	0.0%
134	CRO + HO2	8.13E+03	4.06E+03	7.82E+03	8.13E+03	4.06E+03	7.81E+03	0.0%	0.1%	0.1%
135	OPEN + hv [2]									
136	OPEN + OH	4.43E+04	2.22E+04	4.26E+04	4.43E+04	2.22E+04	4.26E+04	0.1%	0.1%	0.0%
137	OPEN + O3	1.49E-02	7.45E-03	1.53E-02	1.49E-02	7.45E-03	1.53E-02	0.0%	0.0%	0.1%
138	OH + XYL	3.70E+04	1.85E+04	3.50E+04	3.71E+04	1.85E+04	3.51E+04	0.4%	0.1%	0.2%
139	OH + MGLY	2.66E+04	1.33E+04	2.56E+04	2.66E+04	1.33E+04	2.56E+04	0.0%	0.0%	0.1%
140	MGLY + hv [2]									
141	O + ISOP	5.32E+04	2.66E+04	5.11E+04	5.32E+04	2.66E+04	5.11E+04	0.0%	0.0%	0.1%
142	OH + ISOP	1.47E+05	7.37E+04	1.34E+05	1.47E+05	7.37E+04	1.34E+05	0.3%	0.0%	0.0%
143	O3 + ISOP	1.90E-02	9.50E-03	2.34E-02	1.90E-02	9.50E-03	2.34E-02	0.0%	0.0%	0.1%
144	NO3 + ISOP	9.96E+02	4.98E+02	1.02E+03	9.96E+02	4.98E+02	1.01E+03	0.0%	0.0%	0.5%
145	OH + ISPD	4.97E+04	2.48E+04	4.77E+04	4.97E+04	2.48E+04	4.77E+04	0.1%	0.1%	0.1%

Reaction		SmogReyes			EPA			Percent Difference [1]		
	Temperature (K)	**298**	**298**	**310**	**298**	**298**	**310**	**298**	**298**	**310**
	Pressure (Atm)	**1**	**0.5**	**1**	**1**	**0.5**	**1**	**1**	**0.5**	**1**
146	O3 + ISPD	1.05E-02	5.25E-03	1.01E-02	1.05E-02	5.25E-03	1.01E-02	0.1%	0.1%	0.1%
147	NO3 + ISPD	1.48E+00	7.39E-01	1.42E+00	1.48E+00	7.39E-01	1.42E+00	0.1%	0.0%	0.1%
148	ISPD + hv [2]									
149	TERP + O	5.32E+04	2.66E+04	5.11E+04	5.32E+04	2.66E+04	5.11E+04	0.0%	0.0%	0.1%
150	TERP + OH	1.00E+05	5.00E+04	9.07E+04	1.00E+05	5.00E+04	9.07E+04	0.0%	0.0%	0.0%
151	TERP + O3	1.13E-01	5.64E-02	1.21E-01	1.13E-01	5.64E-02	1.21E-01	0.2%	0.0%	0.1%
152	TERP + NO3	9.84E+03	4.92E+03	9.25E+03	9.84E+03	4.92E+03	9.24E+03	0.0%	0.0%	0.1%
153	SO2 + OH	1.31E+03	5.11E+02	1.20E+03	1.31E+03	5.11E+02	1.20E+03	0.3%	0.0%	0.3%
154	OH + ETOH	4.71E+03	2.36E+03	4.67E+03	4.71E+03	2.36E+03	4.67E+03	0.1%	0.1%	0.0%
155	OH + ETHA	3.55E+02	1.77E+02	3.92E+02	3.55E+02	1.77E+02	3.92E+02	0.1%	0.2%	0.0%
156	NO2 + ISOP	2.22E-04	1.11E-04	2.13E-04	2.22E-04	1.11E-04	2.13E-04	0.1%	0.1%	0.1%
Maximum Difference								**0.9%**	**0.6%**	**1.2%**

Table Notes

1. Differences are calculated as the absolute difference between SmogReyes and EPA values divided by the EPA value.
2. Photolysis reactions (with a reactant hv) are not compared.

BOX MODEL COMPARISONS

Comparing the results of box model simulations checked the CMAQ implementation of the CB05 mechanism reactions together with photolysis data and rate constant data. SmogReyes implemented CB05 in the OZIPM box model and set up calculations for the three temperature and pressure conditions as were used for the rate constant comparison shown in Table 3-2. EPA set up a box model version of CMAQ to match as closely as possible the conditions of the OZIPM tests. There was generally good agreement between the concentrations predicted by the two box models suggesting that the mechanism implementation was correct in both models. Example comparisons for 298 K and 1 atmosphere are shown in Figure 3-7 (NO, NO_2 and O_3) and Figure 3-8 (HONO and HO_2). Figures 3-9 and 3-10 show similar comparisons at different temperatures and pressures. These comparisons confirm that CB05 is implemented correctly in the CMAQ model.

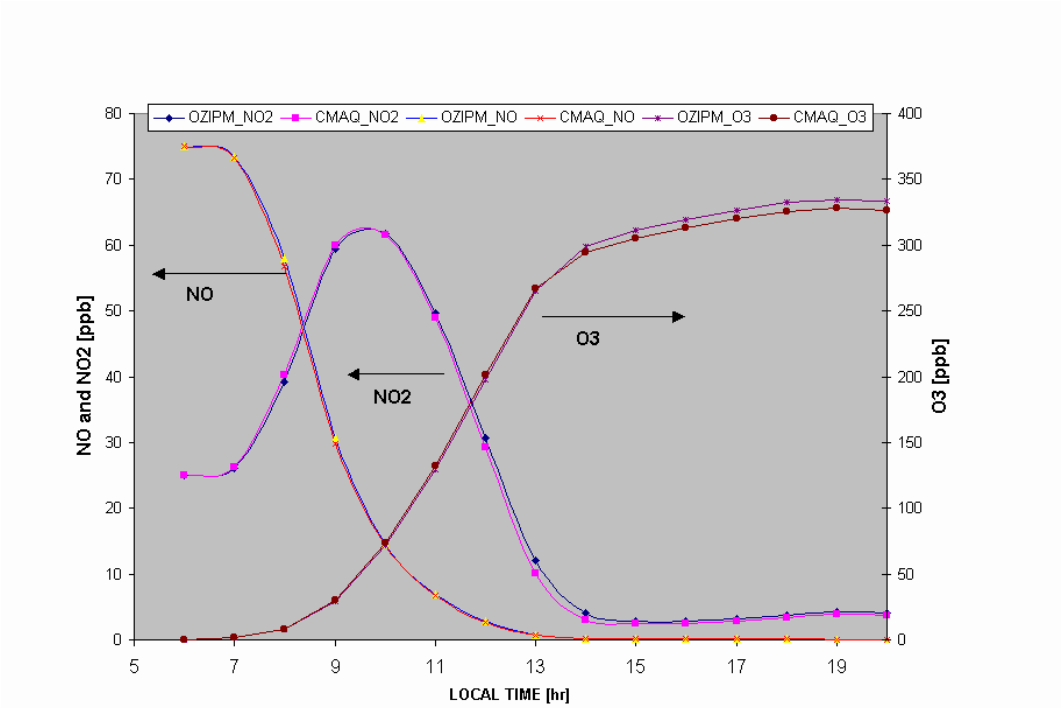

Figure 3-7. Comparison of results from the CMAQ and OZIPM box models for NO, NO_2 and O_3 at 298 K and 1 atmosphere.

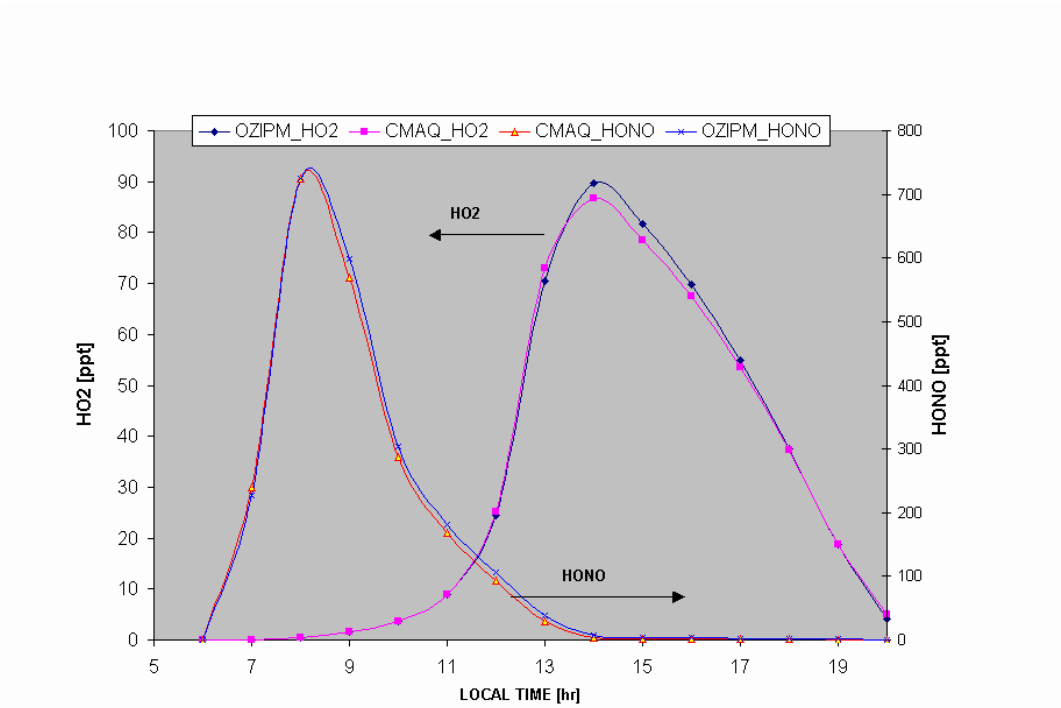

Figure 3-8. Comparison of results from the CMAQ and OZIPM box models for HONO and HO_2 at 298 K and 1 atmosphere.

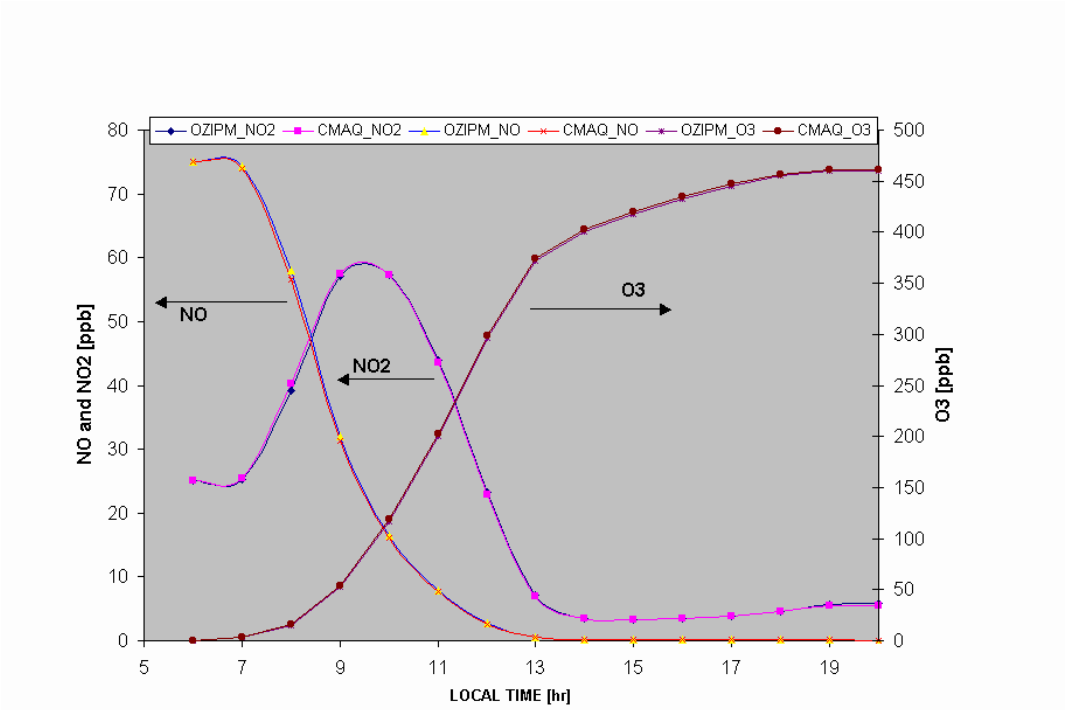

Figure 3-9. Comparison of results from the CMAQ and OZIPM box models for NO, NO_2 and O_3 at 298 K and 0.5 atmosphere.

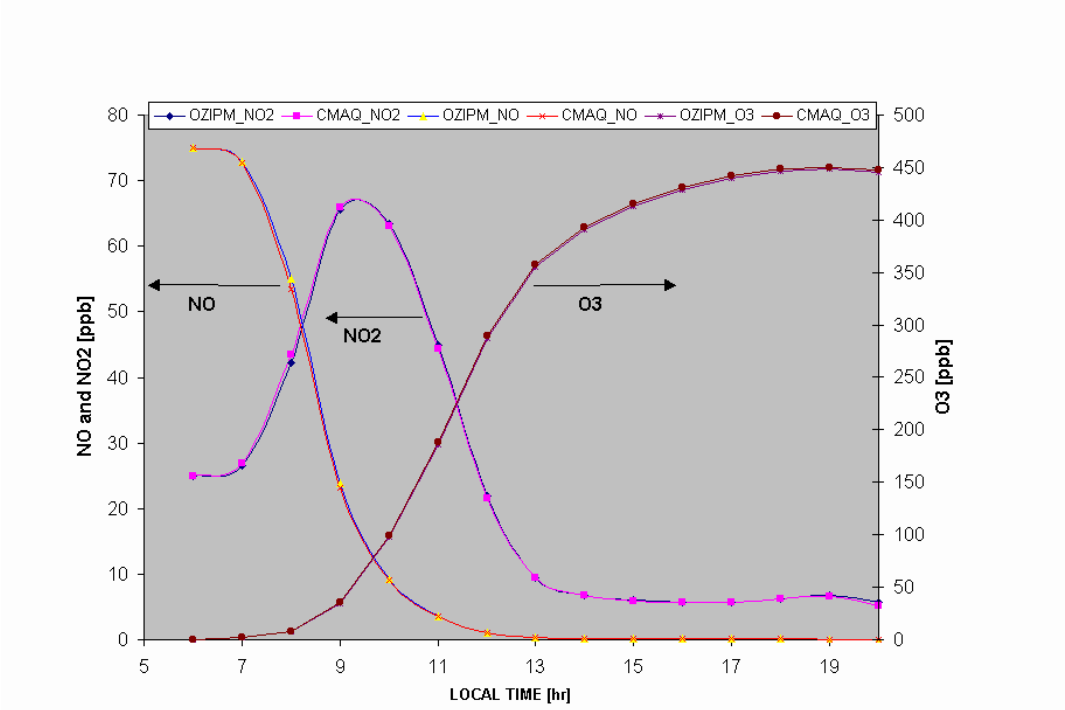

Figure 3-10. Comparison of results from the CMAQ and OZIPM box models for NO, NO_2 and O_3 at 310K and 1 atmosphere.

4. MECHANISM EVALUATION

UNC CHAMBER

The University of North Carolina (UNC) operates a smog chamber facility as described in the CB4-2002 report (Jeffries, Voicu and Sexton; 2002). For this project, UNC provided a database of chamber experiments along with software (called Morpho) to simulate chamber experiments and assistance in using the data and software. The CB05 mechanism was implemented in the Morpho software and simulation results were compared to experimental data as shown below and in Appendix B.

Updated UNC Wall Reaction Mechanism

The chemical mechanism used to simulate a chamber experiment must include reactions for both the gas-phase chemistry taking place in the chamber and the effects of the chamber walls. Chamber walls can provide both sources and sinks for reactive species. The role of the chamber walls is most apparent in experiments that are sensitive to input of radicals and/or reactive nitrogen species from the chamber walls, such as experiments with carbon monoxide (CO).

Jeffries, Voicu and Sexton (2002) revised the UNC chamber mechanism in the process of developing the CB4-2002. Nonetheless, the chamber characterization experiments from CB4-2002 still show biases for ozone and nitrogen species as shown in CO experiments in Figures 4-1 and 4-2 (from Jeffries, Voicu and Sexton; 2002). We reviewed and updated the chamber wall mechanism, as described below, to improve performance in chamber characterization experiments before beginning the evaluation of the CB05 mechanism. The improvement in the wall reaction mechanism can be seen in Figures 4-1 and 4-2 by comparing the CB05 (top) and CB4-2002 (bottom) simulations. Results of additional UNC chamber characterization experiments with CB05 are included in Appendix B.

The wall mechanism developed by Jeffries, Voicu and Sexton (2002) was modified in four ways:

(1) The deposition rate of N_2O_5 was increased by a factor of 9 in order to more accurately simulate the observed NO_2 data in experiments with only NOx and high CO. These experiments have essentially no PAN that normally might confound the data analysis.
(2) Radicals from wall nitrous acid (HONO) photolysis were changed from a mechanism using N_2O_4 on the walls to a mechanism based on NO, NO_2, and water on the walls.
(3) A pathway releasing NO_2 from nitric acid on the walls ($WHNO_3$) was added.
(4) Loss of PNA (HO_2NO_2) to the walls was added. This loss primarily impacts the highest CO experiments.

The original Jeffries, Voicu and Sexton (2002) wall reactions and the revised reactions used in this study are compared in Tables 4-1 and 4-2.

Table 4-1. Wall reactions from the Jeffries, Voicu and Sexton (2002) UNC chamber mechanisms that were changed for this project.

Label	Reactants	Products	Rate Expression
W1	N2O5 + WH2O	2.0 * WHNO3	2.6E-18
W2	NO2 + H2O	WNO2	1.0E-22
W3	WNO2	NO2	6.6E-7
W4	WNO2+WNO2	WN2O4	1.0E-10
W5	WN2O4 + WH2O	WHONO + WHNO3	1.0E-14

Table 4-2. New wall reactions for the UNC chamber used in this project.

Label	Reactants	Products	Rate Expression
W1	N2O5 + WH2O	2.0 * WHNO3	2.34E-17
W2	NO2 + H2O	WNO2	1.0E-23
W3	WNO2	NO2	1.0E-4
W4	NO + H2O	WNO	1.5E-23
W5	WNO	NO	1.0E-4
W6	WNO+WNO2	2.0 * WHONO	2.0E-14
W7	WHNO3	NO2	5.0E-6
W8	PNA + WH2O	WHNO3	1.0E-17

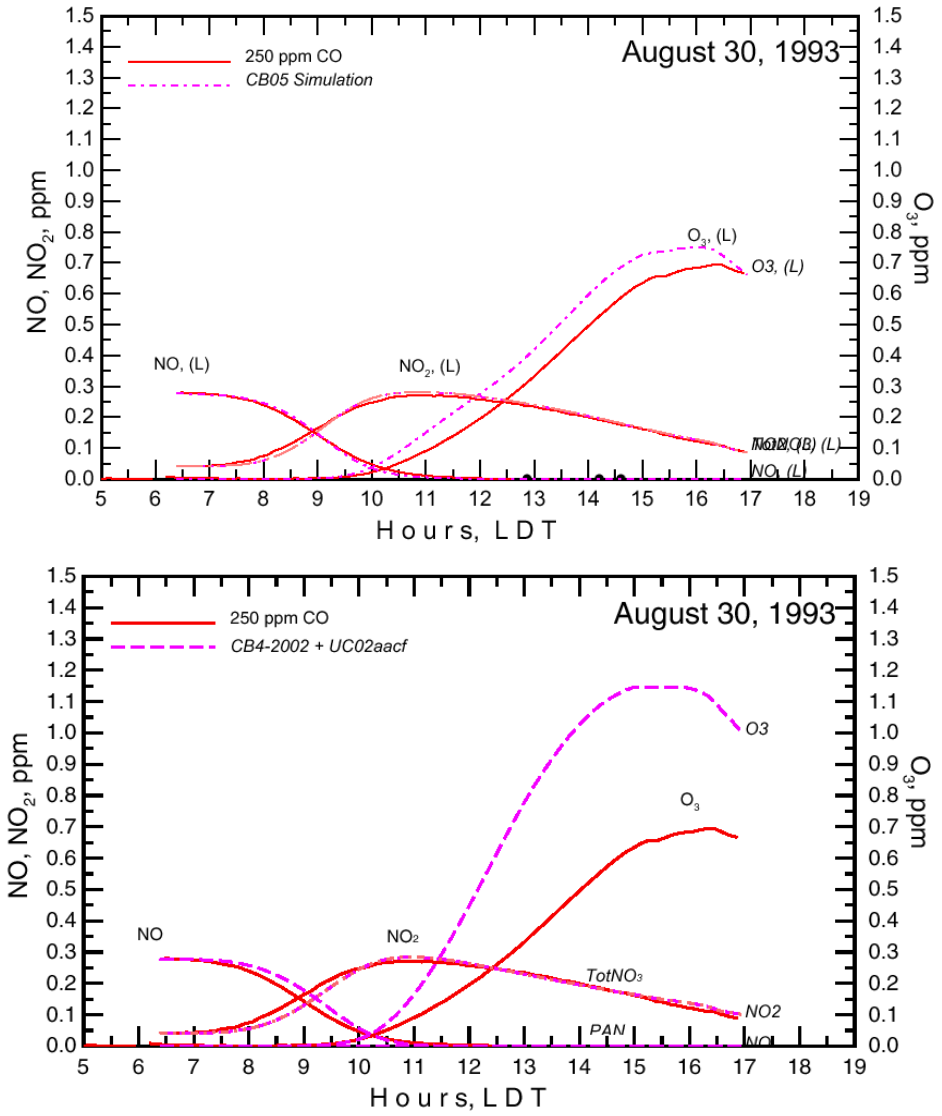

Figure 4-1. Comparison of CB05 (top) and CB4-2002 (bottom) simulations of UNC carbon monoxide experiment August 30, 1993 (red).

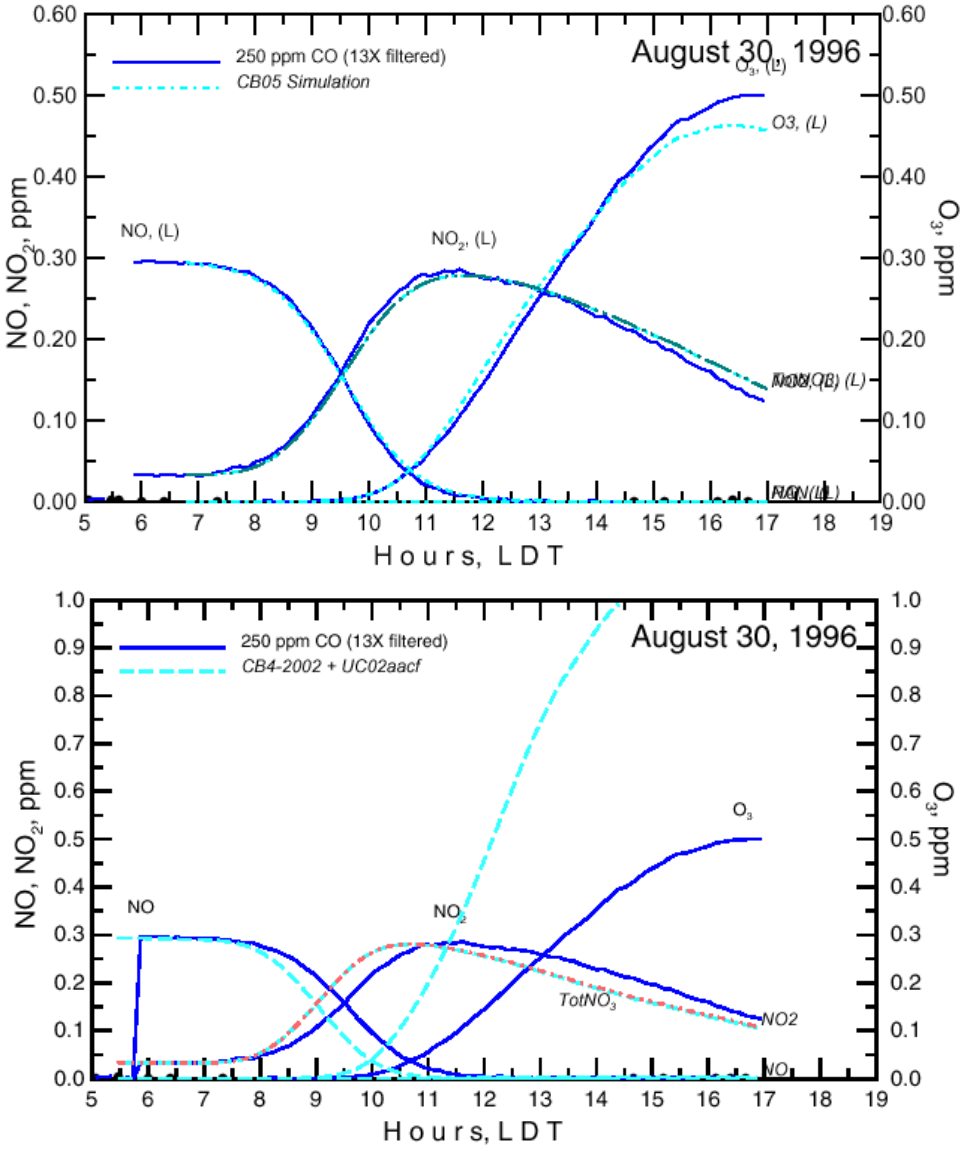

Figure 4-2. Comparison of CB05 (top) and CB4-2002 (bottom) simulations of UNC carbon monoxide experiment August 30, 1996 (blue).

ALDX Mechanism Update

One of the CB05 updates discussed in Section2 is the inclusion of a higher aldehyde species in addition to acetaldehyde. The impact of adding a higher aldehyde species (ALDX) to CB05 can be seen in performance for UBC chamber experiments for aldehydes larger than acetaldehyde. Figure 4-3 compares the performance of CB05 and CB4-2002 in simulating an experiment from September 4, 1997 (red chamber) with trimethylacetaldehyde and propionaldehyde. CB4-2002 represents these aldehydes using ALD2 and produces ozone too slowly, although the final ozone level is simulated quite well. CB05 produces ozone more rapidly because of greater radical production from ALDX photolysis than ALD2 photolysis. The rate of NO to NO_2 conversion also is simulated better by CB05 than CB4-2002.

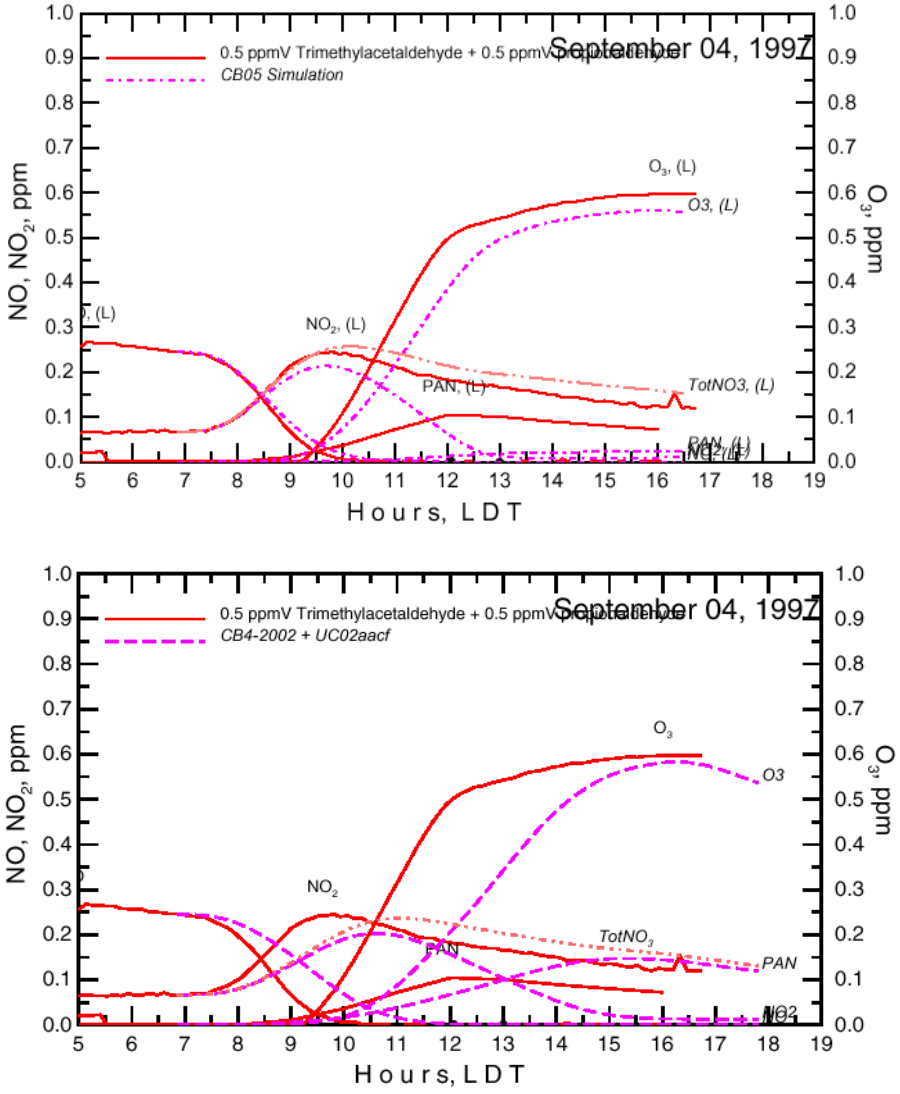

Figure 4-3. Comparison of CB05 (top) and CB4-2002 (bottom) simulations of UNC experiment of September 4, 1997 (red chamber) with trimethylacetaldehyde and propionaldehyde.

Including ALDX in CB05 also improves performance for olefins larger than propene. For example propionaldehyde is a product of 1–butene reactions and butyraldehyde is a product of 1-pentene reactions. Figure 4-4 compares CB05 and CB4-2002 performance for an experiment from October 16, 1996 (blue chamber) with propene, 1-butene and 1-pentene. The rate of ozone production and the rate of NO to NO_2 conversion are simulated much better by CB05 using ALDX than by CB4-2002 using ALD2 to represent the aldehyde products of olefin reactions.

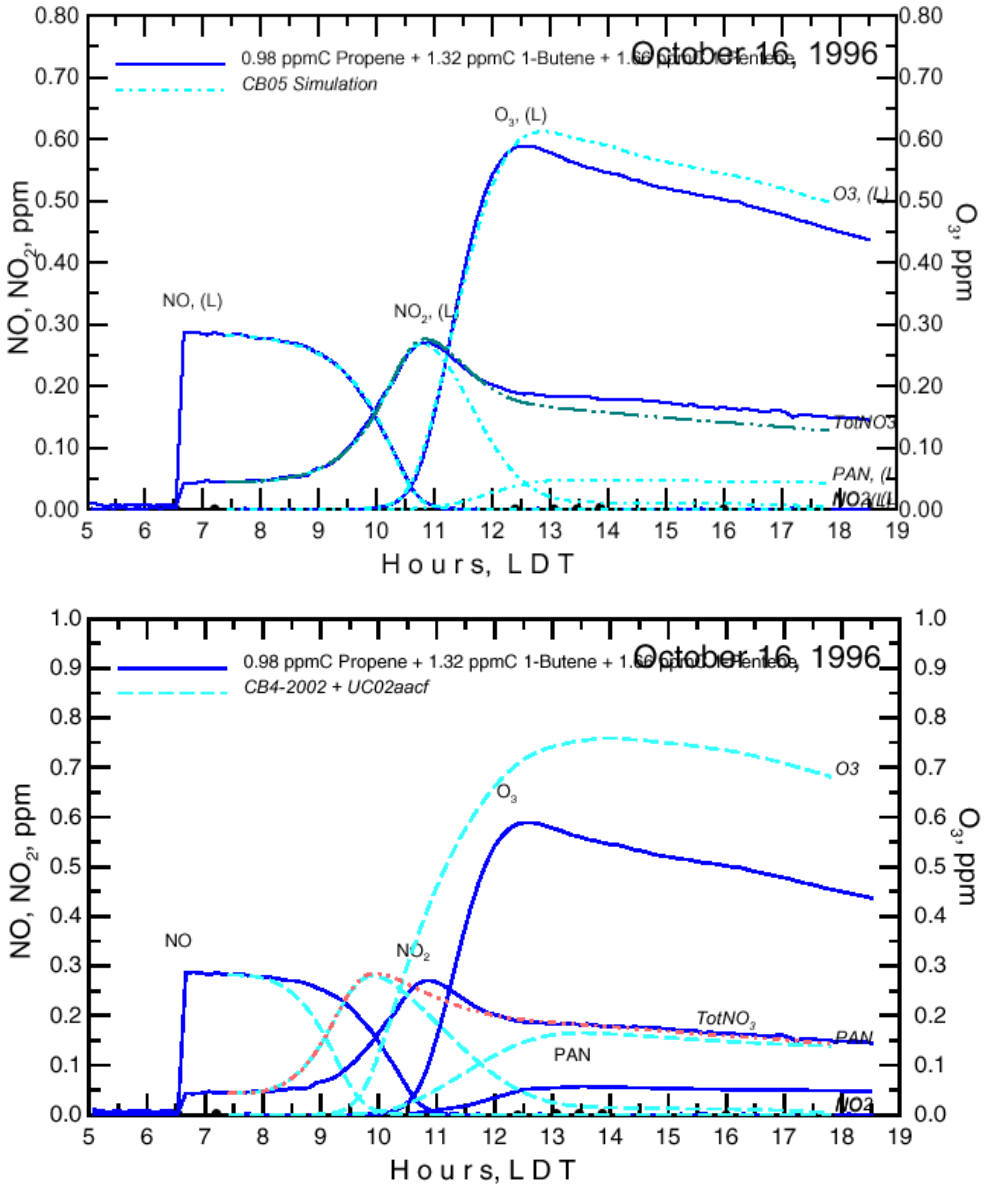

Figure 4-4. Comparison of CB05 (top) and CB4-2002 (bottom) simulations of UNC experiment October 16, 1996 (blue chamber) with propene, 1-butene and 1-pentene.

IOLE Mechanism Update

Including IOLE in CB05 also improves performance for internal olefins (i.e., RHC=CHR) compared to the CB4 surrogate representation of 2 ALD2. Figure 4-5 compares CB05 and CB4-2002 performance for an experiment from September 14, 1996 (blue chamber) with an equimolar mixture of all butene isomers (1-butene, cis-2-butene, trans-2-butene, isobutene). CB05 does better than CB4-2002 in simulating the rate of ozone production, the final ozone level and the rate of NO to NO_2 conversion. CB05 produces ozone more rapidly because of radical production from IOLE reactions and formation of ALDX as a product in addition to ALD2.

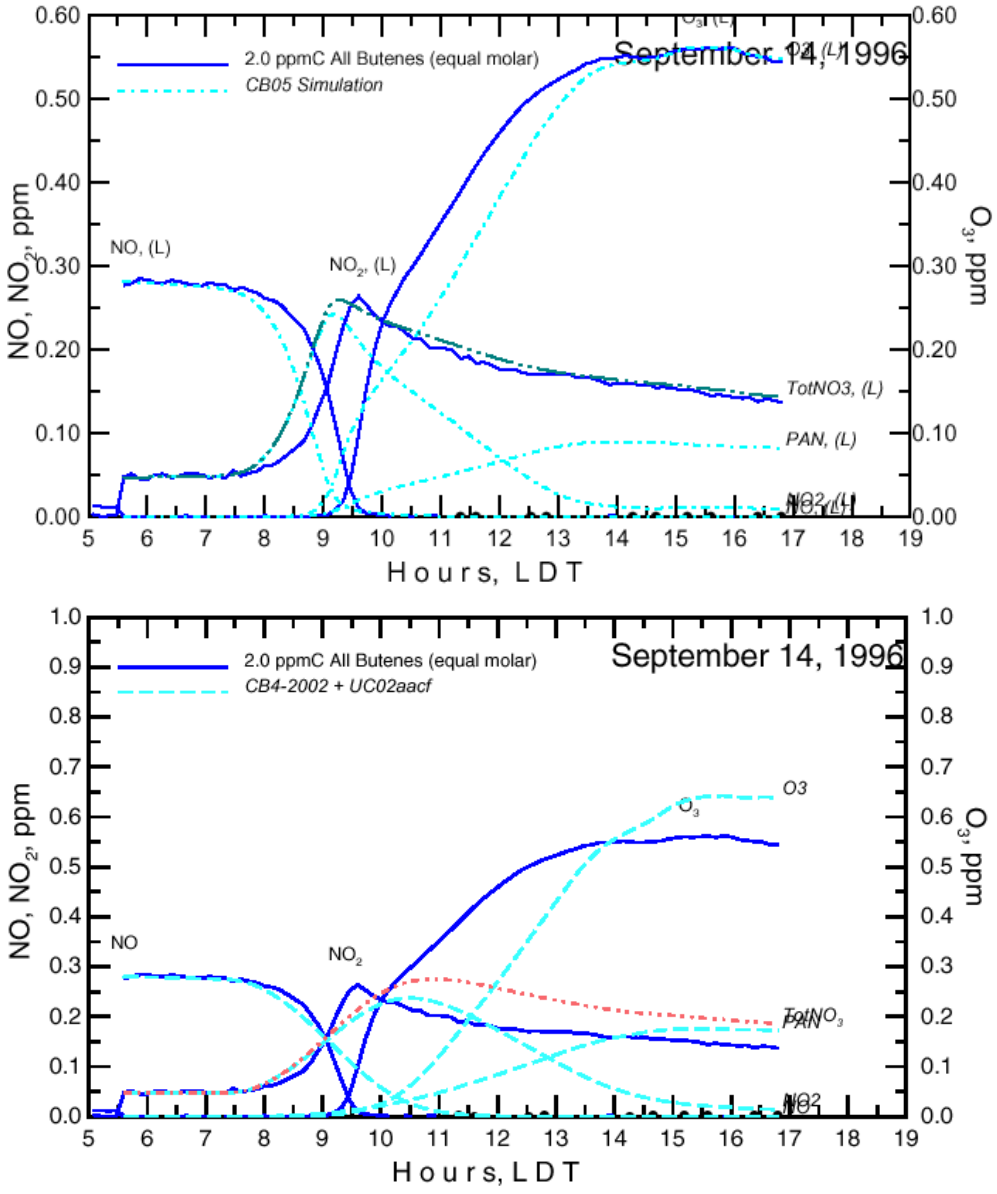

Figure 4-5. Comparison of CB05 (top) and CB4-2002 (bottom) simulations of UNC experiment September 14, 1996 (blue chamber) with an equimolar mixture of all butene isomers (1-butene, cis-2-butene, trans-2-butene, isobutene).

Summary of CB05 Performance for UNC Chamber Experiments

Results of CB05 simulations for UNC chamber experiments are shown in Appendix B. Experiments are grouped according to the VOC introduced into the red chamber. Each experiment is identified by date and chamber (red or blue) and further details on each experiment are given in Jeffries, Voicu and Sexton (2002).

The performance of CB05 against the UNC chamber data is summarized as follows:

Chamber Background. The chamber background experiments mostly reflect the wall mechanism and performed well.

Carbon monoxide. The CO experiments reflect the wall mechanism and core inorganic chemistry in CB05 and performed well with a couple of exceptions that are not understood.

Formaldehyde. The formaldehyde experiments test formaldehyde and basic radical chemistry. CB05 performed very well.

Methane. Methane experiments are somewhat sensitive to the chamber wall mechanism and any impurity in the methane because methane has very low reactivity. CB05 performed well with a couple of exceptions that are not understood

Acetaldehyde (ALD2). Acetaldehyde experiments add PAN formation and additional radical reactions to the chemistry tested by methane and formaldehyde experiments. CB05 performed well for experiments with acetaldehyde and acetaldehyde mixtures.

Higher aldehydes (ALDX). CB05 performed well for experiments with higher aldehyde mixtures. As discussed above, ALDX is an area of improvement in CB05 over CB4.

Ethene (ETH). Ethene experiments test ethene and formaldehyde chemistry. CB05 performed quite well for ethene experiments.

Terminal olefins (OLE). Terminal olefins test the OLE chemistry for alk-1-enes and rely upon ADLX, ALD2 and formaldehyde chemistry. CB05 performed quite well for OLE experiments.

Olefin mixtures (IOLE and OLE). Internal olefins test the IOLE chemistry for alk-2-enes and similar compounds and rely upon ADLX, ALD2 and formaldehyde chemistry. CB05 performed well for IOLE experiments.

Alkanes (PAR). Alkane experiments test the PAR chemistry in addition to the aldehyde and inorganic chemistry. CB05 over predicted ozone in one butane experiments but not others. CB05 performed well for alkanes higher than butane.

Aromatics (TOL and XYL). Aromatics chemistry is complex and includes several species specific to aromatics, but also relies upon simpler aldehyde chemistry. CB05 performance showed more scatter for aromatics than other species. CB05 generally under-predicted the initial rise in ozone and the peak ozone, but did not show a clear

trend toward over or under prediction of the final ozone formation. This result differs from the UCR chamber evaluation presented below.

Isoprene. Isoprene is an explicit species in CB05 that involves the aldehyde and basic inorganic chemistry. CB05 tended to under predict ozone formation in isoprene experiments. This result is surprising as the isoprene chemistry was not overtly changed from the previous CB4 mechanisms (e.g., CB4-2002). The current CB05 isoprene mechanism was implemented as a translation of the SAPRC one-product isoprene mechanism. This should be revisited, possibly by implementing a "three product" mechanism with methacorlein and methylvinyl ketone as explicit products (Carter 1996).

Urban Mixtures. CB05 tended to under predict ozone formation in many but not all experiments with the UNC synthetic urban mixture. Further investigation would be needed to understand this performance.

UCR CHAMBER

The University of California at Riverside (UCR) operates several smog chambers including a new chamber (the "EPA chamber"), described by Carter et al., 2005, which is capable of experiments at lower NOx levels than the earlier chambers. Dr. Carter of UCR performed chamber simulations to evaluate both the CB05 and the SAPRC99 "fixed parameter" mechanisms (Carter, 2000) for this study. Results from several simulations in the EPA chamber are shown in Figures 4-6 to 4-15. The results are summarized as follows. CB05 and SAPRC99 performance was similar for experiments with CO, formaldehyde and ethene. CB05 performed somewhat better than SAPRC99 for propene although both mechanisms performed quite well. CB05 and SAPRC99 performance was similar and good for butane.

The CB05 and SAPRC99 fixed parameter version (Carter, 2000) were compared against experiments from several chambers at UCR. Dr. Carter at UCR performed the UCR chamber simulations for both CB05 and SAPRC99 and provided the results to the CB05 mechanism developers.

Over 350 UCR experiments for individual compounds and compound mixtures were used to evaluate the mechanisms as listed in Tables 4-3 and 4-4. Each group of experiments was compared by displaying the bias in predicted oxidant production (O3-NO) with experiment time, as seen in Figure 4-16. The bias values (prediction minus observation divided by observation) are assigned to ranges (bins) and counted. Good performance is shown by most of the counts being in the bins with low bias. Separate lines are shown for each hour of the experiment (1 to 6 hours) to reveal biases in the rate of oxidant production (early hours) versus biases in the final amount of oxidant (late hours).

Different compounds test different parts of the photochemical mechanisms, as discussed above in the evaluation against UNC chamber data. Compounds are ordered in Figure 4-16 and the discussion below so as to involve progressively more of the mechanism in the evaluation.

Carbon Monoxide (CO). The CO experiments were used by UCR to adjust the chamber wall mechanism for CB05. The UCR chamber wall mechanisms differ by chamber and were

not reevaluated in detail for CB05. A single parameter that controls the production of radicals by wall reactions was adjusted (upward) for CB05 compared to SAPRC99.

Formaldehyde. CB05 showed a slight under-prediction bias for formaldehyde in contrast to SAPRC99, which showed neutral bias. This may be related to differences in the OH plus NO2 rate constant between CB05 and SAPRC99 (CB05 rate is slightly higher). Note that CB05 and SAPRC99 are using the same photolysis data for formaldehyde so this is not a factor in the different performance of the two mechanisms.

Acetaldehyde. Both mechanisms performed well for acetaldehyde with CB05 performing exceptionally well.

Ethene. CB05 and SAPRC99 performance for ethene was similar with both mechanisms showing a slight positive bias. The similarity in CB05 and SAPRC99 performance for ethane is surprising given the difference in performance for formaldehyde (see above) because ethene experiments are very sensitive to the formaldehyde mechanism.

Propene. Both CB05 and SAPRC99 tended to under-predict oxidant production for propene in the UCR chambers, especially in the early experiment hours. CB05 had less under-prediction of the final oxidant levels from propene than SAPRC99.

Trans-2-butene. This compound tests the new IOLE chemistry in CB05. CB05 performed very well for trans-2-butene. SAPRC99 tended to under-estimate the initial oxidant production rate but then performed similar to CB05 in predicting the final oxidant levels.

Isoprene. CB05 and SAPRC99 performed similarly and well for isoprene with near zero bias being the most frequent performance. CB05 had a slightly broader bias distribution than SAPRC99. This may be because SAPRC99 has a more complex "3-product" mechanism than the CB05 "1-product" mechanism. The CB05 1-product mechanism is a translation of the SAPRC 1-product mechanism.

n-Butane. CB05 had a narrower and negative bias distribution whereas SAPRC99 had a broader and positive bias distribution for n-butane. For both mechanisms, near-zero bias was the most frequent outcome for the final oxidant levels in n-butane experiments.

n-Octane. Both CB05 and SAPRC99 tended to under-predict oxidant production from n-octane, with greater negative bias for SAPRC99 than CB05.

Toluene. CB05 under-predicted the initial rate of oxidant formation from toluene but tended to produce the right final oxidant levels. SAPRC99 tended to slightly under-predict the initial oxidant production rate but slightly over-predict the final oxidant levels for toluene. Thus, SAPRC99 has closer to zero overall bias for toluene than CB05.

m-Xylene. CB05 tended to under-predict the initial rate of oxidant formation from m-xylene and slightly under-predict the final oxidant levels. SAPRC99 performance for m-xylene was very good and most often showed zero bias for oxidant levels throughout experiments.

o-Xylene. Both CB05 and SAPRC99 showed a lot of scatter in oxidant bias for o-xylene. CB05 had less scatter and tended to under-predict the final oxidants whereas SAPRC99 had more scatter and tended to over-predict the final oxidant levels for o-xylene.

1,2,4-Trimethylbenzene. Both CB05 and SAPRC99 showed scattered oxidant bias for 1,2,4-Trimethylbenzene. CB05 tended to under-predict the final oxidants whereas SAPRC99 tended to over-predict the final oxidant levels for 1,2,4-trimethylbenzene.

Alpha-pinene and beta-pinene. The new CB05 terpene mechanism is a translation of the SAPRC99 lumped terpene mechanism, so CB05 and SAPRC99 are expected to show similar performance for alpha- and beta-pinene, as was the case. Performance for alpha-pinene was much better than for beta-pinene illustrating the difficulty in representing oxidant formation from both species using a single lumped terpene mechanism.

Surrogate mixtures. Oxidant performance was evaluated for two different types of multi-species mixtures (surrogate mixtures) employed at UCR that are referred to as the "EPA Surrogate" and the "Full Surrogate." CB05 and SAPRC99 performance for surrogate mixtures is quite similar. For the "EPA Surrogate" experiments, both mechanisms show scattered negative bias with a greater tendency to under-predict the early oxidant production rate and lesser bias for the final oxidant levels. The assessment for the "Full Surrogate" runs is similar except that the CB05 bias is less scattered and marginally closer to neutral than SAPRC99. Overall, CB05 shows less scatter but SAPRC99 has marginally less negative bias than CB05 for the final oxidant levels in surrogate mixture experiments. Neither mechanism performed clearly better than the other in the surrogate mixture experiments.

The area of most difference between CB05 and SAPRC99 is aromatics chemistry. The SAPRC99 aromatics chemistry performs much better than CB05 against the UCR chamber data CB05 predicts less ozone formation from aromatics than SAPRC99, especially for toluene, and therefore systematically under predicts the UCR chamber ozone in aromatics experiments. CB05 showed less tendency to under predict ozone in UNC aromatics chamber experiments than UCR experiments. There appears to be a systematic difference in the aromatics experiments between the UCR and UNC chambers that may be related to the chambers or the design of the experiments. This could be investigated by evaluating the SAPRC99 mechanism against UNC chamber experiments. Further work is warranted to understand differences in the UCR and UNC aromatics experiments and differences between the aromatics mechanisms.

Table 4-3. Compounds and numbers of UCR experiments included in the comparison between CB05 and SAPRC99 mechanism performance.

Compound	Number of Experiments
Carbon monoxide	18
Formaldehyde	24
Acetaldehyde	12
Ethene	39
Propene	89
t-2-Butene	12
Isoprene	18
Butane	10
Octane	5
Toluene	28
m-Xylene	27
o-Xylene	13
123-trimethylbenzene	9
Alpha-Pinene	11
Beta-Pinene	9
EPA surrogate mixture	25
Full surrogate mixture	18

Table 4-4. Numbered UCR chamber experiments used to evaluate the CB05 and SAPRC99 mechanisms, by compound.

CO	Form-aldehyde	Acet-aldehyde	Ethene	Propene		trans-2-Butene	Isoprene	Butane	Octane	Toluene	m-Xylene	o-Xylene	1,2,3-tri-methyl-benzene	a-Pinene	b-Pinene	EPA Surrogate	Full Surrogate
18	24	12	39	89		12	18	10	5	28	27	13	9	11	9	25	18
CTC031	ITC1549	DTC150A	ITC1555	ETC440	XTC081	EC146	ITC511	ETC484	EPA114B	ITC534	DTC073A	DTC207A	DTC201A	ETC420	ETC421	EPA080A	DTC251A
CTC061	ITC1554	DTC150B	ITC926	ETC449	XTC082	EC147	ITC811	ETC488	EPA095A	ITC699	DTC188A	DTC207B	DTC203A	ETC443	ETC433	EPA080B	DTC251B
CTC090A	ITC864	DTC152B	ITC936	DTC026A	XTC097	EC157	ITC812	ETC094	EPA083B	ITC828	DTC188B	DTC208A	DTC203B	ETC444	ETC434	EPA081A	DTC455A
CTC090B	ETC378	DTC387B	ETC220	DTC026B	XTC113	ETC493	DTC053A	ETC097	EPA085B	DTC042A	DTC189A	DTC208B	DTC204A	ETC446	ETC435	EPA081B	DTC455B
EPA057A	ETC441	XTC083	ETC221	DTC128A	CTC012	ETC501	DTC053B	ETC135	EPA113B	DTC042B	DTC189B	DTC209A	DTC204B	ETC447	ETC442	EPA082A	DTC474A
EPA057B	DTC149A	XTC092	ETC381	DTC128B	CTC018	ETC307	DTC056A	ETC224		DTC151A	DTC191A	DTC209B	CTC056	XTC095	XTC099	EPA082B	DTC474B
EPA058A	DTC149B	CTC014	ETC439	DTC129A	CTC023	ETC309	DTC056B	ETC389		DTC155A	DTC191B	CTC038	CTC091B	OTC318A	OTC318B	EPA083A	DTC488A
EPA058B	DTC218A	CTC015	ETC464	DTC129B	CTC049	DTC043B	XTC093	ETC393		DTC158A	DTC192A	CTC039	CTC093A	ETC508	DTC051B	EPA084B	DTC488B
EPA061A	DTC218B	CTC032	ETC466	DTC205A	CTC059	DTC021B	XTC101	DTC019B		DTC170A	DTC192B	CTC046	CTC093B	DTC045B	DTC048A	EPA085A	DTC616A
EPA061B	DTC270A	CTC072	ETC467	DTC205B	CTC078	DTC069A	EC520	DTC031A		XTC106	DTC193A	CTC068		DTC044A		EPA086A	DTC616B
EPA070A	DTC270B	EC164	ETC469	DTC246A	CTC083A	DTC041A	EC522			CTC026	DTC193B	CTC081		DTC034B		EPA095B	CTC149A
EPA070B	DTC387A	EC254	ETC471	DTC288A	CTC083B	DTC033A	EC524			CTC034	CTC029	CTC091A				EPA096A	CTC149B
EPA071A	XTC086		ETC473	DTC288B	CTC086A		EC527			CTC048	CTC035	EC288				EPA096B	CTC165A
EPA071B	CTC016		ETC476	DTC301A	CTC086B		EC669			CTC065	CTC036					EPA097A	CTC165B
EPA103A	CTC024		ETC479	DTC301B	CTC115A		OTC309A			CTC079	CTC066					EPA097B	CTC171A
EPA103B	CTC077		ETC482	DTC331A	CTC115B		OTC309B			EC264	CTC080					EPA098A	CTC171B
EPA140A	CTC095A		ETC486	DTC331B	CTC132A		OTC316A			EC266	CTC094A					EPA098B	OTC277A
EPA140B	CTC095B		ETC497	DTC346A	CTC132B		OTC316B			EC269	CTC094B					EPA100A	OTC277B
	CTC116A		ETC505	DTC346B	CTC147A					EC270	ETC196					EPA101A	
	CTC116B		DTC041B	DTC371A	CTC147B					EC271	ETC207					EPA101B	
	CTC133A		DTC043A	DTC371B	CTC153A					EC273	ETC301					EPA108B	
	CTC133B		DTC044B	DTC393A	CTC153B					EC293	DTC025A					EPA110B	
	CTC176A		DTC045A	DTC393B	CTC163A					EC327	DTC068B					EPA113A	
	CTC176B		DTC046B	DTC405A	CTC163B					EC340	DTC035A					EPA114A	
			DTC047A	DTC405B	CTC170A					OTC299A	DTC067B					EPA123A	
			DTC048B	DTC417A	CTC170B					OTC299B	CTC109A						
			DTC050A	DTC417B	CTC191A					OTC300A	CTC128A						
			DTC051A	DTC431A	CTC191B					OTC300B							
			DTC072B	DTC431B	CTC203A												
			XTC105	DTC443A	CTC203B												
			XTC112	DTC443B	CTC219A												
			EC142	DTC458A	CTC219B												
			EC143	DTC458B	CTC234A												
			EC156	DTC472A	CTC234B												
			EC285	DTC472B	CTC245A												
			EC286	DTC483A	CTC245B												
			EC287	DTC483B	CTC264A												
			EPA073A	DTC503A	CTC264B												
			EPA073B	DTC503B	OTC272A												
				DTC526A	OTC272B												
				DTC526B	OTC295A												
				DTC578A	OTC295B												
				DTC578B	OTC298A												
				DTC597A	OTC298B												
				DTC597B													

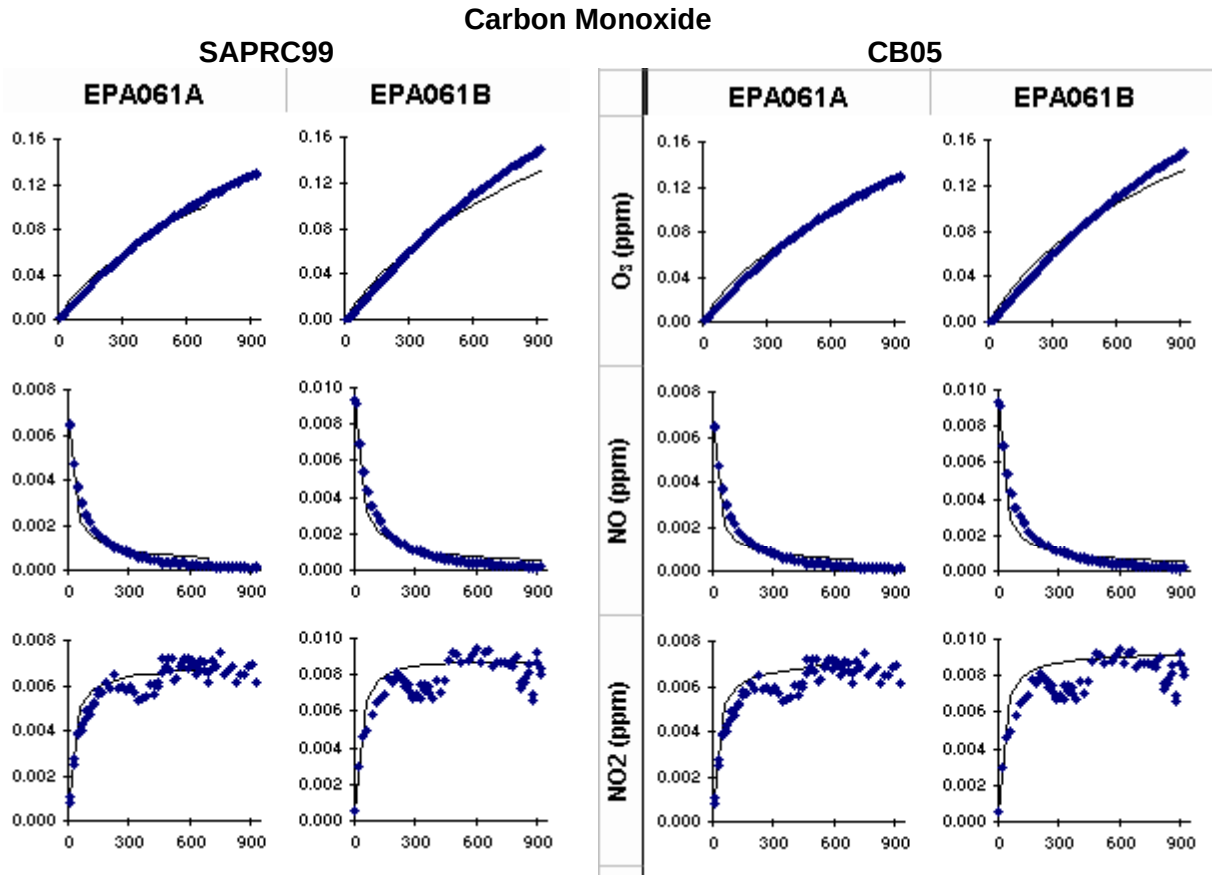

Figure 4-6. SAPRC99 (left) and CB05 (right) simulation of a carbon monoxide experiment in the EPA chamber at UCR.

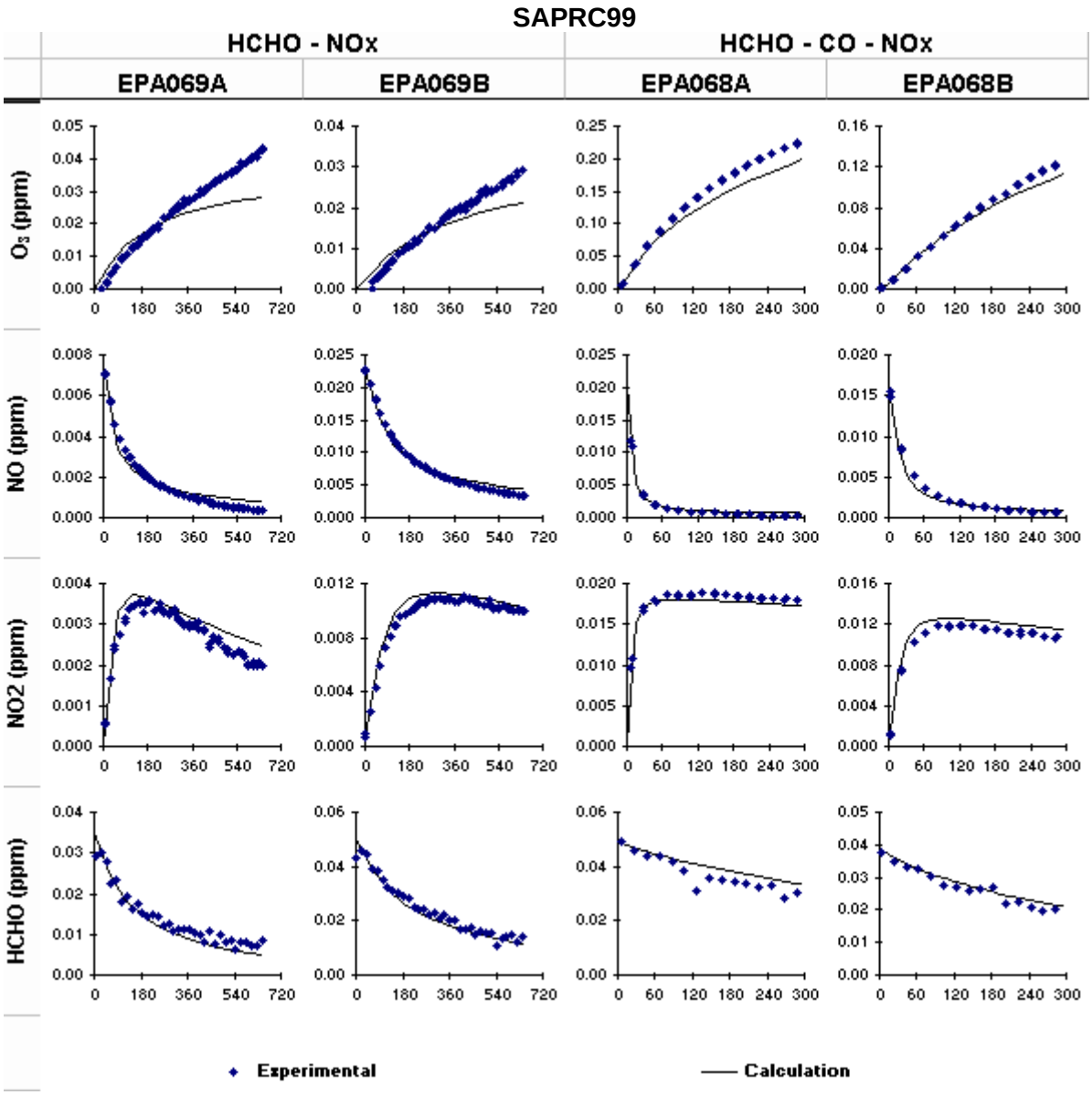

Figure 4-7. SAPRC99 simulation of four formaldehyde experiments in the EPA chamber at UCR.

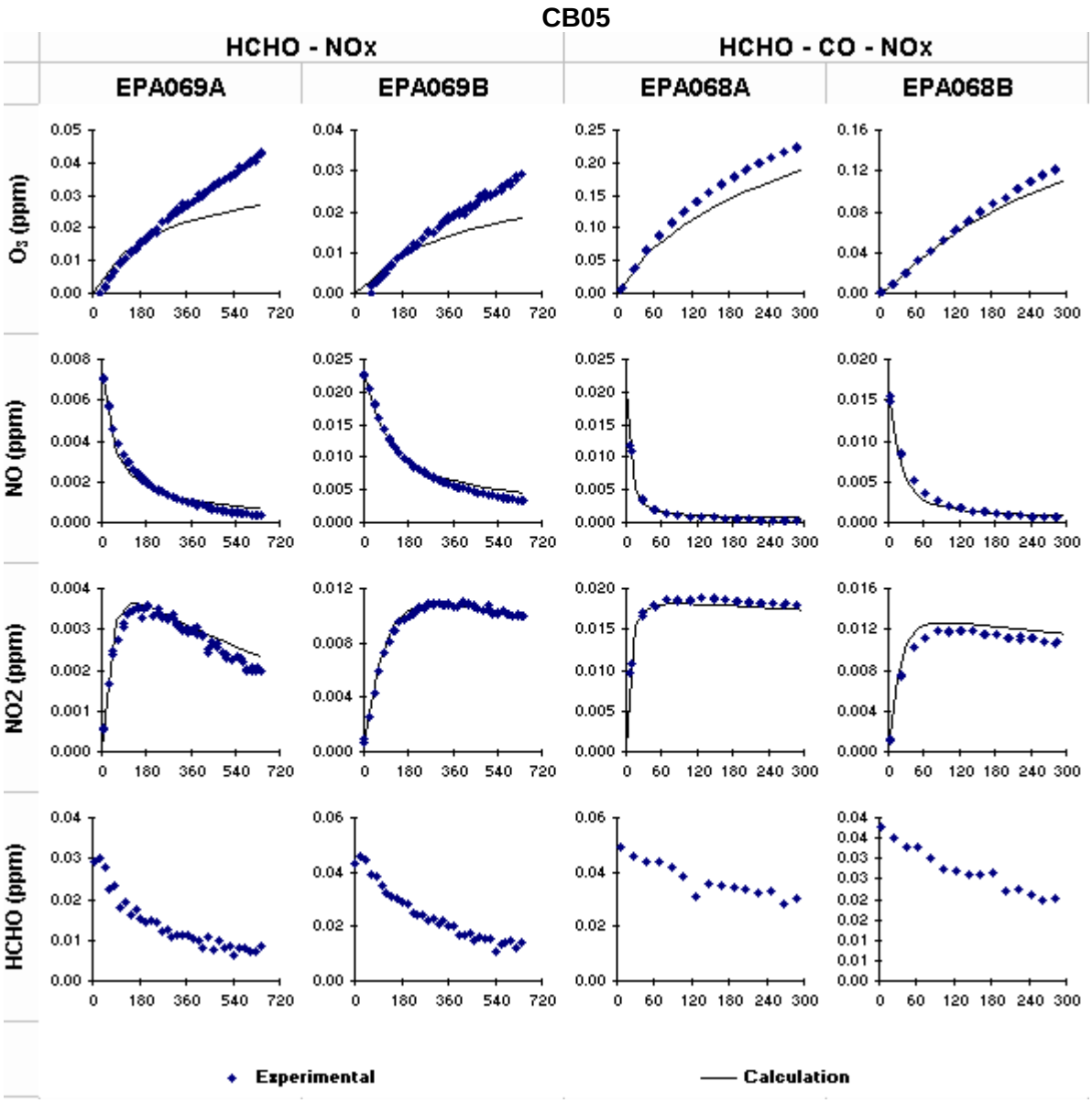

Figure 4-8. CB05 simulation of four formaldehyde experiments in the EPA chamber at UCR.

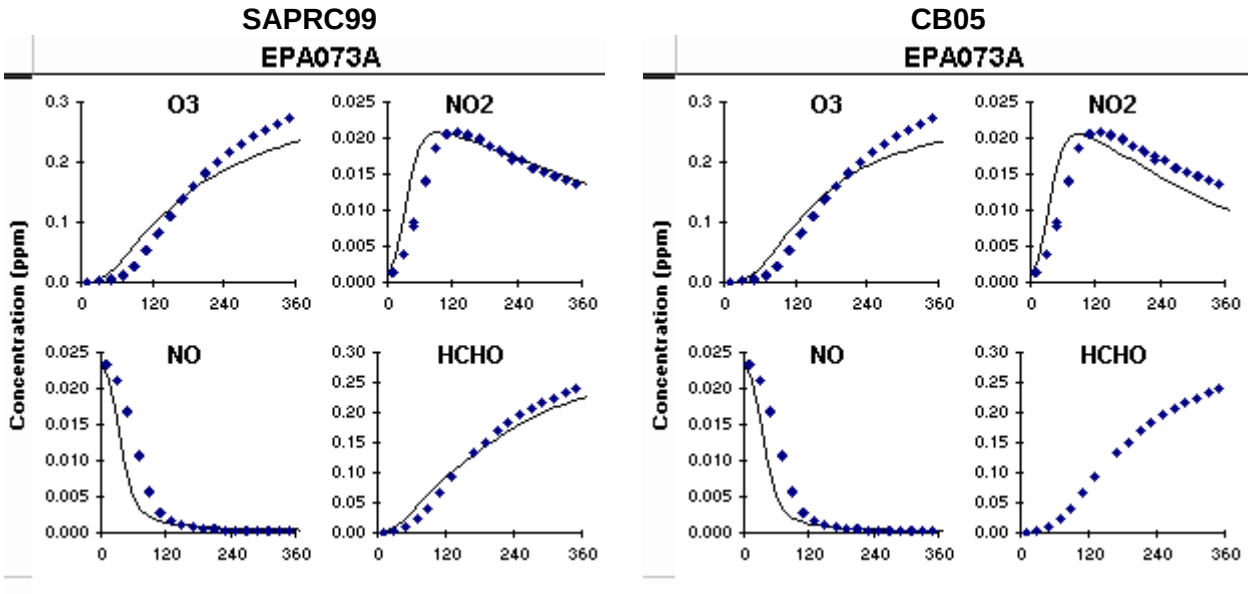

Figure 4-9. SAPRC99 (left) and CB05 (right) simulation of an ethene experiment in the EPA chamber at UCR.

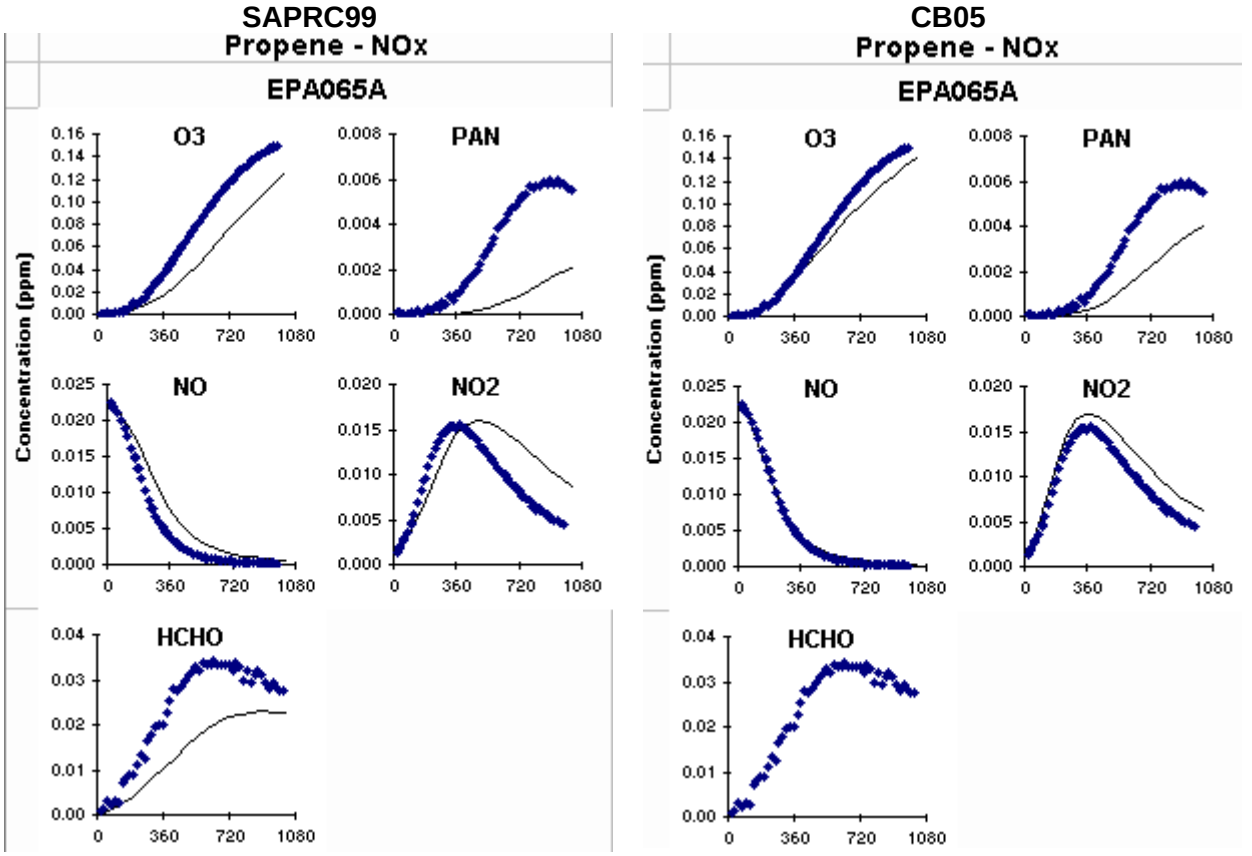

Figure 4-10. SAPRC99 (left) and CB05 (right) simulation of a propene experiment in the EPA chamber at UCR.

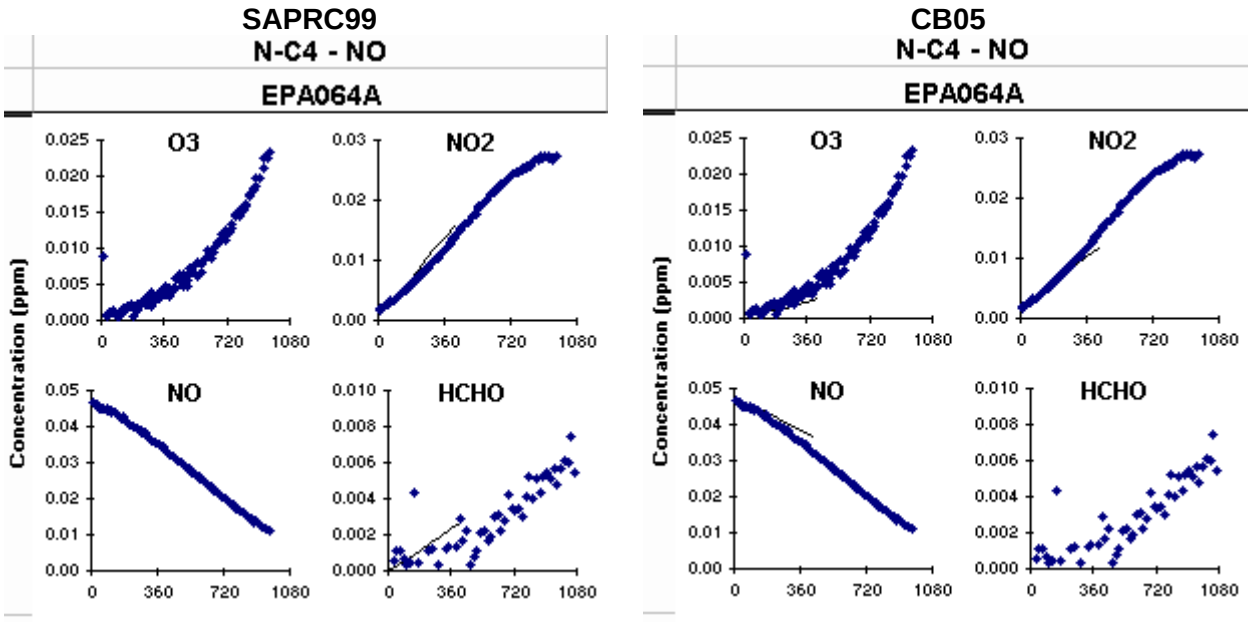

Figure 4-11. SAPRC99 (left) and CB05 (right) simulation of a butane experiment in the EPA chamber at UCR.

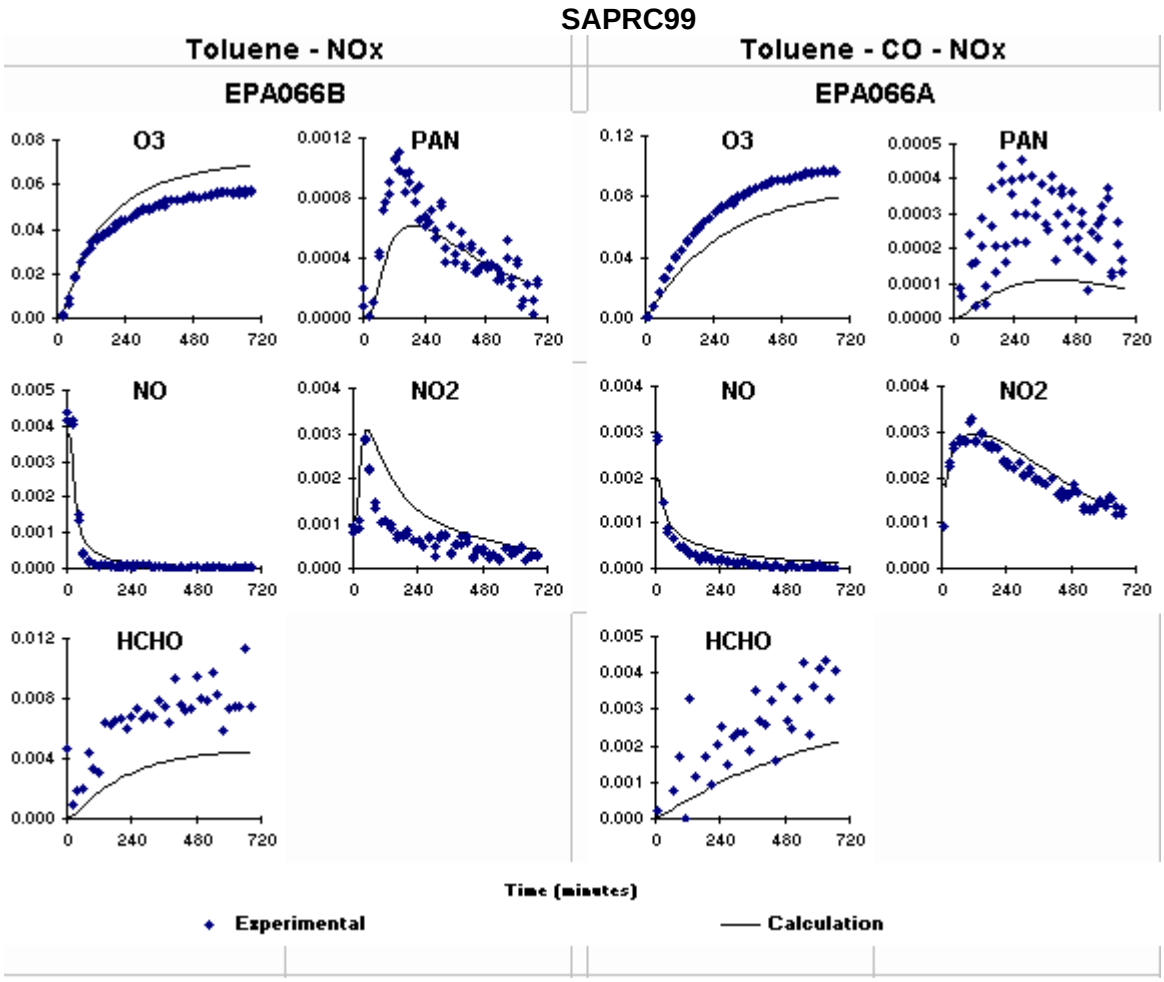

Figure 4-12. SAPRC99 simulation of two toluene experiments in the EPA chamber at UCR.

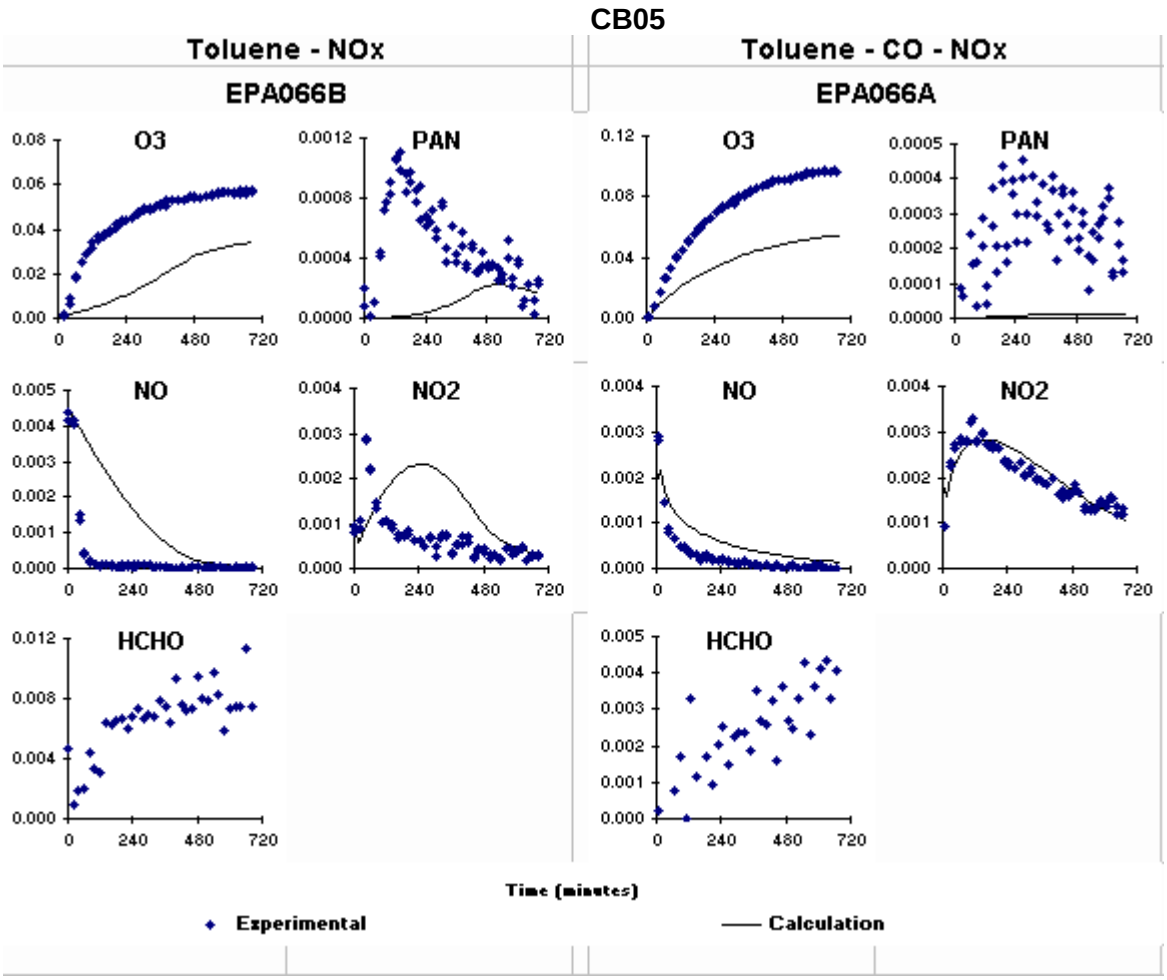

Figure 4-13. CB05 simulation of two toluene experiments in the EPA chamber at UCR.

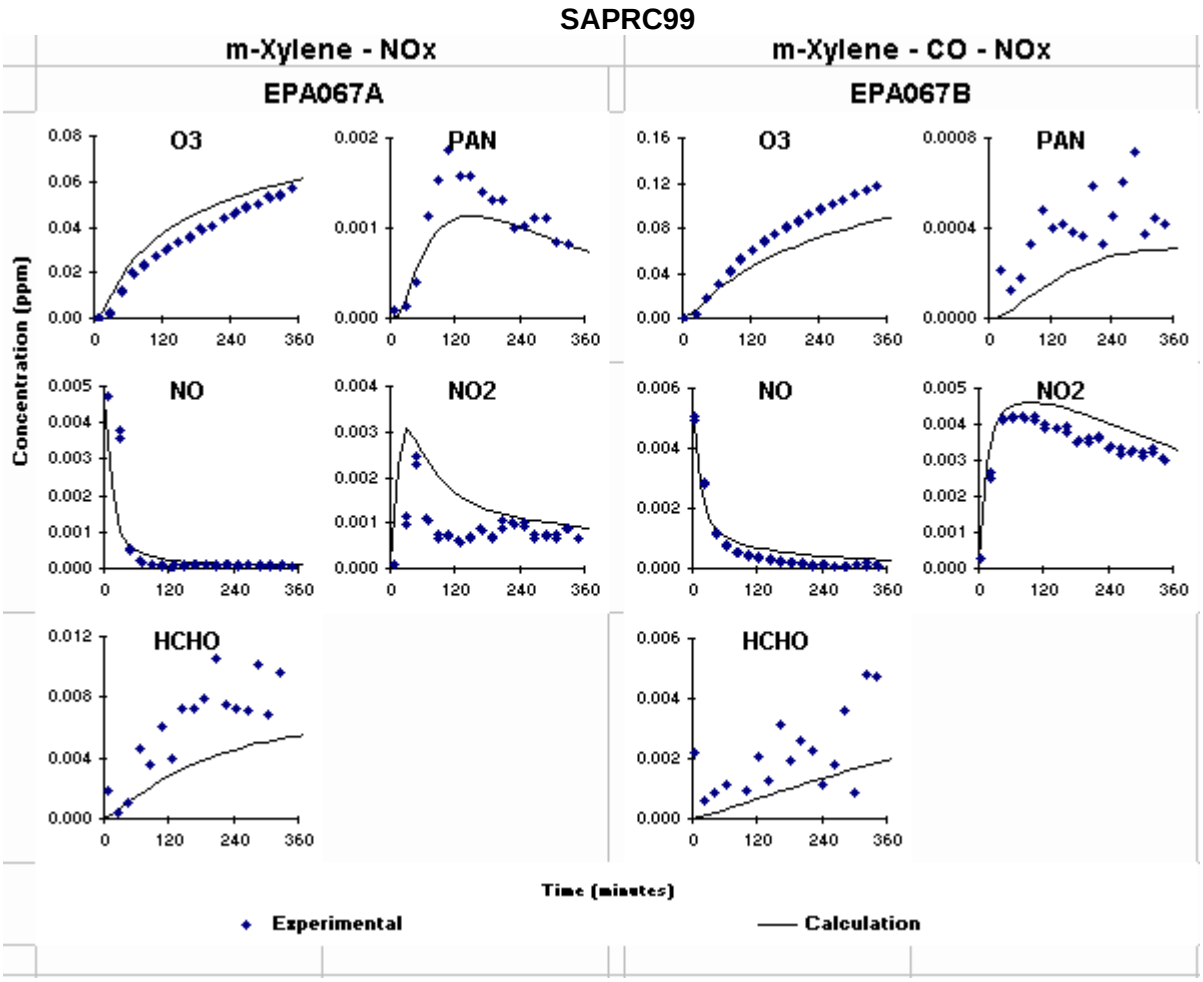

Figure 4-14. SAPRC99 simulation of two xylene experiments in the EPA chamber at UCR.

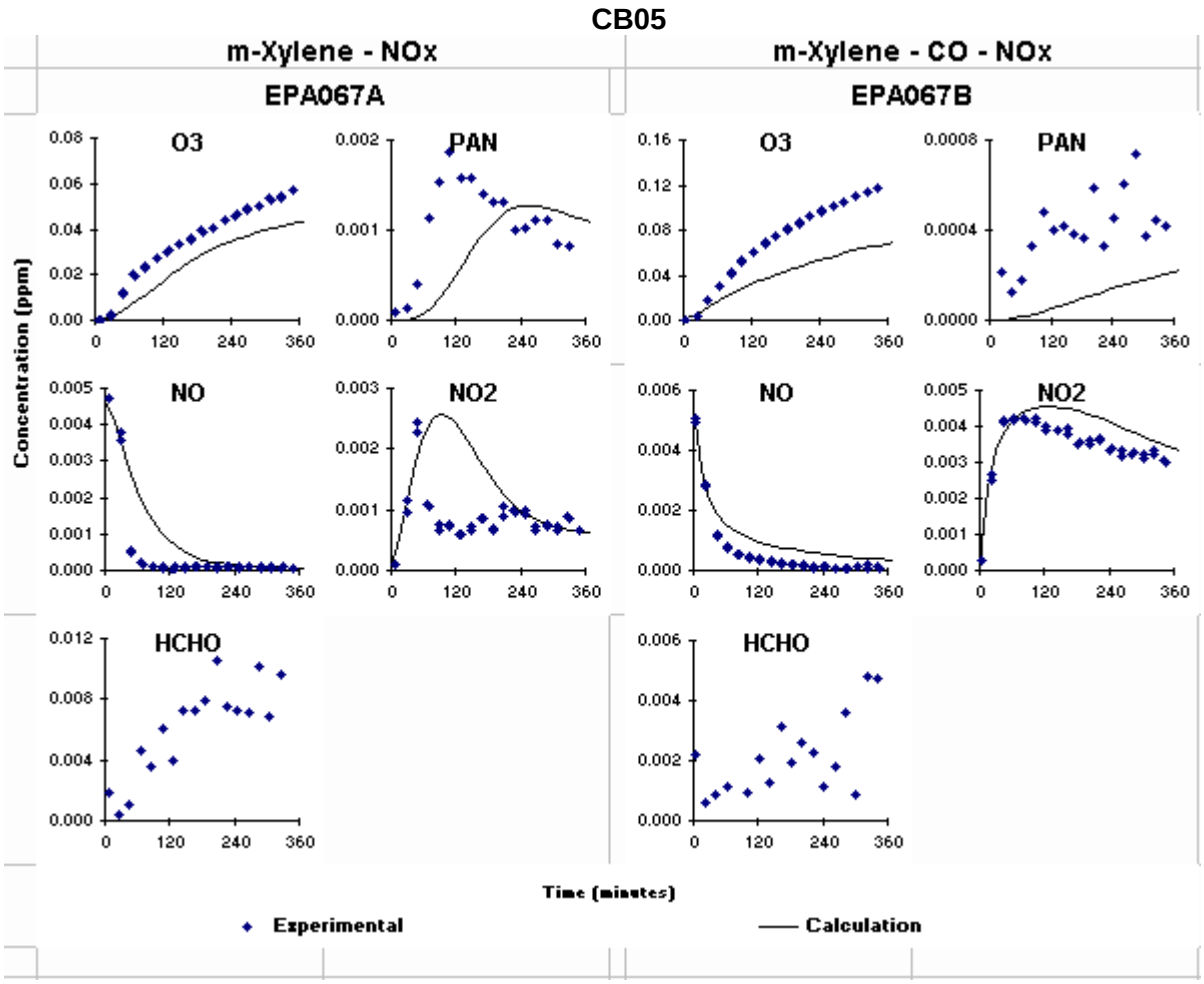

Figure 4-15. CB05 simulation of two xylene experiments in the EPA chamber at UCR.

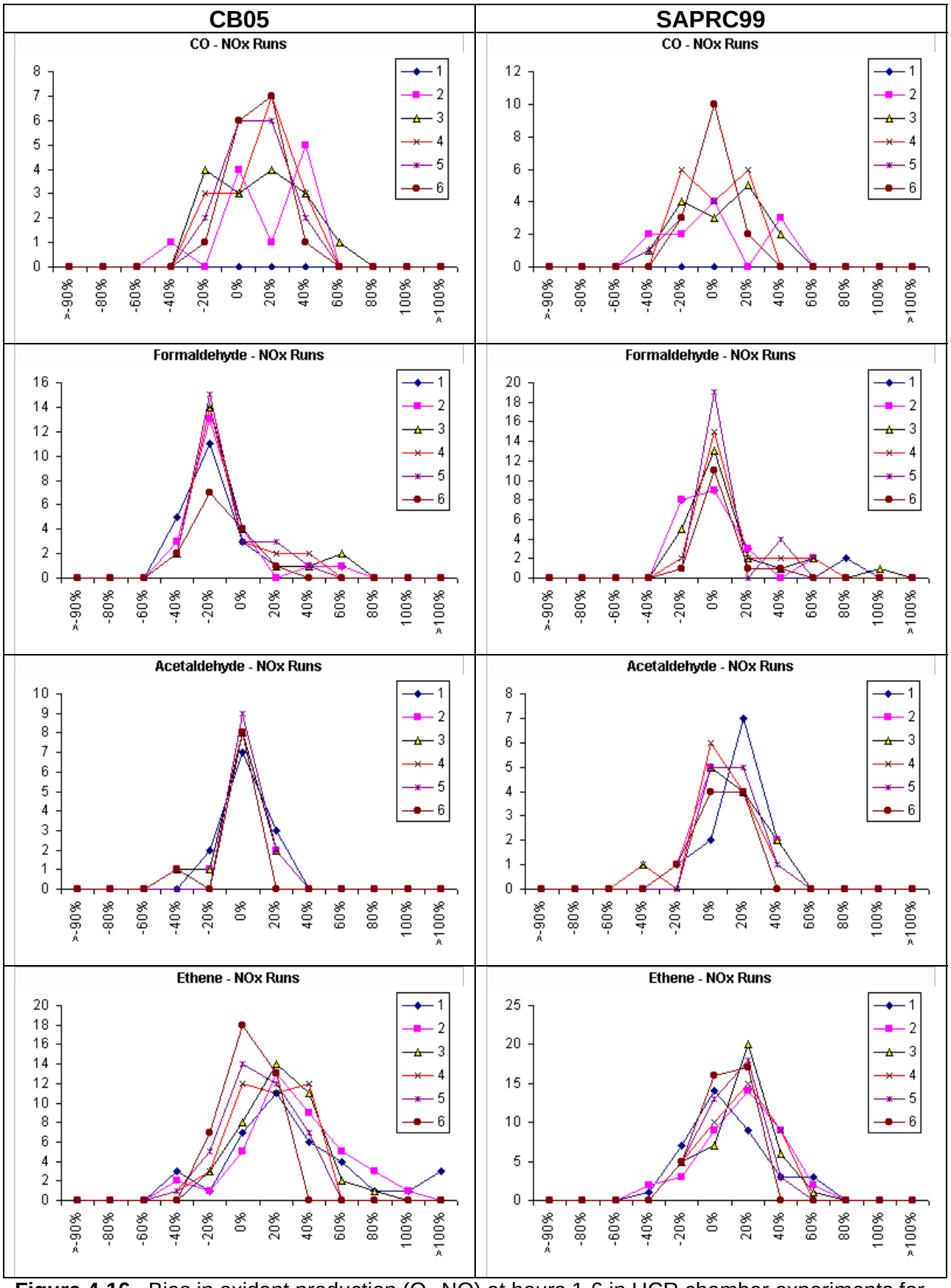

Figure 4-16. Bias in oxidant production (O_3-NO) at hours 1-6 in UCR chamber experiments for the CB05 and SAPRC99 mechanisms, by compound.

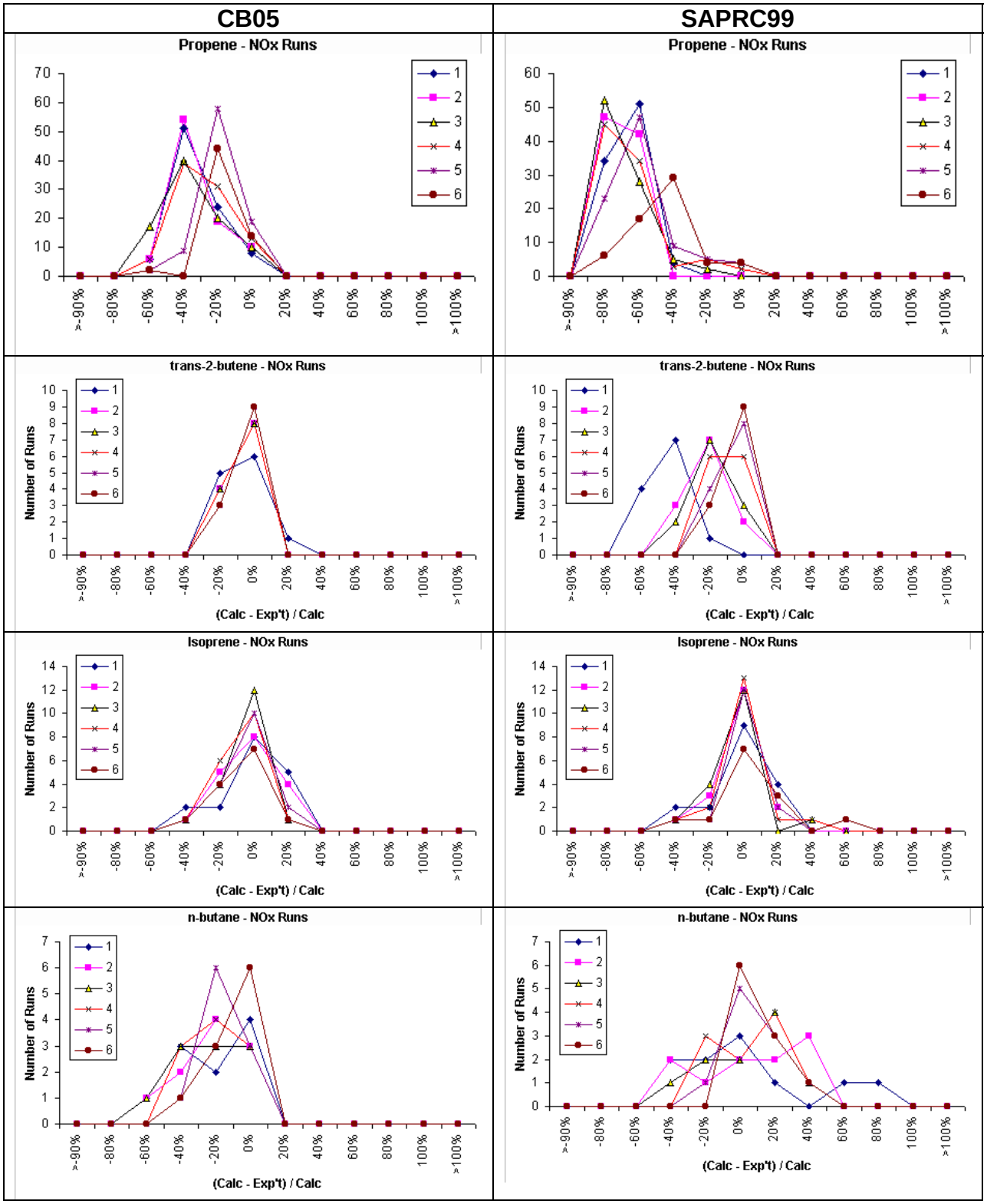

Figure 4-16. (continued). Bias in oxidant production (O_3-NO) at hours 1-6 in UCR chamber experiments for the CB05 and SAPRC99 mechanisms, by compound.

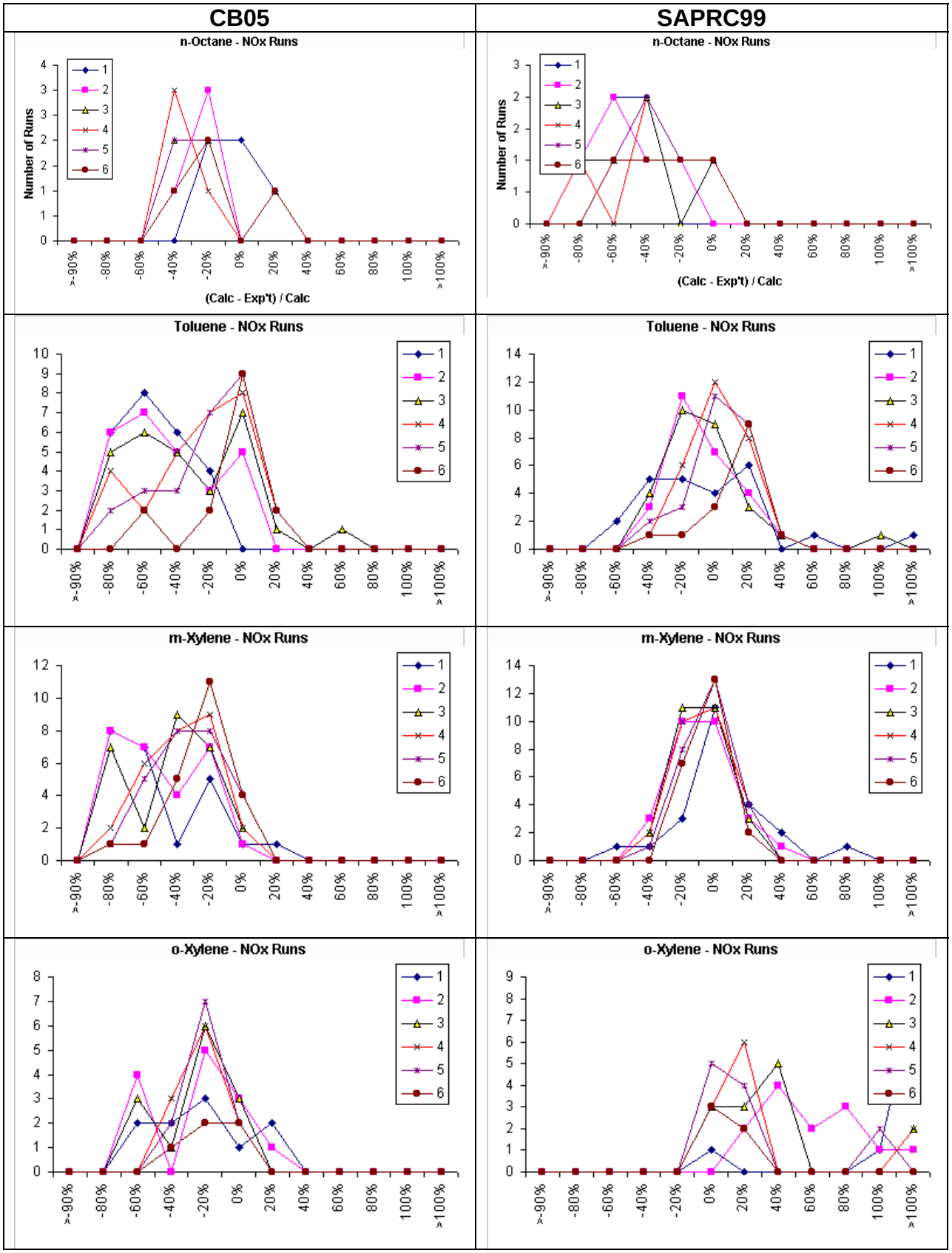

Figure 4-16. (continued). Bias in oxidant production (O_3-NO) at hours 1-6 in UCR chamber experiments for the CB05 and SAPRC99 mechanisms, by compound.

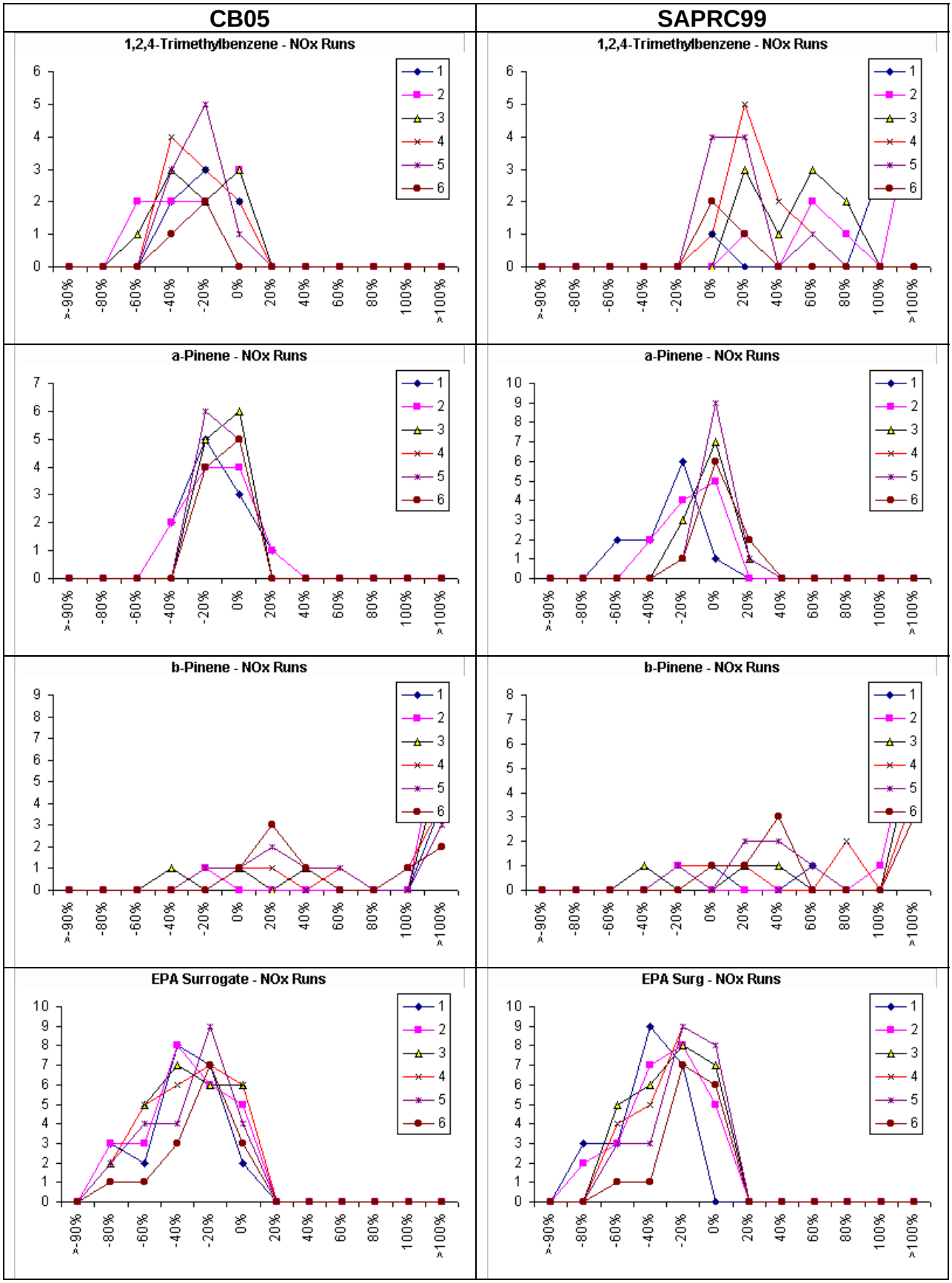

Figure 4-16. (continued). Bias in oxidant production (O_3-NO) at hours 1-6 in UCR chamber experiments for the CB05 and SAPRC99 mechanisms, by compound.

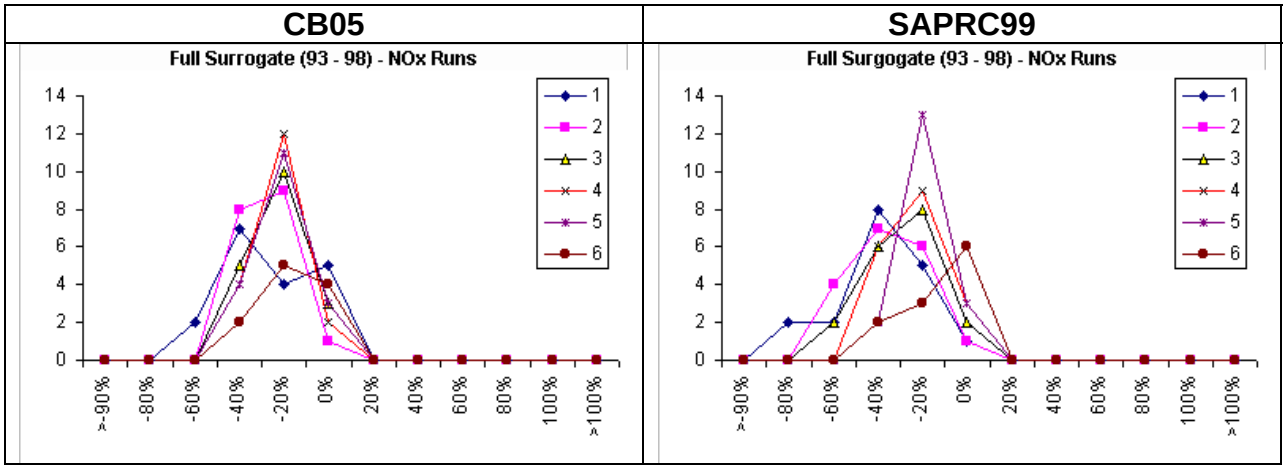

Figure 4-16. (concluded). Bias in oxidant production (O_3-NO) at hours 1-6 in UCR chamber experiments for the CB05 and SAPRC99 mechanisms, by compound.

5. SUMMARY AND RECOMMENDATIONS

The Carbon Bond mechanism has been updated for use in EPA atmospheric modeling studies. The starting point for this study was version 4 of the Carbon Bond mechanism (CB4) developed in the late 1980s (Gery et al., 1989) as updated in the mid 1990s for EPA's "OTAG" ozone transport assessment study. The new version of the Carbon Bond mechanism is called CB05 because it was developed in 2005.

The CB05 is a condensed mechanism of atmospheric oxidant chemistry that provides a basis for computer modeling studies of ozone, particulate matter (PM), visibility, acid deposition and air toxics issues. Updates in CB05 compared to earlier CB4 mechanisms are:

- Updated rate constants based on recent (2003 – 2005) IUPAC and NASA evaluations.
- An extended inorganic reaction set for urban to remote tropospheric conditions.
- NOx recycling reactions to represent the fate of NOx over multiple days.
- Explicit organic chemistry for methane and ethane.
- Explicit methylperoxy radical, methyl hydroperoxide and formic acid.
- Lumped higher organic peroxides, organic acids and peracids.
- Internal olefin (R-HC=CH-R) species called IOLE.
- Higher aldehyde species ALDX making ALD2 explicitly acetaldehyde.
- Higher peroxyacyl nitrate species from ALDX called PANX.
- Lumped terpene species called TERP.
- Optional mechanism extension for reactive chlorine chemistry.
- Optional extended mechanism with explicit reactions for air-toxics.

The core CB05 mechanism has 51 species and 156 reactions. The CB05 was evaluated against smog chamber data from the Universities of North Carolina (UNC) and California at Riverside (UCTR). An updated wall reaction mechanism was developed for the UNC chamber that improved performance in experiments that are sensitive to chamber radical sources. The addition of higher aldehyde (ALDX) and internal olefin (IOLE) species to CB05 improved mechanism performance for simulating these species groups. The addition of organic peroxide species improves the simulation of oxidants that are involved in PM sulfate formation. The addition of explicit methylperoxy radical improves the simulation of hydrogen peroxide under low NOx conditions.

Two CB05 mechanism extensions were developed. The optional reactive chlorine chemistry mechanism can be used in conjunction with the CB05 core mechanism to model the impact of Cl_2 and/or HOCl emissions on oxidant formation and VOC decay rates. The optional explicit species extension can be used in conjunction with the CB05 (or another) core mechanism to model the following toxic species: primary formaldehyde, primary acetaldehyde, 1,3-butadiene, primary and secondary acrolein. Other optional explicit species are toluene, o-xylene, m-xylene, p-xylene, apha-pinene and beta-pinene. These include the main precursors to secondary organic aerosol (SOA) and could be used as the basis for refined modeling approach for SOA that is independent of the core mechanism selected (e.g., CB4, CB05 or SAPRC99).

Recommendations

- Terpene experiments from UNC should be implemented in the UNC "Morpho" chamber simulation software and used to evaluate, and possibly update, the CB05 terpene mechanism.

- The SAPRC99 mechanism should be evaluated against UNC chamber experiments using the Morpho software and updated UNC chamber wall mechanisms.

- There should be a comparative study of UCR and UNC chamber experiments, especially for aromatics, to understand apparent chamber differences.

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Appendix A

Assignments from VOC Species to CB05 Model Species

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
ALKANES - examples																			
methane	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	16.04	1
propane	0	1.5	0	0	0	0	0	0	0	0	0	1.5	0	0	0	0	0	44.1	1.5
ethane	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	30.07	2
n-butane	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	58.12	4
2,2-dimethylpropane	0	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	72.15	4
2-methylpropane; isobutane	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	58.12	4
2-methylpropane; isobutane	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	58.12	4
n-pentane	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	72.15	5
2-methyl-butane	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	72.15	5
2,2-dimethylbutane	0	5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	86.18	5
isomers of pentane	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	72.15	5
cyclopentane	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	70.14	5
c5 paraffin	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	72.15	5
dimethylbutane	0	5.75	0	0	0	0	0	0	0	0	0	0.25	0	0	0	0	0	86.18	5.75
isomers of hexane	0	5.83	0	0	0	0	0	0	0	0	0	0.17	0	0	0	0	0	86.18	5.83
2,3-dimethylbutane	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	86.18	6
cyclohexane	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	84.16	6
1,6-Diisocyanatohexane	0	6	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	168.2	6
2-methylpentane	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	86.18	6
3-methylpentane	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	86.18	6
methylcyclopentane	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	84.16	6
methylpentane	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	86.18	6
3,3-dimethylpentane	0	6	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	100.21	6
n-hexane	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	86.18	6
dimethylpentane	0	6.75	0	0	0	0	0	0	0	0	0	0.25	0	0	0	0	0	100.21	6.75
c7 paraffins	0	6.81	0	0	0	0	0	0	0	0	0	0.19	0	0	0	0	0	100.21	6.81
isomers of heptane	0	6.81	0	0	0	0	0	0	0	0	0	0.19	0	0	0	0	0	100.21	6.81
n-octane	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	114.23	7
c7 cycloparaffins	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	98.19	7
methyl hexane	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100.21	7
n-decane	0	7	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	142.29	7
n-heptane	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100.21	7
methylcyclohexane	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	98.19	7
2,4-dimethylpentane	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100.21	7
2,2,4-trimethylpentane	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	114.23	7
2,3-dimethylpentane	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100.21	7
2,3,3-trimethylpentane	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	114.23	7
dimethylcyclopentane	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	98.19	7
ethylcyclopentane	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	98.19	7
n-nonane	0	7	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	128.26	7
2-methylhexane	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100.21	7
2,2-dimethylhexane	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	114.23	7
3-methylhexane	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100.21	7
trimethylpentane	0	7.33	0	0	0	0	0	0	0	0	0	0.67	0	0	0	0	0	114.23	7.33
isomers of octane (c8 paraffin)	0	7.62	0	0	0	0	0	0	0	0	0	0.38	0	0	0	0	0	114.23	7.62

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
methylnonane	0	7.75	0	0	0	0	0	0	0	0	0	2.25	0	0	0	0	0	142.29	7.75
dimethylhexanes	0	7.83	0	0	0	0	0	0	0	0	0	0.17	0	0	0	0	0	114.23	7.83
c8 cycloparaffins	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	112.22	8
3-methylheptane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.23	8
2-methylheptane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.23	8
4-methylheptane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.23	8
methylheptane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.23	8
n-undecane	0	8	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	156.31	8
n-dodecane	0	8	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	170.34	8
ethylcyclohexane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	112.22	8
cis-1,4-dimethylcyclohexane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	112.22	8
2,3,4-trimethylpentane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.23	8
cis-1-methyl-3-ethylcyclopentane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	112.22	8
isopropylcyclopentane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	112.22	8
trimethylcyclopentane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	112.22	8
c8 alkyl cyclohexanes	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	112.22	8
dimethylcyclohexanes	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	112.22	8
2,2,4-trimethylhexane	0	8	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	128.26	8
2,4-dimethylhexane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.23	8
2,5-dimethylhexane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.23	8
2,3-dimethylhexane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.23	8
ethylhexane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.23	8
2,2,5-trimethylhexane	0	8	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	128.26	8
cis-bicyclo[3.3.0]octane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	110.2	8
aliphatics	0	8.08	0	0	0	0	0	0	0	0	0	0.62	0	0	0	0	0	122.89	8.08
diethylcyclohexane	0	8.5	0	0	0	0	0	0	0	0	0	1.5	0	0	0	0	0	140.27	8.5
isomers of nonane (c9 paraffin)	0	8.75	0	0	0	0	0	0	0	0	0	0.25	0	0	0	0	0	128.26	8.75
trimethylhexanes	0	8.8	0	0	0	0	0	0	0	0	0	0.2	0	0	0	0	0	128.26	8.8
propenylcyclohexane	0	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	124.23	9
methyloctanes	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
c9 cycloparaffins	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
methyldodecanes	0	9	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	184.37	9
2,4-dimethylheptane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
3,5-dimethylheptane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
2,5-dimethylheptane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
2,3-dimethylheptane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
ethylheptane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
ethylbicycloheptane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	124.23	9
dimethylheptanes	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
2-methyloctane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
3-methyloctane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
4-methyloctane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
propylcyclohexane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
1,1,3-trimethylcyclohexane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
ethyldimethylpentane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
tetramethylcyclopentane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
c9 alkyl cyclohexanes	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
ethylmethylcyclohexanes	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
2,3,5-trimethylhexane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
ethylmethylhexane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
n-tridecane	0	9	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	184.37	9
isopropylcyclohexane (2-methylethyl cycloh	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
Bicyclo[4.3.0]nonane (octahydroindene)	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	124.23	9
unk c9 paraffin	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.26	9
methylcyclooctane	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
isomers of decane (c10 paraffins)	0	9.25	0	0	0	0	0	0	0	0	0	0.75	0	0	0	0	0	142.29	9.25
c6 substituted cyclohexane	0	9.33	0	0	0	0	0	0	0	0	0	2.67	0	0	0	0	0	168.32	9.33
isomers of undecane (c11 paraffins)	0	9.5	0	0	0	0	0	0	0	0	0	1.5	0	0	0	0	0	156.31	9.5
methyldecanes	0	9.5	0	0	0	0	0	0	0	0	0	1.5	0	0	0	0	0	156.31	9.5
dimethyloctanes	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
n-tetradecane	0	10	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	198.39	10
n-pentadecane	0	10	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	212.42	10
isomers of tridecane (c13 paraffins)	0	10	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	184.37	10
2,4,5-trimethylheptane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
methylethylheptane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
trimethylheptanes	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
ethyloctane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
2,4-dimethyloctane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
3,4-dimethyloctane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
2,3-dimethyloctane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
2,6-dimethyloctane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
dimethylethylcyclohexane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	140.27	10
isopropylmethylcyclohexane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	140.27	10
butylcyclohexane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	140.27	10
cyclopentylcyclopentane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	138.25	10
c10 alkyl cyclohexanes	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	140.27	10
methyl propylcyclohexanes	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	140.27	10
tetramethylhexane	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.29	10
decalins (mixed cis,trans)	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	138.25	10
c5 substituted cyclohexane	0	10.25	0	0	0	0	0	0	0	0	0	0.75	0	0	0	0	0	154.3	10.25
dimethylnonanes	0	10.4	0	0	0	0	0	0	0	0	0	0.6	0	0	0	0	0	156.31	10.4
isomers of dodecane (c12 paraffins)	0	10.67	0	0	0	0	0	0	0	0	0	1.33	0	0	0	0	0	170.34	10.67
isomers of tetradecane (c14 paraffins)	0	10.75	0	0	0	0	0	0	0	0	0	3.25	0	0	0	0	0	198.39	10.75
trimethyloctanes	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	156.31	11
hexadecane	0	11	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	226.45	11
n-heptadecane	0	11	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	240.48	11
c16 branched alkanes	0	11	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	226.45	11
dimethylundecanes	0	11	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	184.37	11
ethylmethyloctane	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	156.31	11
n-pentylcyclohexane	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	154.3	11
ethyl propylcyclohexanes	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	154.3	11
diethylmethylcyclohexanes	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	154.3	11
dimethyldecane	0	11	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	170.34	11
2-methyldecane	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	156.31	11

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
methyldecalins	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	152.28	11
methylundecane	0	11.2	0	0	0	0	0	0	0	0	0	0.8	0	0	0	0	0	170.34	11.2
isomers of pentadecane (c15 paraffins)	0	11.25	0	0	0	0	0	0	0	0	0	3.75	0	0	0	0	0	212.42	11.25
ethyldimethyloctane	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	170.34	12
dimethylbutylcyclohexane	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	168.32	12
c2 alkyl decalin	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	166.31	12
nonadecane	0	13	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	268.53	13
trimethyldecane	0	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	184.37	13
methylpropylnonane	0	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	184.37	13
eicosane	0	14	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	282.56	14
isomers of heptadecane (c17 paraffins)	0	15	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	240.48	15
isomers of octadecane (c18 paraffins)	0	16.5	0	0	0	0	0	0	0	0	0	1.5	0	0	0	0	0	254.5	16.5
ALKENES - examples																			
ethylene	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	28.05	2
propylene	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	42.08	3
1,2-propadiene	0	0	1.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	40.07	3
trans-2-butene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	56.11	4
cis-2-butene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	56.11	4
2-methylpropene (isobutene)	0	3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	56.11	4
isomers of butene	0	1	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	56.11	4
1-butene	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	56.11	4
4-vinylcyclohexene	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	108.18	4
1,2-butadiene {methylallene}	0	1	1.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	54.09	4
1,3-butadiene	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	54.09	4
methylbutene	0	3.33	0.33	0	0	0.33	0	0	0	0	0	0	0	0	0	0.33	0	70.14	4.98
1,3-cyclopentadiene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.25	0	0	66.1	5
methylbutadiene	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	68.12	5
isoprene	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	68.12	5
trans-2-pentene	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	70.14	5
cis-2-pentene	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	70.14	5
2-methyl-2-butene	0	3	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	70.14	5
2-methyl-1-butene	0	4	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	70.14	5
isomers of pentene	0	2.4	0.2	0	0	0.2	0	0	0	0	0	0	0	0	0	1	0	70.14	5
3-methyl-1-butene	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	70.14	5
1-pentene	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	70.14	5
1,4-pentadiene	0	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	68.12	5
cyclopentene	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	68.12	5
normal pentene isomers	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	70.14	5
piperylene {1,3-pentadiene} (mixed isomers	0	0	0.5	0	0	0	0	0	0	0	0	0	0	0	1	0	0	68.12	5
cyclohexene	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	82.15	6
cis-3-hexene	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	84.16	6
2-hexenes	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	84.16	6
4-methyl-trans-2-pentene	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	84.16	6
trans-3-hexene	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	84.16	6
trans-2-hexene	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	84.16	6
cis-2-hexene	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	84.16	6

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
1-methylcyclopentene	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	82.15	6
dimethylbutene	0	3.5	0	0	0	0.5	0	0	0	0	0	0	0	0	0	1	0	84.16	6
2-methyl-2-pentene	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	84.16	6
3-methyl-trans-2-pentene	0	4	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	84.16	6
2,3-dimethyl-1-butene	0	5	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	84.16	6
2-ethyl-1-butene	0	5	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	84.16	6
2-methyl-1-pentene	0	5	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	84.16	6
c6 olefins (hexene isomers)	0	3	0.33	0	0	0	0	0	0	0	0	0	0	0	0	1.17	0	84.16	6
methylpentenes	0	3.5	0.5	0	0	0	0	0	0	0	0	0	0	0	0	0.75	0	84.16	6
hexadiene	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	82.15	6
methylcyclopentadiene	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	80.13	6
1-hexene	0	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	84.16	6
3-methyl-1-pentene	0	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	84.16	6
4-methyl-1-pentene	0	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	84.16	6
methylcyclohexene	0	3	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	96.17	7
methylhexadiene	0	3	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	96.17	7
3-ethyl-2-pentene	0	5	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	98.19	7
1-methyl cyclohexene	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	96.17	7
2,4,4-trimethyl-1-pentene	0	6	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	112.22	7
c7 olefins	0	4	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	98.19	7
ethylpentene	0	5	0.5	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0	98.19	7
dimethylpentene	0	4.5	0.75	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0	98.19	7
methylcyclohexadiene	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	94.16	7
1-heptene	0	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	98.19	7
ethylcyclopentene	0	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	96.17	7
dimethylcyclopentenes	0	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	96.17	7
3-heptene (mixed cis,trans)	0	3	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	98.19	7
methylhexenes	0	4	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	98.19	7
heptenes	0	3.33	0.17	0	0	0	0	0	0	0	0	0	0	0	0	1.67	0	98.19	7.01
c8 olefins	0	4.67	0.5	0	0	0	0	0	0	0	0	0.33	0	0	0	1	0	112.22	7.67
cis-2-octene	0	4	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	112.22	8
2,4,4-trimethyl-2-pentene (beta diisobutyl	0	6	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	112.22	8
dimethylhexadiene	0	2	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	110.2	8
tetramethylcyclobutene	0	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	110.2	8
1-octene	0	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	112.22	8
butoxybutene	0	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	128.22	8
octatriene	0	0	2	0	0	0	0	0	0	0	0	0	0	0	1	0	0	108.18	8
trimethylpentadiene	0	4	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	110.2	8
methyl heptene	0	5.33	0.67	0	0	0	0	0	0	0	0	0	0	0	0	0.67	0	112.22	8.01
trans-2-nonene	0	5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	126.24	9
4-nonene (mixed isomers)	0	5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	126.24	9
c9 olefins	0	6	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	126.24	9
nonadiene	0	3	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	124.23	9
ethylheptene	0	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
trimethylhexene	0	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
1-nonene	0	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.24	9
c10 olefins	0	6.17	0.33	0	0	0	0	0	0	0	0	0.5	0	0	0	1.33	0	140.27	9.49

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
3-carene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
d-limonene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
a-pinene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
b-pinene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
terpinene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
myrcene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
dimethyloctenes	0	6	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	140.27	10
propylheptenes	0	7	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	140.27	10
methylnonenes	0	7	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	140.27	10
ethyloctenes	0	7	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	140.27	10
c12 olefins	0	7	0.5	0	0	0	0	0	0	0	0	2	0	0	0	1	0	168.32	10
4-phenyl-1-butene	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	132.21	10
trans-1-phenylbutene	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	132.21	10
1-decene	0	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	140.27	10
b-phellandrene {1(7)-2-p-menthadiene}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
dl-limonene {dipentene}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
terpene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
methyldecenes	0	8	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	154.3	11
c11 olefins	0	8	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	154.3	11
1-undecene	0	9	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	154.3	11
trimethylnonene	0	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	168.32	12
1-Dodecene	0	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	168.32	12
trimethyldecenes	0	10	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	182.35	13
caryophyllene	0	9	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	204.36	15
ALKYNES - examples																			
acetylene	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	26.04	1
1-propyne	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	40.07	3
1-butyne (ethylacetylene)	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	54.09	4
2-butyne	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	54.09	4
1-pentyne	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	68.12	5
pentenyne	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	66.1	5
hexyne	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	82.15	6
methylheptyne (6-methyl-2-heptyne)	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	110.2	8
dimethyloctyne	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	138.25	10
ALDEYHDES - examples																			
benzaldehyde	0	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	106.12	0
p-tolualdehyde {4-methylbenzaldehyde}	0	0	0	0	0	0	0	0	0	0	0	8	0	0	0	0	0	120.15	0
formaldehyde	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	30.03	1
acetaldehyde	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	44.05	2
glyoxal	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	58.04	2
total c2-c5 aldehydes	0	0.65	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	53.11	2.65
acrolein (2-propenal)	0	0	0.5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	56.06	3
propionaldehyde	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	58.08	3
methyl glyoxal	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	72.06	3
butyraldehyde	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	72.11	4

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
isobutyraldehyde	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	72.11	4
crotonaldehyde	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	70.09	4
n-pentanal (n-valeraldehyde)	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	86.13	5
isovaleraldehyde (3-methylbutanal)	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	86.13	5
2-furfural	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	96.09	5
2-Hexenal	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	98.15	6
hexanal (hexanaladehyde)	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	100.16	6
2,4-hexadienal	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	96.13	6
methylhexanal	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	114.19	7
trans, trans-2,4-heptadienal	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	110.16	7
ethylhexaldehyde	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	128.22	8
ALCOHOLS - examples																			
carvomenthol (2-p-menthanol) (2-methyl-5-(	0	0	0	0	0	0	0	0	0	0	0	10	0	0	0	0	0	156.27	0
methyl alcohol	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	32.04	1
phenol (carbolic acid)	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	94.11	1
ethyl alcohol	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	46.07	2
ethylene glycol	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	62.07	2
2-Methylaminoethanol	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	75.11	3
n-propyl alcohol	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	60.1	3
isopropyl alcohol	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	60.1	3
tert-butyl alcohol	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	74.12	3
propylene glycol	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	76.1	3
glycerol	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	92.1	3
2-methoxyethanol {methyl cellosolve} {egme	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	76.1	3
diglycolamine (2-(2-aminoethoxy)ethanol)	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	105.14	4
n-butyl alcohol	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	74.12	4
isobutyl alcohol	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	74.12	4
sec-butyl alcohol	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	74.12	4
1,4-butanediol	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	90.12	4
butandiol	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	90.12	4
diethylene glycol (2,2'-oxybisethanol)	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	106.12	4
2-ethoxyethanol {cellosolve} {egee}	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	90.12	4
misc. alcohols	0	4.74	0	0	0	0	0	0	0	0	0	0.1	0	0	0	0	0	85.64	4.74
amyl alcohols	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	88.15	5
furfuryl alcohol	0	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	98.1	5
n-pentanol	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	88.15	5
1-ethoxy-2-propanol	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	104.15	5
isoamyl alcohol (3-methyl-1-butanol)	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	88.15	5
bis-phenol a	0	5	0	0	0	0	0	0	0	0	0	10	0	0	0	0	0	228.29	5
methyl carbitol {2-(2-methoxyethoxy)ethano	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	120.15	5
diisopropylene glycol	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	134.18	6
diethyl aminoethanol	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	117.19	6
2-Ethyl-1,3-hexanediol	0	6	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	146.23	6
triethylene glycol	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	150.18	6
2-Hexyloxyethanol	0	6	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	146.23	6
cyclohexanol	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100.16	6

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
hexylene glycol (2-methylpentane-2,4-diol)	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	118.18	6
1-hexanol (n-hexanol)	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	102.18	6
4-methyl-2-pentanol (methyl isobutyl carbi	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	102.18	6
diacetone alcohol (4-hydroxy-4-methyl-2-pe	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	116.16	6
butyl cellosolve {2-butoxyethanol} {egbe}	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	118.18	6
carbitol {degee} {2-(2-ethoxyethoxy)ethano	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	134.18	6
benzyl alcohol	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	108.14	7
2,2,4-Trimethyl-1,3-Pentanediol	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	146.23	7
1-heptanol	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	116.2	7
dimethylpentanol (2,3-dimethyl-1-pentanol)	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	116.2	7
o-cresol (2-methyl-benzenol)	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	108.14	7
biphenylol {2-phenylphenol}	0	0	0	1	0	0	0	0	0	0	0	5	0	0	0	0	0	170.21	7
cresols	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	108.14	7
octanol isomers	0	7.25	0	0	0	0	0	0	0	0	0	0.75	0	0	0	0	0	130.23	7.25
c8 phenols	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	122.17	8
xylenol	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	122.17	8
2-(2-butoxyethoxy)ethanol {butyl carbitol	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	162.23	8
methylheptanol	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	130.23	8
2-ethyl-1-hexanol	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	130.23	8
dimethylbenzylalcohol	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	136.19	9
c9 phenols	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	136.19	9
trimethylcyclohexanol	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.24	9
dimethylheptanol (2,6-dimethyl-2-heptanol)	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	144.26	9
ethyldimethylphenol	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	150.22	10
c10 alkylphenols	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	150.22	10
2-N,N-Dibutylaminoethanol	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	173.3	10
1-decanol	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	158.29	10
3,7-dimethyl-1-octanol	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	158.29	10
a-terpineol	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	154.25	10
c11 alkylphenols	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	164.25	11
nonylphenol	0	8	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	220.36	15
ETHERS - examples																			
ethylene oxide	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	44.05	1
dimethyl ether	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	46.07	2
propylene oxide	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	58.08	2
dimethoxymethane (methylal)	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	76.1	3
ethyl ether	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	74.12	4
methyl t-butyl ether (mtbe)	0	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	88.15	4
tetrahydrofuran	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	72.11	4
1,4-dioxane	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	88.11	4
propylene glycol methyl ether {1-methoxy-2	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	90.12	4
ethyl t-butyl ether	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	102.18	5
ethyl isopropyl ether	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	88.15	5
t-amylmethylether (tame)	0	5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	102.18	5
ethylene glycol propyl ether {2-propoxyet	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	104.15	5
4,4-Dimethyl-3-oxahexane	0	4	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	116.2	6

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
diisopropyl ether	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	102.18	6
propylene glycol n-propyl ether	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	118.18	6
acetal (1,1-diethoxyethane)	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	118.18	6
ethylfuran	0	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	96.13	6
di(propylene glycol) methyl ether	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	148.2	7
dibutyl ether	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	130.23	8
2-butyltetrahydrofuran	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	128.22	8
KETONES - examples																			
carvone	0	0	0	0	0	0	0	0	0	0	0	10	0	0	0	0	0	150.22	0
acetone	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	58.08	3
methyl ethyl ketone (mek) (2-butanone)	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	72.11	4
1-methyl-2-pyrrolidinone	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0	99.13	5
Methyl Isopropyl Ketone	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	86.13	5
methyl n-butyl ketone	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100.16	6
methyl isobutyl ketone	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100.16	6
cyclohexanone	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	98.15	6
dimethylcyclobutanone	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	98.15	6
methyl amyl ketone	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.19	7
2-methyl-3-hexanone	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.19	7
propylcyclohexanone	0	7	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	140.23	7
heptanone	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114.19	7
methylacetophenone	0	1	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	134.18	8
trimethylcyclopentanone	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.2	8
dihydroxynapthalenedione	0	2	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	190.16	9
nonenone	0	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	140.23	9
2,2,4,4-tetramethyl-3-pentanone	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	142.24	9
c4 substituted cyclohexanone	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	154.25	10
9,10-anthraquinone	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	208.22	14
1-aminoanthraquinone	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	223.23	14
ORGANIC ACIDS - examples																			
formic acid	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	46.03	0
oxalic acid	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	90.04	0
acetic acid	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	60.05	1
benzoic acid	0	1	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	122.12	1
terephthalic acid (p-benzenedicarboxylic a	0	1	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	166.13	1
propionic acid	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	74.08	2
acrylic acid	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	72.06	2
methyacrylic acid	0	1	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	86.09	3
butanoic acid	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	88.11	3
3-Methylbutanoic acid	0	3	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	102.13	3
isobutyric acid	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	88.11	3
adipic acid	0	4	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	146.14	4
2-ethylhexanoic acid	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	144.21	7
Phenylacetic Acid	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	136.15	7
dimethylethylbenzoic acid	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	150.18	9

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
ESTERS - examples																			
methyl formate	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	60.05	1
phthalic anhydride	0	1	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	148.12	1
acetic anhydride	0	2	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	102.09	2
methyl acetate	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	74.08	2
vinyl acetate	0	1	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	86.09	3
ethyl acetate	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	88.11	3
methyl acrylate	0	1	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	86.09	3
dimethylterephthalate	0	3	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	194.19	3
dimethyl phthalate	0	3	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	194.19	3
Isopropyl Formate	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	88.11	3
maleic anhydride	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	98.06	4
propyl acetate	0	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	102.13	4
isopropyl acetate	0	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	102.13	4
ethyl acrylate	0	2	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	100.12	4
methyl methacrylate	0	2	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	100.12	4
hydroxypropyl acrylate	0	2	1	0	0	0	0	0	0	0	0	2	0	0	0	0	0	130.14	4
dimethyl succinate (dimethyl butaneoate)	0	4	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	146.14	4
misc. esters	0	4.11	0	0	0	0	0	0	0	0	0	1	0	0	0	0.01	0	104.38	4.13
c5 ester	0	4.33	0	0	0	0	0	0	0	0	0	0.67	0	0	0	0	0	102.13	4.33
propylene glycol monomethyl ether acetate	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	132.16	5
n-butyl acetate	0	5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	116.16	5
isobutyl acetate	0	5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	116.16	5
2-ethoxyethyl acetate {cellosolve acetate}	0	5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	132.16	5
pentanedioic acid, dimethyl ester (dimethy	0	5	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	160.17	5
n-Propyl Propionate	0	5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	116.16	5
n-butyl benzoate	0	5	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	178.23	5
methyl isobutyrate	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	102.13	5
amyl acetate	0	6	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	130.19	6
n-butyl acrylate	0	4	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	128.17	6
dimethyl adipate (dimethylhexanedioate)	0	6	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	174.2	6
isobutyl acrylate {2-propenoic acid}	0	4	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	128.17	6
butyl methacrylate	0	5	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	142.2	7
dipropyl phthalate	0	7	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	250.3	7
2-butoxyethyl acetate (ethylene glycol but	0	5	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	160.21	7
ethylhexanoate (ethyl n-hexanoate)	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	144.21	7
substituted c9 ester (c12)	0	7	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	216.32	7
substituted c7 ester (c12)	0	7	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	216.32	7
methylethylpentanoate	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	144.21	7
methyl amyl acetate (4-methyl-2-pentanol a	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	144.21	7
isobutyl isobutyrate	0	7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	144.21	7
dipropylene glycol methyl ether acetate	0	6	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	190.24	8
2-Ethyl-Hexyl Acrylate	0	6	1	0	0	0	0	0	0	0	0	3	0	0	0	0	0	184.28	8
butylisopropylphthalate	0	8	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	264.32	8
dibutyl phthalate	0	9	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	278.35	9
diethylene glycol butyl ether acetate {2-2	0	9	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	204.27	9

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
isoamyl isobutyrate	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	158.24	9
methyl c11 ester	0	11	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	212.33	11
methyl dodecanoate {methyl laurate}	0	12	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	214.35	12
methyl c12 ester	0	12	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	228.38	12
methyl myristate {methyl tetradecanoate}	0	14	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	242.4	14
methyl c13 ester	0	14	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	242.4	14
methyl c15 ester	0	16	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	270.46	16
AROMATIC COMPOUNDS - examples																			
benzene	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	78.11	1
nitrobenzene	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	123.11	1
aniline {aminobenzene}	0	0	0	0	0.75	0	0	0	0	0	0	0	0	0	0	0	0	93.13	6
toluene	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	92.14	7
methylphenanthrenes	0	0	0	1	0	0	0	0	0	0	0	8	0	0	0	0	0	192.26	7
c2 alkylphenanthrenes	0	0	0	1	0	0	0	0	0	0	0	3	0	0	0	0	0	206.28	7
c2 alkylanthracenes	0	0	0	1	0	0	0	0	0	0	0	3	0	0	0	0	0	206.28	7
biphenyl {phenyl benzene}	0	0	0	1	0	0	0	0	0	0	0	5	0	0	0	0	0	154.21	7
o-xylene	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	106.17	8
m-xylene	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	106.17	8
p-xylene	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	106.17	8
m-xylene and p-xylene	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	106.17	8
benzo[ghi]fluoranthene	0	0	0	0	1	0	0	0	0	0	0	10	0	0	0	0	0	226.28	8
benzo(a)anthracene	0	0	0	0	1	0	0	0	0	0	0	10	0	0	0	0	0	228.29	8
chrysene	0	0	0	0	1	0	0	0	0	0	0	10	0	0	0	0	0	228.29	8
benzo(c)phenanthrene	0	0	0	0	1	0	0	0	0	0	0	10	0	0	0	0	0	228.29	8
methylbenzphenanthrene	0	0	0	0	1	0	0	0	0	0	0	11	0	0	0	0	0	242.32	8
styrene	0	0	0.5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	104.15	8
methylbenzanthracenes	0	0	0	0	1	0	0	0	0	0	0	11	0	0	0	0	0	242.32	8
isomers of xylene	0	0.25	0	0.25	0.75	0	0	0	0	0	0	0	0	0	0	0	0	106.17	8
ethylbenzene	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	106.17	8
methyl biphenyl (mixed) {phenyltoluene}	0	0	0	0	1	0	0	0	0	0	0	5	0	0	0	0	0	168.24	8
methylchrysenes	0	0	0	0	1	0	0	0	0	0	0	11	0	0	0	0	0	242.32	8
indene	0	0	0.5	0	1	0	0	0	0	0	0	0	0	0	0	0	0	116.16	9
1,3,5-trimethylbenzene	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
1,2,4-trimethylbenzene	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
1,2,3-trimethylbenzene	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
trimethylbenzenes	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
ethyltoluenes {methylethylbenzenes}	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
o-ethyltoluene	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
m-ethyltoluene	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
p-ethyltoluene	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
c9 alkyl benzenes	0	1.38	0	0.38	0.62	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
t-butylbenzene	0	2	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	134.22	9
Isomers of propylbenzene	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
n-propylbenzene	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
cumene (isopropyl benzene)	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	120.2	9
methyl styrene (mixed) {vinyl toluene}	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	118.18	9

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
indan	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	118.18	9
cumene hydroperoxide	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	152.19	9
Butylbenzene isomers	0	2.9	0	1	0	0	0	0	0	0	0	0.1	0	0	0	0	0	134.22	9.9
c3/c4/c5 alkylbenzenes	0	2.25	0	0.32	0.68	0	0	0	0	0	0	0	0	0	0	0	0	133.24	9.93
methylindans	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	132.21	10
camphene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	136.24	10
methylindene	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	130.19	10
divinyl benzene {vinyl styrene}	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	130.19	10
1,3-diethylbenzene (meta)	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
1,2-diethylbenzene (ortho)	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
1,2,3,4-tetramethylbenzene	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
ethyldimethylbenzenes	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
tetramethylbenzenes	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
1-methyl-2-tert-butylbenzene	0	2	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	148.25	10
1-methyl-4-isopropylbenzene	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
1-methyl-3n-propylbenzene	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
1-methyl-3-isopropylbenzene	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
napthalene	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	128.17	10
dihydronaphthalene	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	130.19	10
1-methyl naphthalene	0	2	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	142.2	10
diethylbenzenes	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
(1-methylpropyl)benzene (sec-butyl benzene	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
n-butylbenzene	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
(2-methylpropyl)benzene	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
ethyl styrene {ethylvinyl benzene}	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	132.21	10
c4 alkylstyrenes	0	1	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	160.26	10
1,3-diethylbenzene (meta)	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
1,2-diethylbenzene (ortho)	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
c10 aromatics	0	2.25	0	0.25	0.75	0	0	0	0	0	0	0	0	0	0	0	0	134.22	10
methylnaphthalenes	0	2.5	0	0	1	0	0	0	0	0	0	0.5	0	0	0	0	0	142.2	10.5
dimethylindans	0	3	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	146.23	11
dimethylindene	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	144.22	11
c3 alkylstyrene	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	146.23	11
c11 unsaturated alkylbenzenes	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	146.23	11
1-(1,1-dimethylethyl)-3,5-dimethylbenzene	0	3	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	162.28	11
methoxynaphthalene	0	3	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	158.2	11
methyldihydronaphthalene	0	3	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	144.22	11
c11 alkylbenzenes	0	3.33	0	0.33	0.67	0	0	0	0	0	0	0	0	0	0	0	0	148.25	11
n-pentylbenzene	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	148.25	11
c2 alkyl indan	0	3	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	146.23	11
ethylindan	0	3	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	146.23	11
diisopropyl benzene (mixed isomers)	0	4	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	162.28	12
acenaphthylene	0	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	152.2	12
c2 alkylnaphthalene	0	4	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	156.23	12
acenaphthene	0	4	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	154.21	12
c12 dialkyl benzenes	0	4	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	162.28	12
dimethyl napthalenes	0	4	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	156.23	12

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
ethylnaphthalenes	0	4	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	156.23	12
trimethylindan	0	4	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	160.26	12
propylnaphthalene	0	5	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	170.26	13
trimethylnaphthalene	0	5	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	170.26	13
fluorene	0	5	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	166.22	13
c13 alkyl benzenes	0	5.33	0	0.33	0.67	0	0	0	0	0	0	0	0	0	0	0	0	176.3	13
anthracene	0	2	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	178.23	14
diphenyl ethane {bibenzyl}	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	182.27	14
methylanthracenes	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	192.26	15
fluoranthene	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	202.26	16
pyrene	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	202.26	16
cyclopentaphenanthrenes	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	204.27	16
cyclopentaanthracenes	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	204.27	16
phenylnaphthalenes	0	1	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	204.27	16
ethyl-phenyl-phenyl-ethane	0	1	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	210.32	16
methylfluoranthenes	0	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	216.28	17
di(ethylphenyl)ethane	0	4	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	238.37	18
cyclopenta[cd]pyrene	0	2	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	228.29	18
HALOGENATED COMPOUNDS - examples																			
methyl chloride	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	50.49	0
carbon tetrachloride	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	153.82	0
dichlorodifluoromethane (f-12)	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	120.91	0
chlorotrifluoromethane (f-13)	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	104.46	0
1,1-dichloroethane	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	98.96	0
1,1,1-trichloroethane	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	133.41	0
1,1,2-trichloroethane	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	133.41	0
dichlorotetrafluoroethane	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	170.92	0
ethyl chloride	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	64.52	0
ethylene dichloride	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	98.96	0
chloropentafluoroethane (f115)	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	154.47	0
hexafluoroethane {f-116}	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	138.01	0
methylene bromide	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	173.85	0
ethylene dibromide	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	187.87	0
methyl bromide	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	94.94	0
1,2-dichloro-1,1,2,2-tetrafluoroethane {cf	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	170.92	0
chlorodifluoromethane (f-22)	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	86.47	0
trifluoromethane (f-23)	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	70.01	0
chlorofluorohydrocarbons	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	187.38	0
trichlorotrifluoroethane-f113	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	187.38	0
chloroform	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	119.38	0
trichlorofluoromethane	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	137.37	0
Iodomethane	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	141.94	0
dichloromethane {methylene chloride}	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	84.93	0
tetrafluoromethane {carbon tetrafluoride}	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	88	0
perchloroethylene	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	165.83	0
2,2-dichloronitroaniline	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	207.02	1

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
bromodinitroaniline {2,4-dinitro-6-bromoan	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	262.03	1
bromodinitrobenzene	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	247.01	1
chlorobenzene	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	112.56	1
o-dichlorobenzene	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	147	1
1,3-dichlorobenzene {m-dichlorobenzene}	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	147	1
p-dichlorobenzene	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	147	1
dichlorobenzenes	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	147	1
trichlorobenzenes (mixed)	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	181.45	1
tetrachlorobenzenes	0	1	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	215.89	1
propylene dichloride	0	1.5	0	0	0	0	0	0	0	0	0	1.5	0	0	0	0	0	112.99	1.5
1,3-Dichloropropane	0	1.5	0	0	0	0	0	0	0	0	0	1.5	0	0	0	0	0	112.99	1.5
vinyl chloride	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	62.5	2
1,1-dichloroethene {vinylidene chloride}	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	96.94	2
trichloroethylene (tce)	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	131.39	2
Chloropropane	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	78.54	3
epichlorohydrin	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	92.53	3
Glycerol alpha-monochlorohydrin	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	110.54	3
chloroprene (2-chloro-1,3-butadiene)	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	88.54	4
1-chlorobutane	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	92.57	4
benzyl chloride	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	126.59	7
Benzoyl chloride	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	140.57	7
3-(chloromethyl)-heptane	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	148.68	8
NITROGEN containing compounds - examples																			
nitroethane	0	0.4	0	0	0	0	0	0	0	0	0	1.6	0	0	0	0	0	75.07	0.4
methylamine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0	31.06	1
pyridine	0	1	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	79.1	1
phenyl isocyanate	0	1	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	119.12	1
acetonitrile	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	41.05	1
hydroxyacetonitrile	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	57.05	1
Monomethyl Hydrazine	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	46.07	1
Nitropropanes	0	1.5	0	0	0	0	0	0	0	0	0	1.5	0	0	0	0	0	89.09	1.5
dimethyl formamide	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	73.1	2
ethylene diamine	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	60.1	2
ethanolamine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	61.08	2
ethylamine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	45.09	2
dimethylamine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	45.09	2
ethyleneamines	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	43.07	2
trimethyl amine	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	59.11	3
tert-butyl amine	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	73.14	3
isopropylamine	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	59.11	3
dimethyl alkyl amines	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	59.11	3
acrylonitrile	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	53.06	3
Isobutyronitrile	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	69.11	3
butyronitrile	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	69.11	3
N,N-Dimethylacetoacetamide	0	2	0	0	0	0	0	0	0	0	0	2	0	0	0	1	0	129.16	4
dimethylacetamide	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	87.12	4

Table 1. Matrix of Assignments from Real Compounds to Carbon Bond 05 (CB05) Model Species

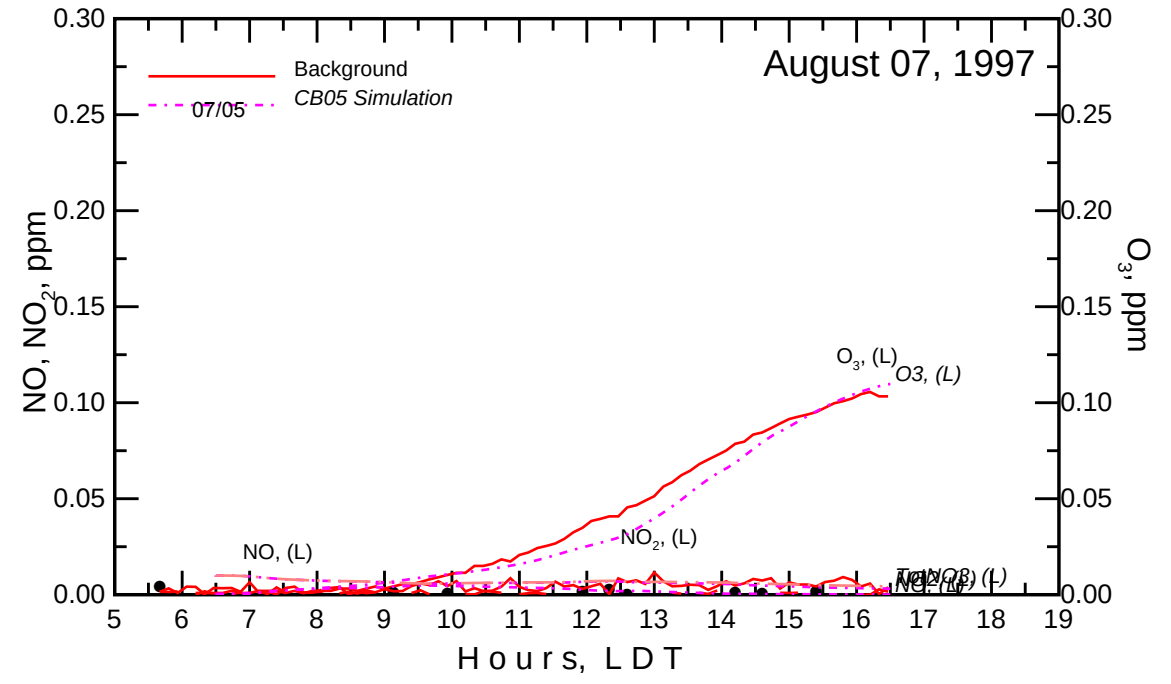
name	NASN	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	NR	CH4	ETHA	IOLE	ALDX	TERP	MW	# carbons
N-(2-Hydroxyethyl)ethylenediamine	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	104.15	4
diethanolamine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	105.14	4
n,n-dimethylethanolamine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	89.14	4
diethylenetriamine	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	103.17	4
diethylamine	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	73.14	4
n-Butylamine	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	73.14	4
2-methyl-3-butenenitrile	0	2	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	81.12	4
methyl glutaronitrile	0	4	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	108.14	4
morpholine (tetrahydro-1,4-oxazin)	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	87.12	4
caprolactam	0	5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	113.16	5
1,4-Diazabicyclo[2.2.2]octane	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	112.18	6
hexamethylenediamine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	116.21	6
cyclohexamine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	99.18	6
hexamethyleneimine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	99.18	6
Diisopropanolamine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	133.19	6
triethanolamine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	149.19	6
triethylene tetramine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	146.24	6
triethylamine	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	101.19	6
n-Hexylamine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	101.19	6
N-aminoethylpiperazine	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	129.21	6
n-phenylaniline {diphenylamine}	0	0	0	1	0	0	0	0	0	0	0	5	0	0	0	0	0	169.23	7
4-methylaniline	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	107.16	7
toluene isocyanate	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	133.15	7
2,4-toluene diisocyanate {tdi}	0	0	0	1	0	0	0	0	0	0	0	2	0	0	0	0	0	174.16	7
2,4-Dinitrotoluene	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	182.14	7
benzothiazole	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	135.19	7
Tetraethylenepentamine	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	189.31	8
4,4-methylene dianiline	0	1	0	1	0	0	0	0	0	0	0	5	0	0	0	0	0	198.27	8
dimethylnaphthyridine	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	158.2	10
SULFUR containing compounds - examples																			
carbonyl sulfide	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	60.07	0
carbon disulfide	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	76.14	1
methyl mercaptan	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	48.11	1
dimethyl sulfide	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	62.13	2
dimethyl disulfide	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	94.2	2
ethyl mercaptan	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	62.13	2
Diethyl Sulfate	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	154.19	4
Thiophene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	84.14	4

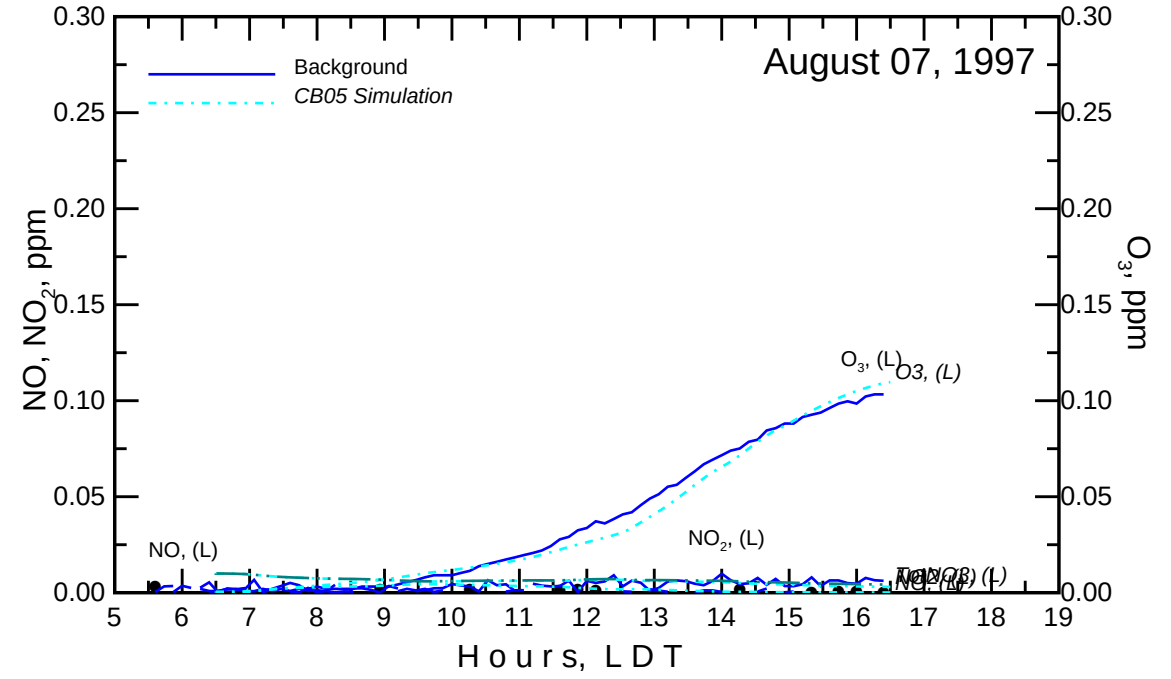
Appendix B

Chamber Simulations for the University of North Carolina (UNC) Chamber with CB05 Organized by Chemical Compound Type

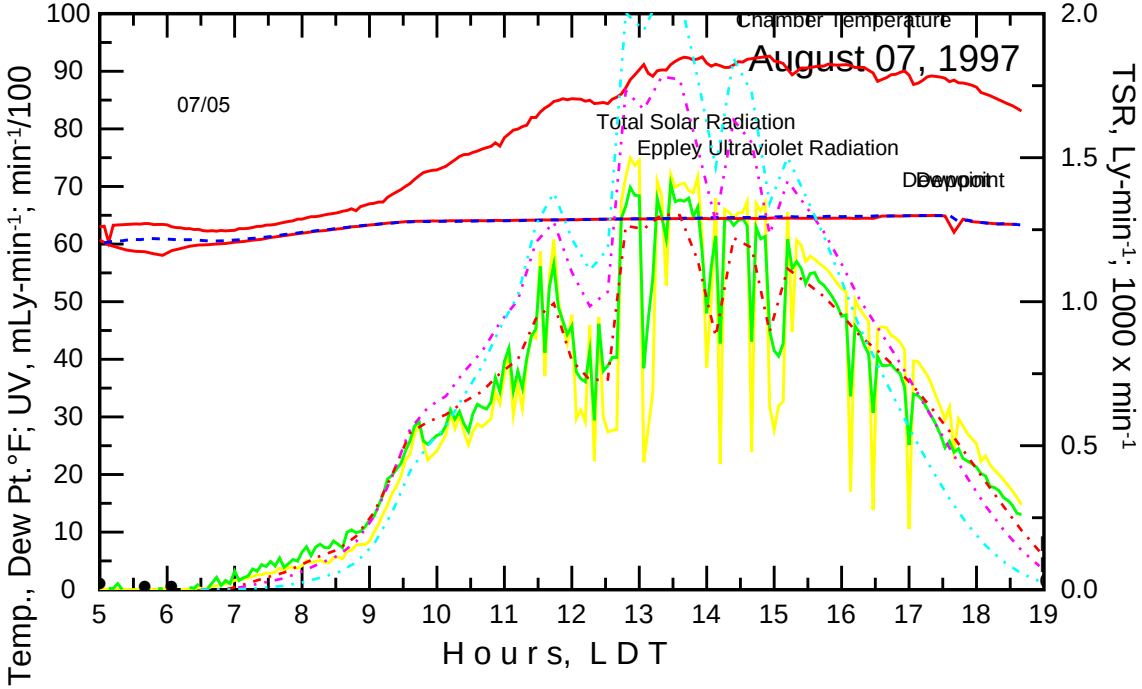
Chamber Background

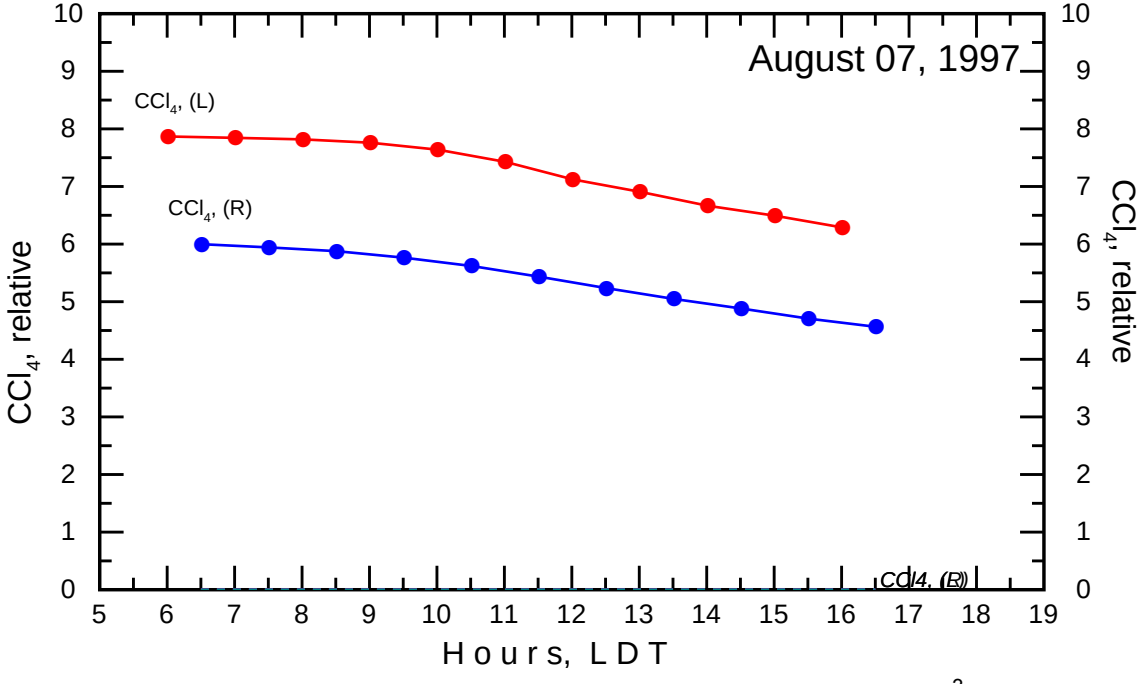
Au 07 97
OC 10 96

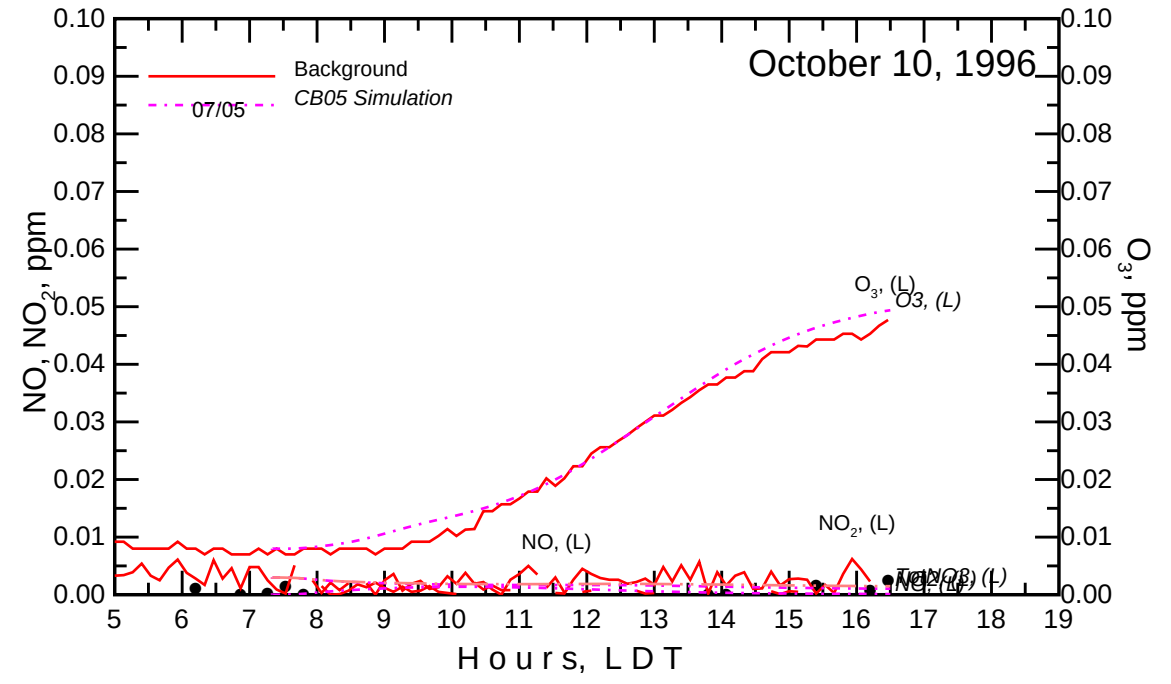

August 07, 1997
Background
CB05 Simulation
07/05
NO, NO2, ppm
O3, ppm
O3, (L)
NO2, (L)
NO, (L)
Hours, LDT

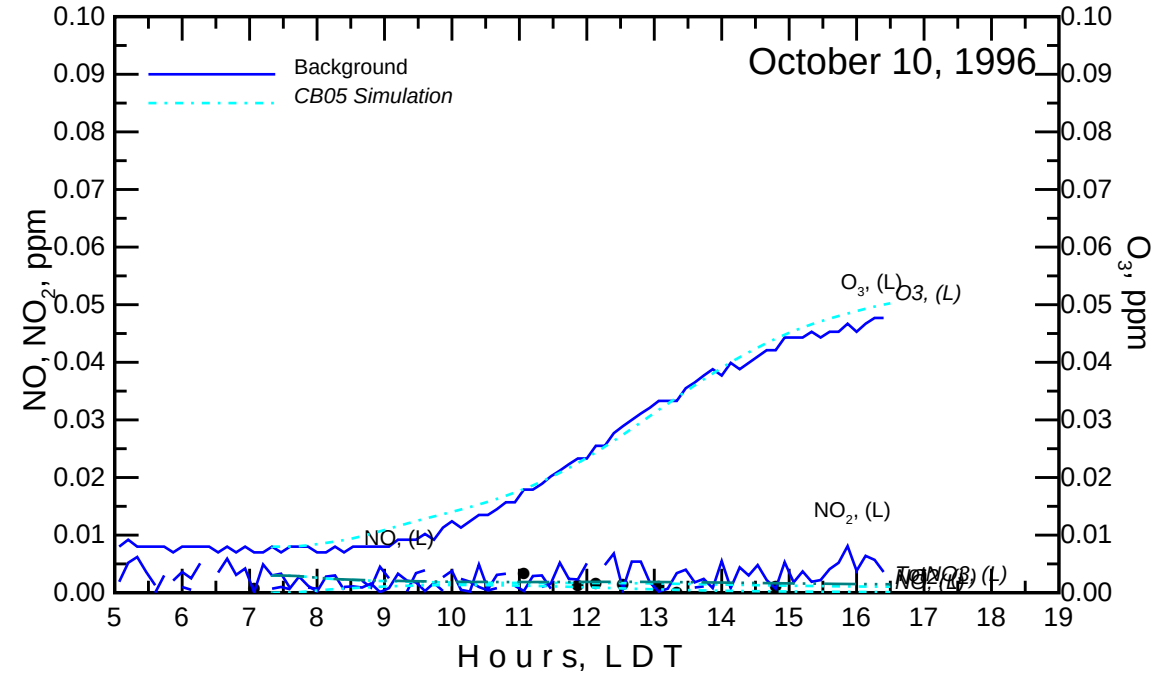

August 07, 1997
Background
CB05 Simulation
NO, NO2, ppm
O3, ppm
O3, (L)
NO2, (L)
NO, (L)
Hours, LDT

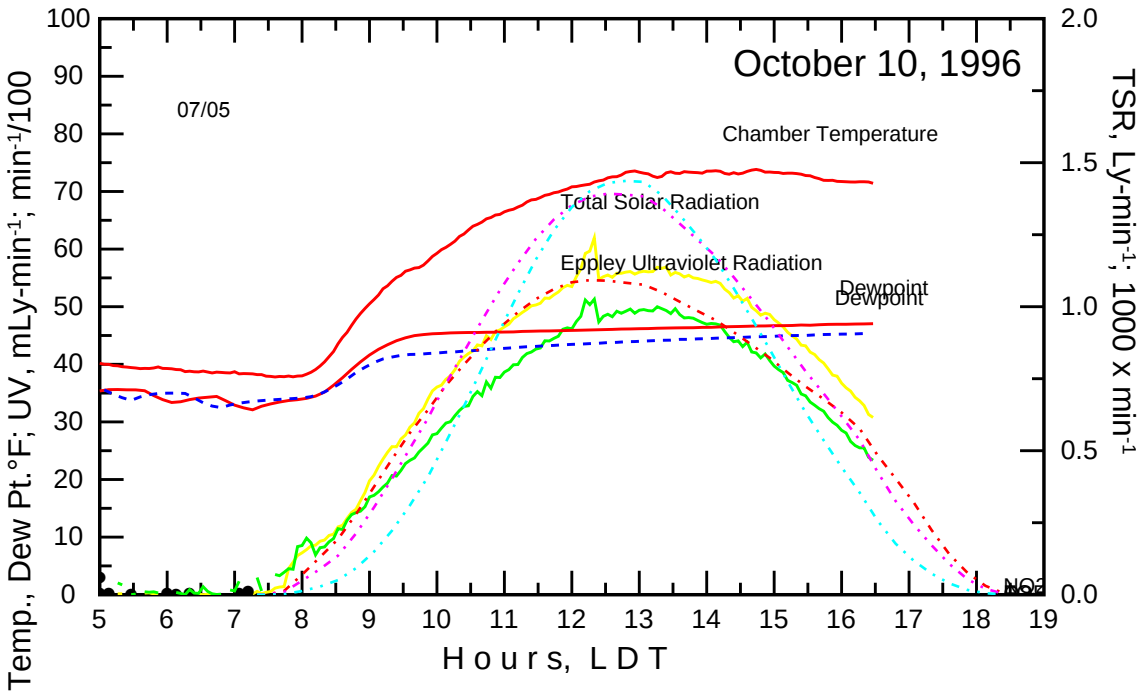
Background

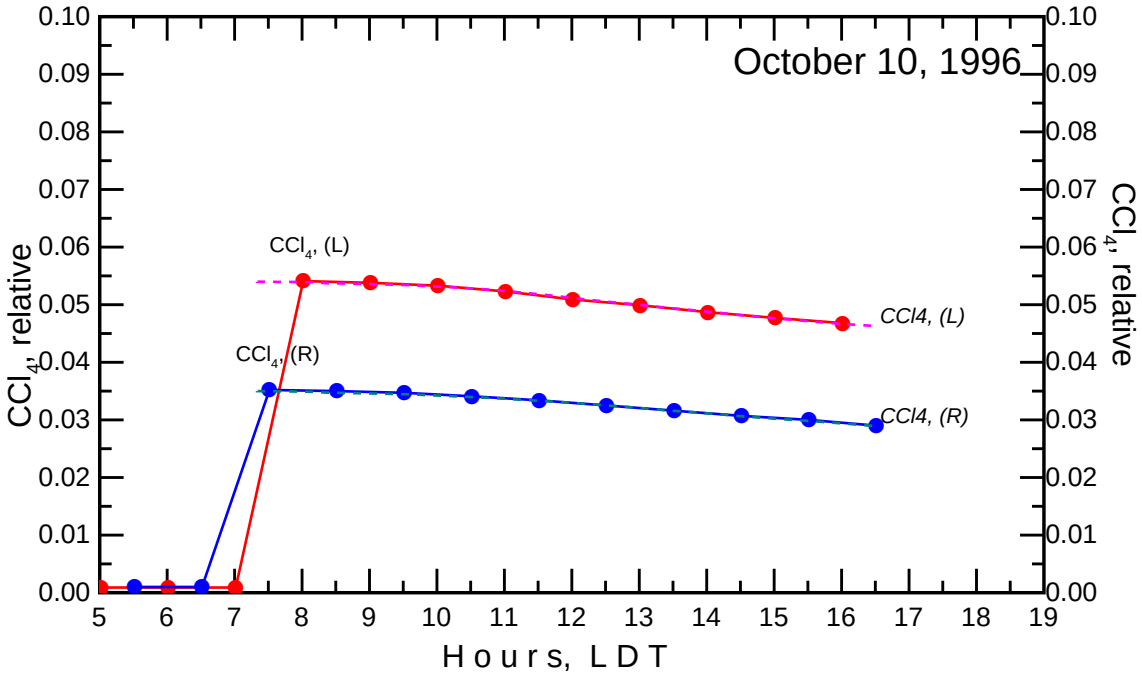

August 07, 1997
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


August 07, 1997
CCl4, (L)
CCl4, (R)
CCl4, relative
Hours, LDT


October 10, 1996
Background
CB05 Simulation
07/05
O3, (L)
NO, (L)
NO2, (L)
TotNO3, (L)
NO, NO2, ppm
O3, ppm
Hours, LDT

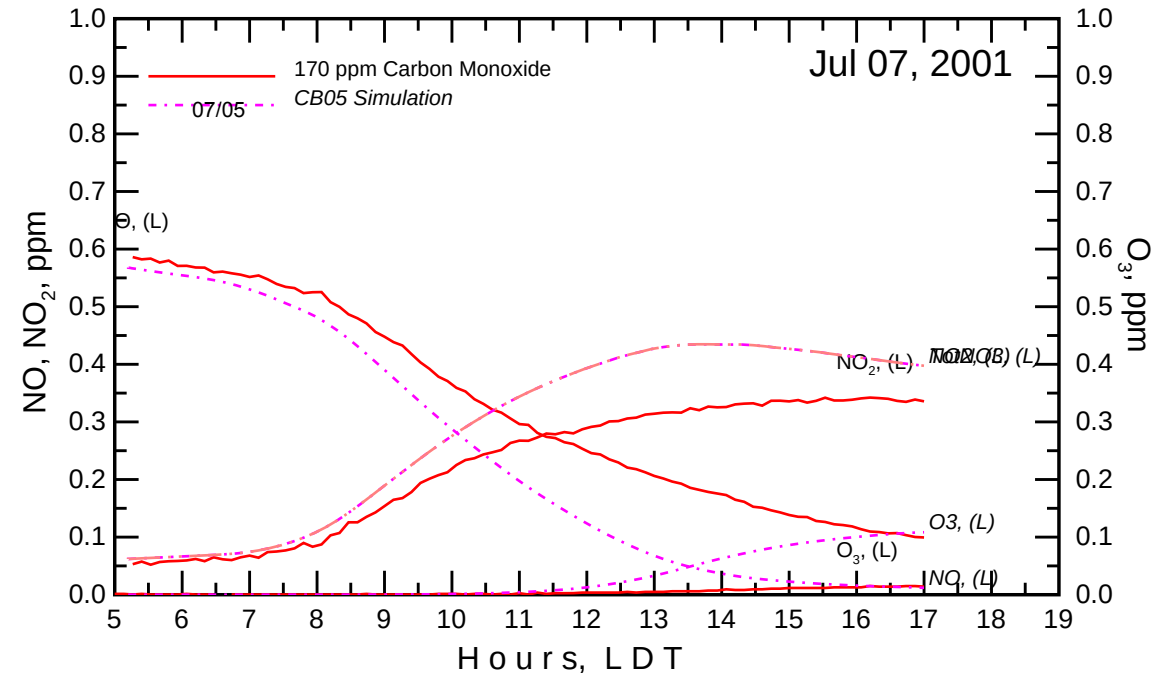

October 10, 1996
Background
CB05 Simulation
O3, (L)
NO, (L)
NO2, (L)
TotNO3, (L)
NO, NO2, ppm
O3, ppm
Hours, LDT

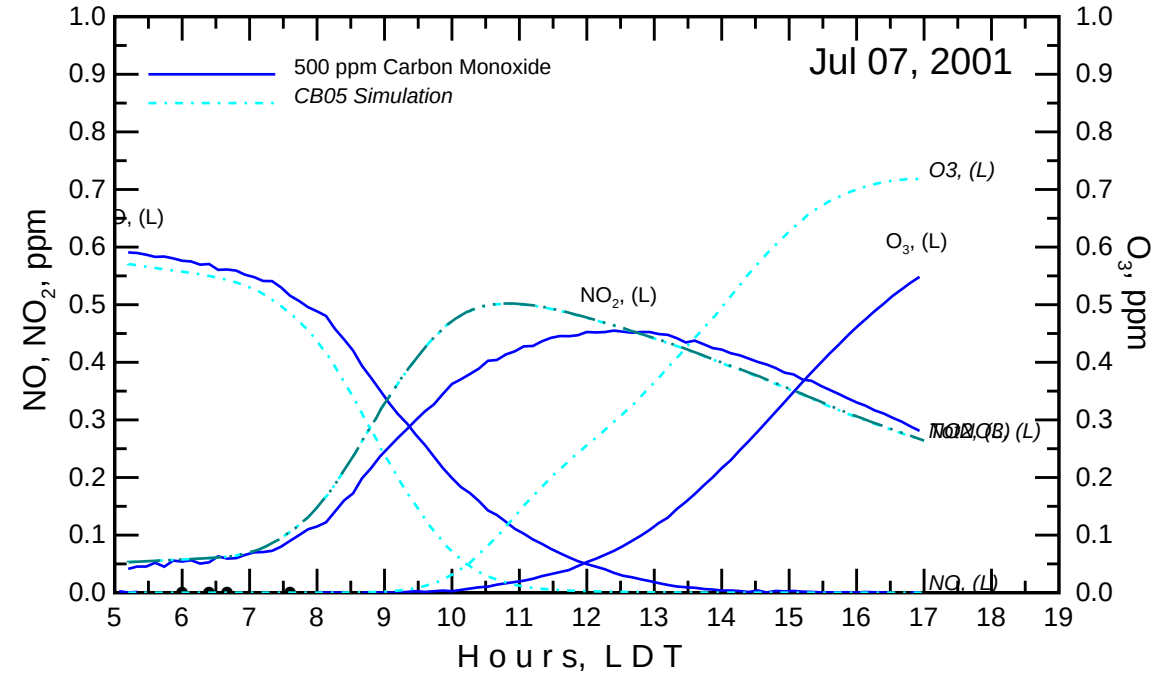

October 10, 1996
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
NO2
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


October 10, 1996
CCl4, (L)
CCl4, (R)
CCl4, (L)
CCl4, (R)
CCl4, relative
CCl4, relative
Hours, LDT

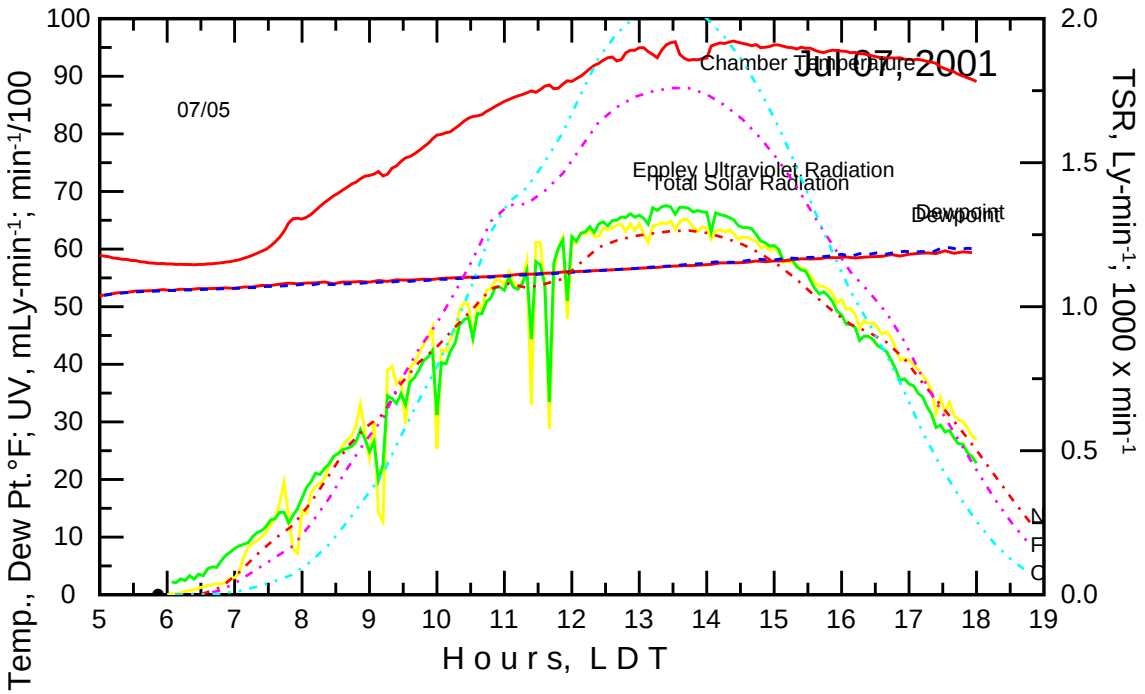
Carbon Monoxide (CO)

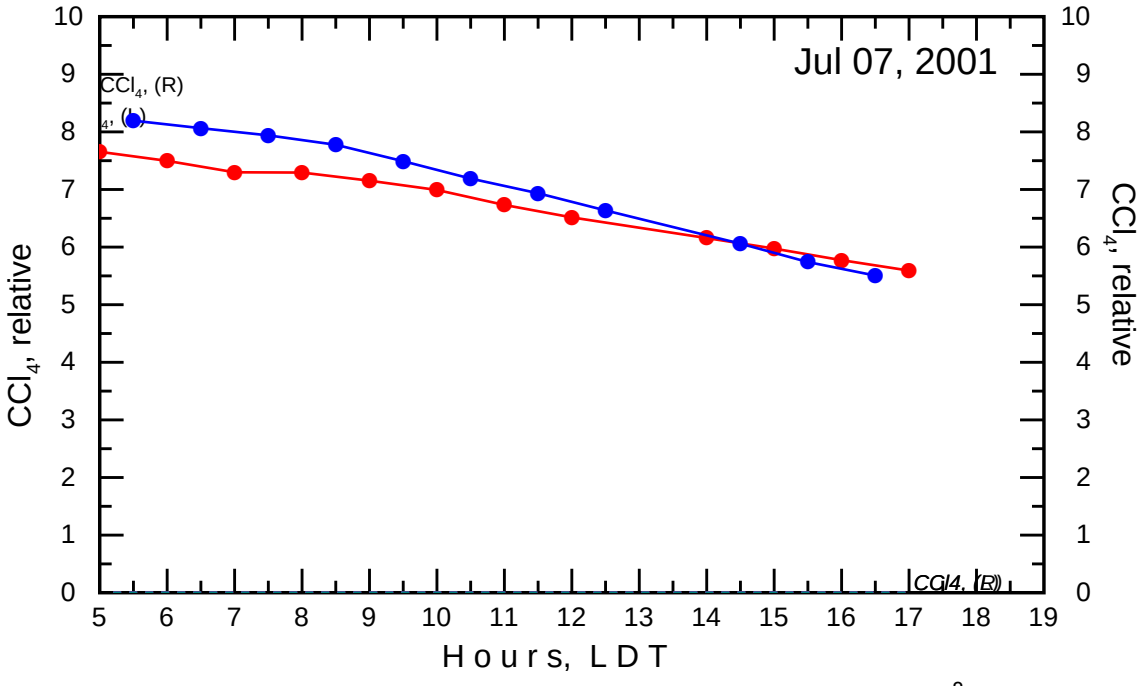
JL 07 01
JL 22 01
AU 30 93
ST 20 00
OC 03 95

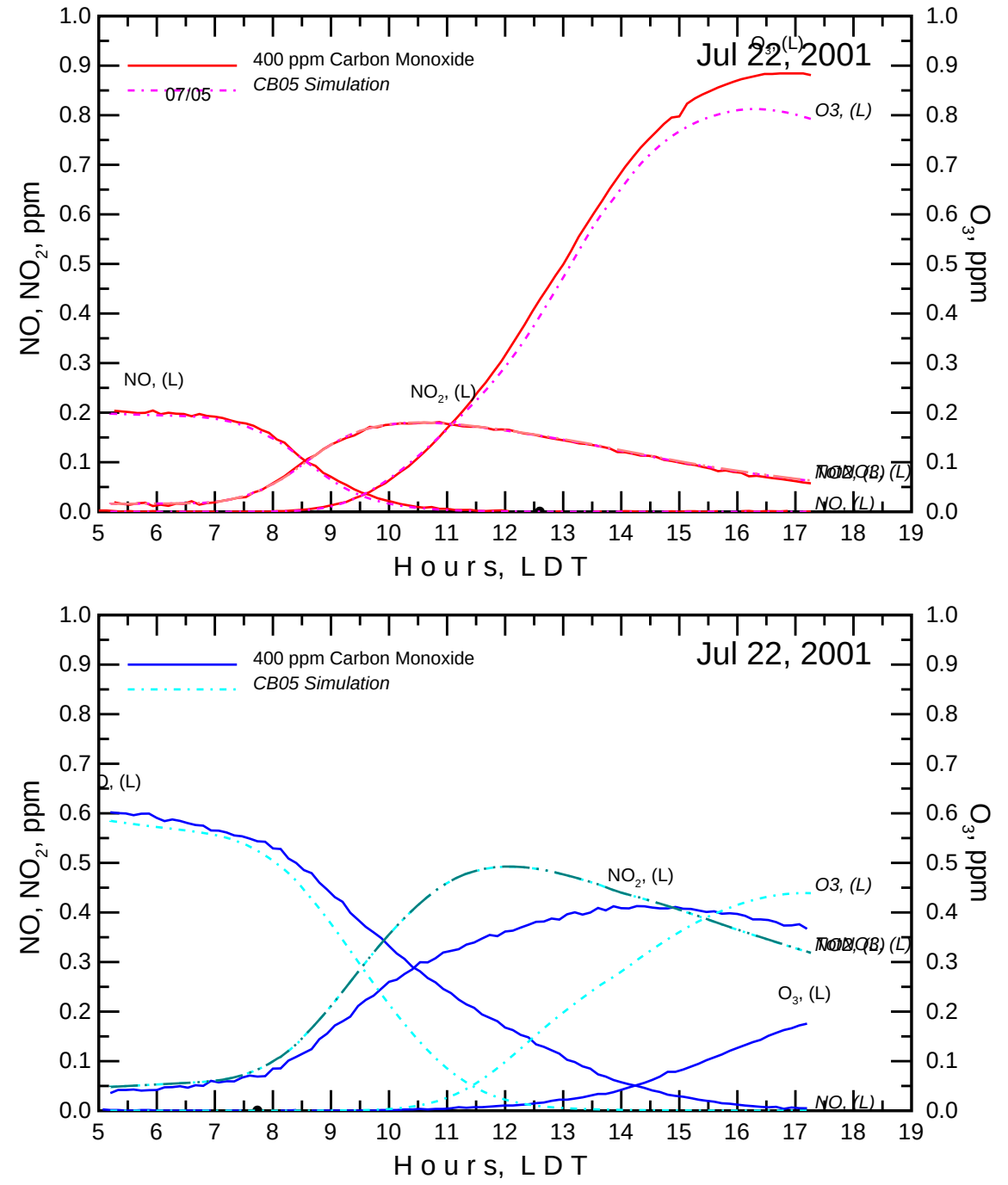




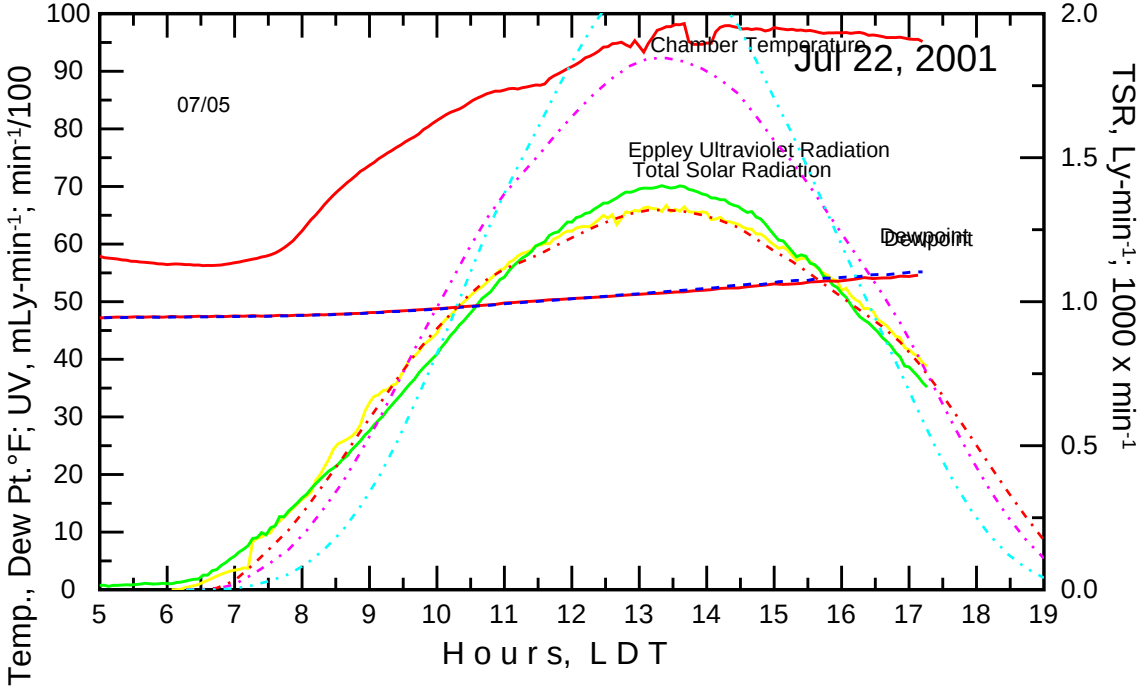
Delta CO (filtered); NOx Matched

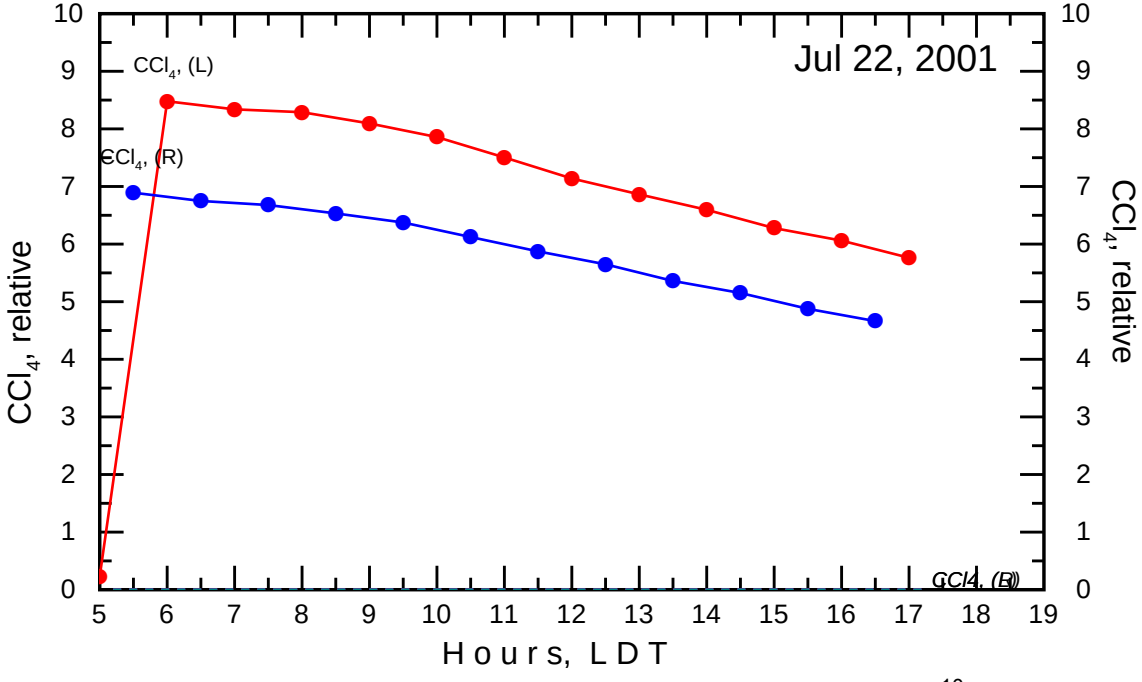

Jul 07, 2001
07/05
Chamber Temperature
Eppley Ultraviolet Radiation
Total Solar Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

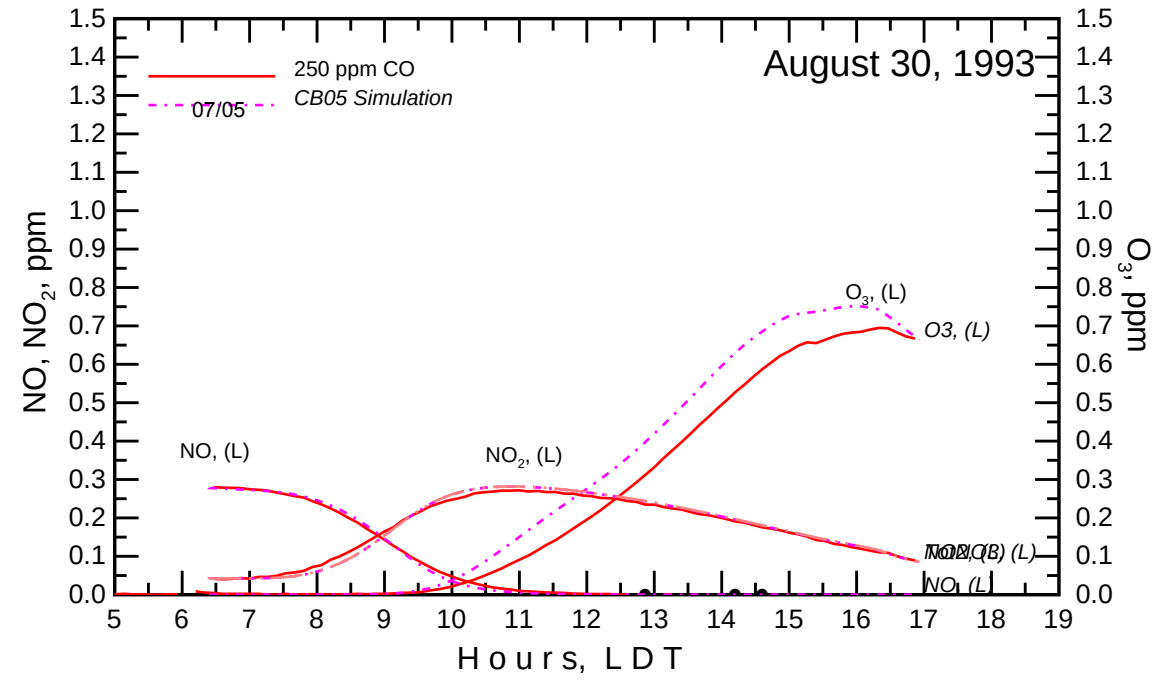

Jul 07, 2001
CCl4, (R)
CCl4, relative
Hours, LDT

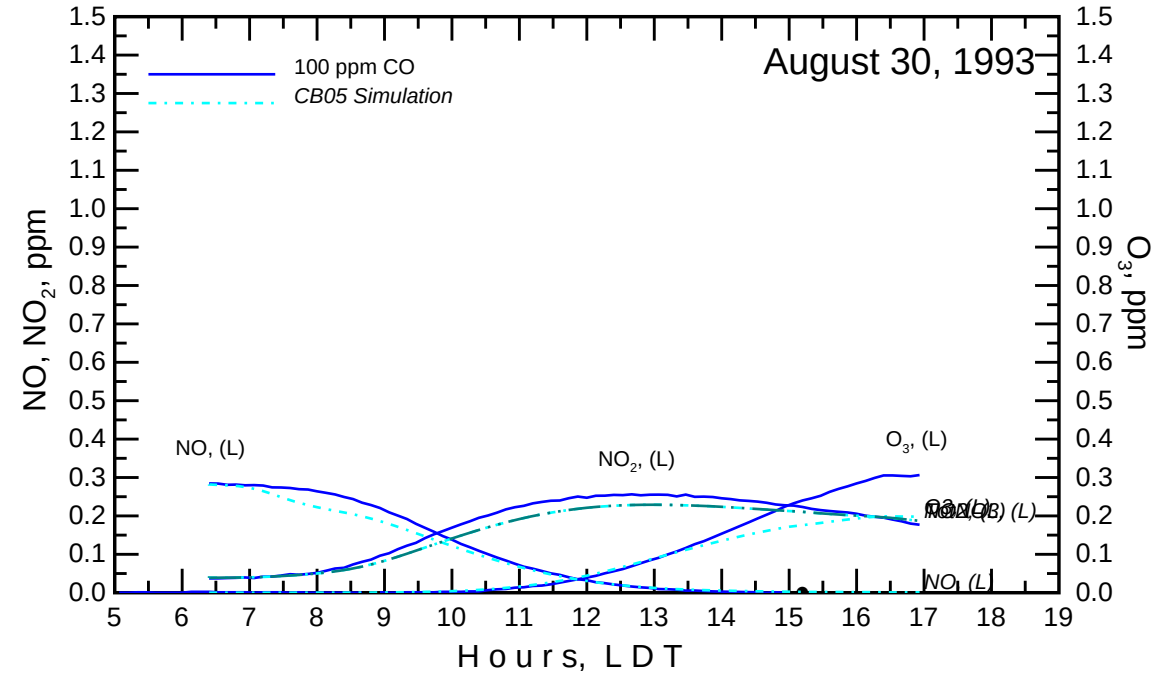


Matched Carbon Monoxide; Delta NOx

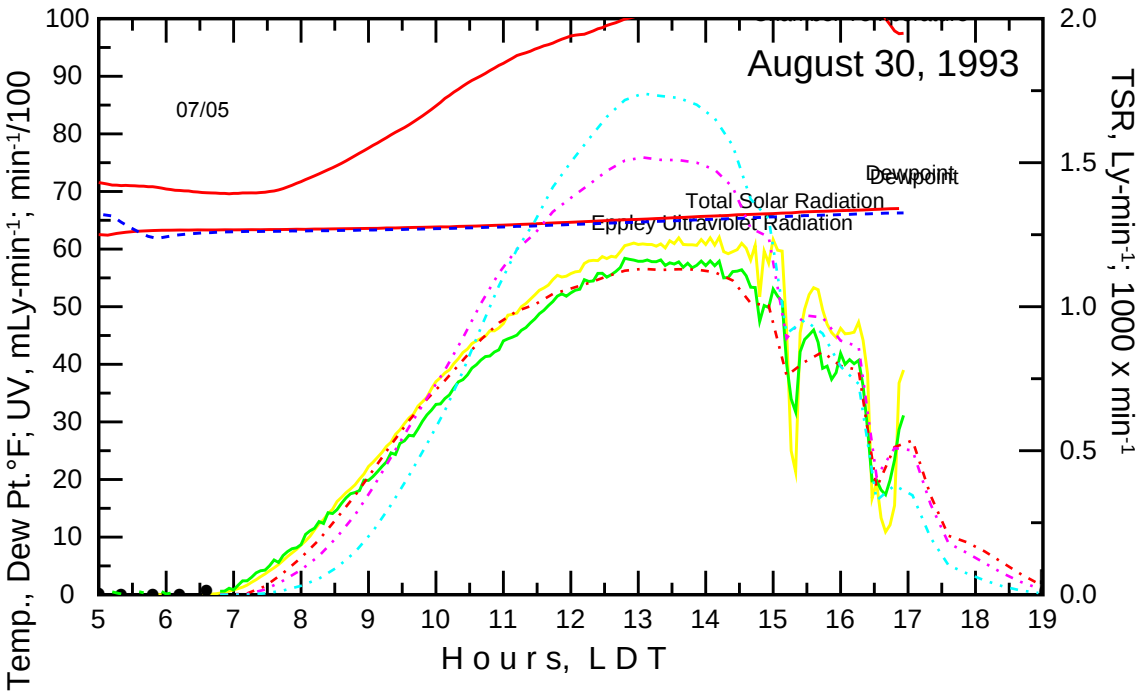

Jul 22, 2001
07/05
Chamber Temperature
Eppley Ultraviolet Radiation
Total Solar Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

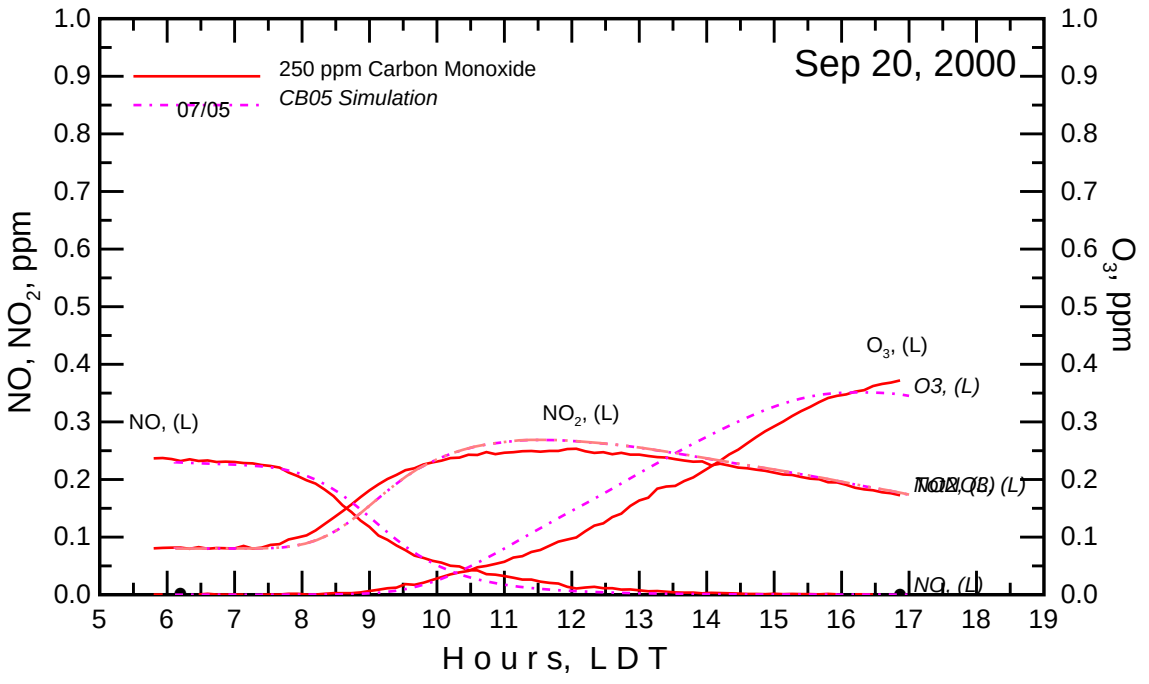

Jul 22, 2001
CCl4, (L)
CCl4, (R)
CCl4, relative
Hours, LDT

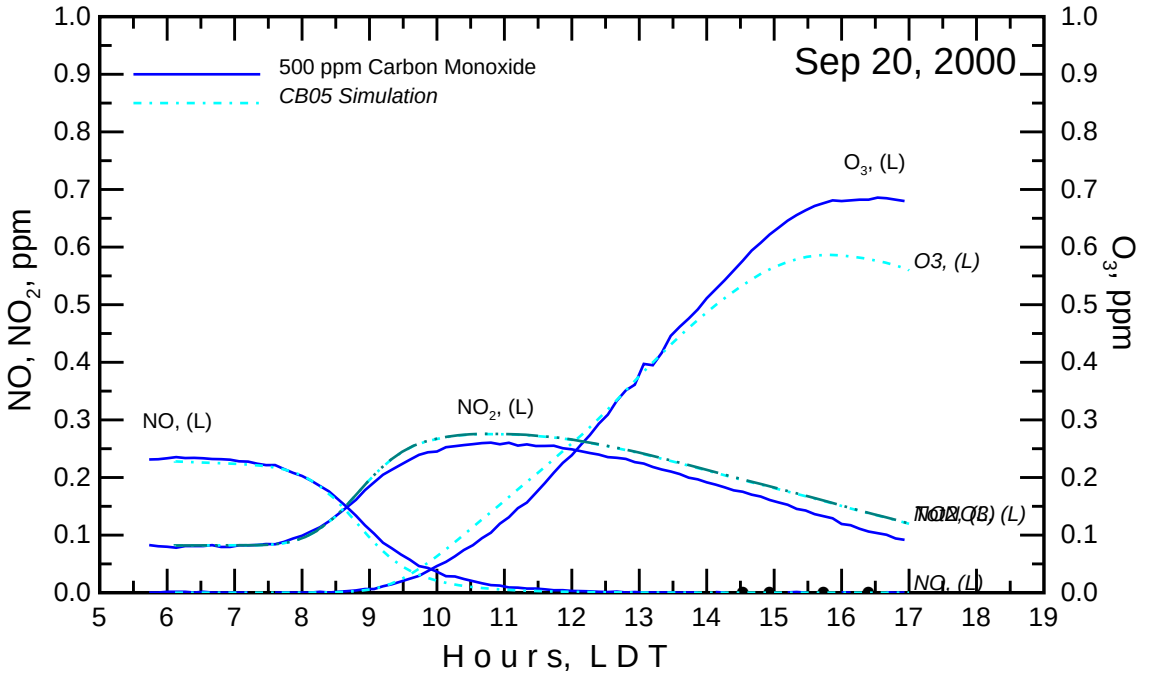

250 ppm CO
CB05 Simulation
07/05
August 30, 1993
NO, NO2, ppm
O3, ppm
O3, (L)
NO, (L)
NO2, (L)
NO, (L)
Hours, LDT


100 ppm CO
CB05 Simulation
August 30, 1993
NO, NO2, ppm
O3, ppm
O3, (L)
NO, (L)
NO2, (L)
NO, (L)
Hours, LDT

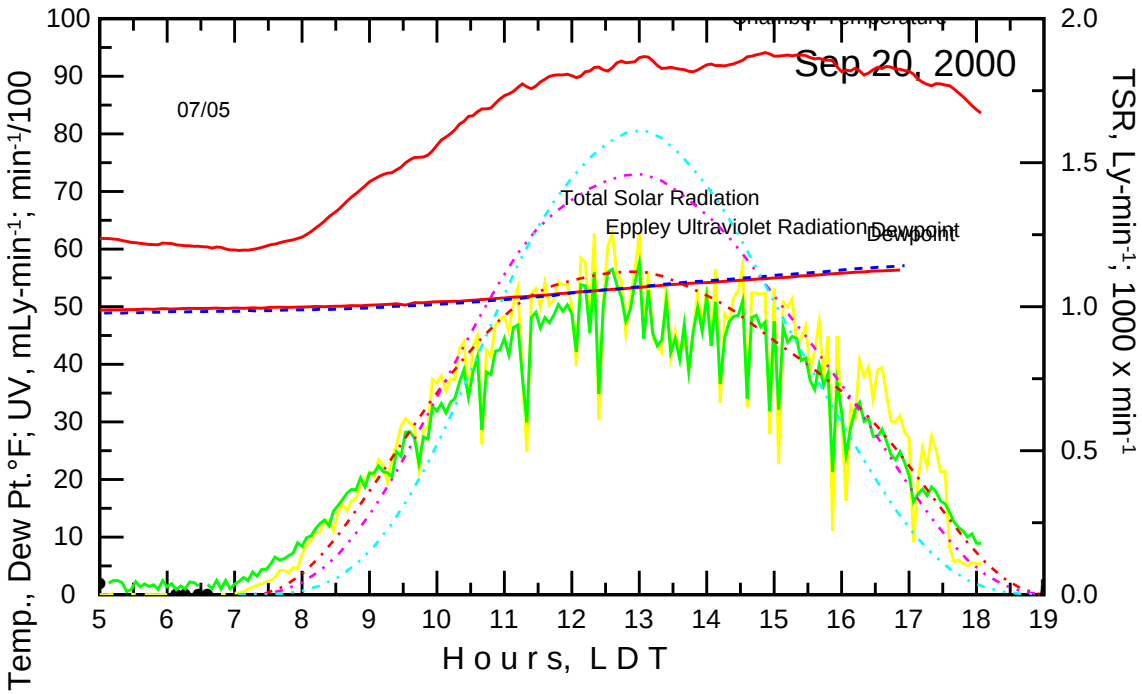
Delta CO

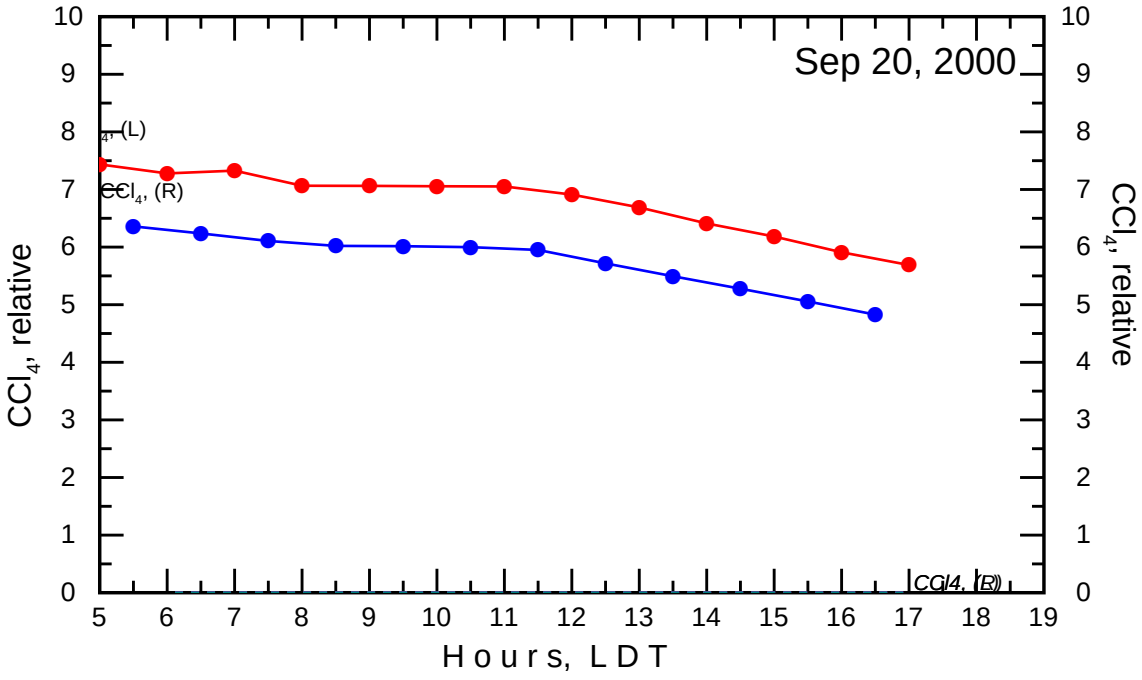

August 30, 1993
07/05
Dewpoint
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

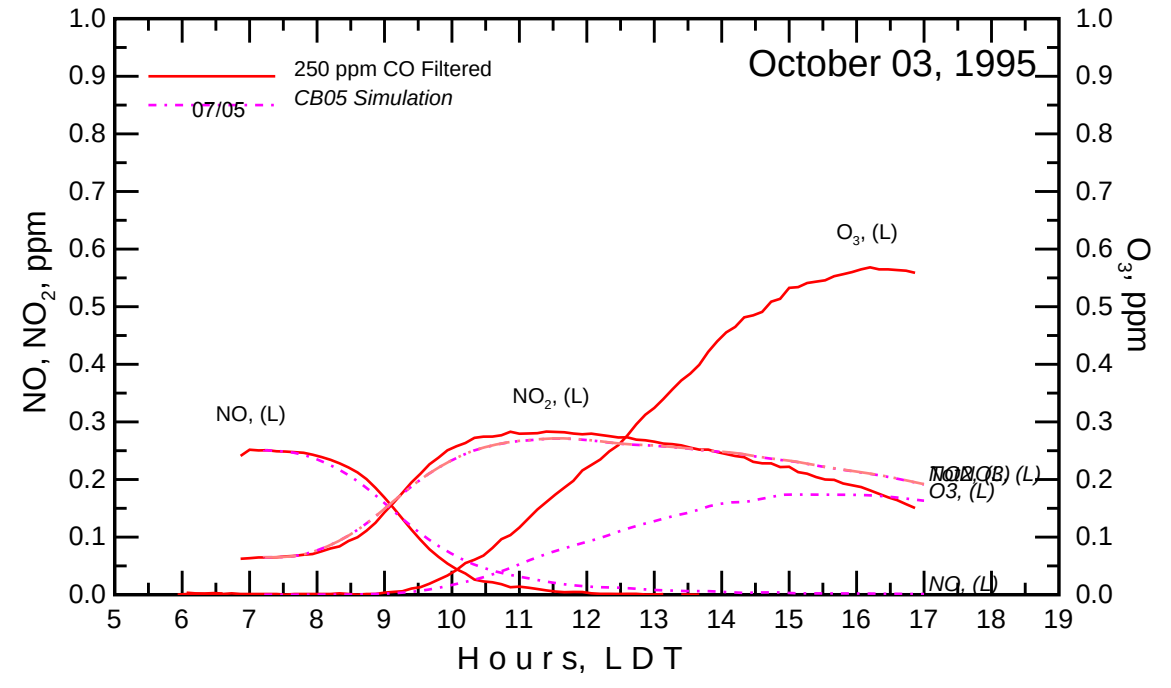


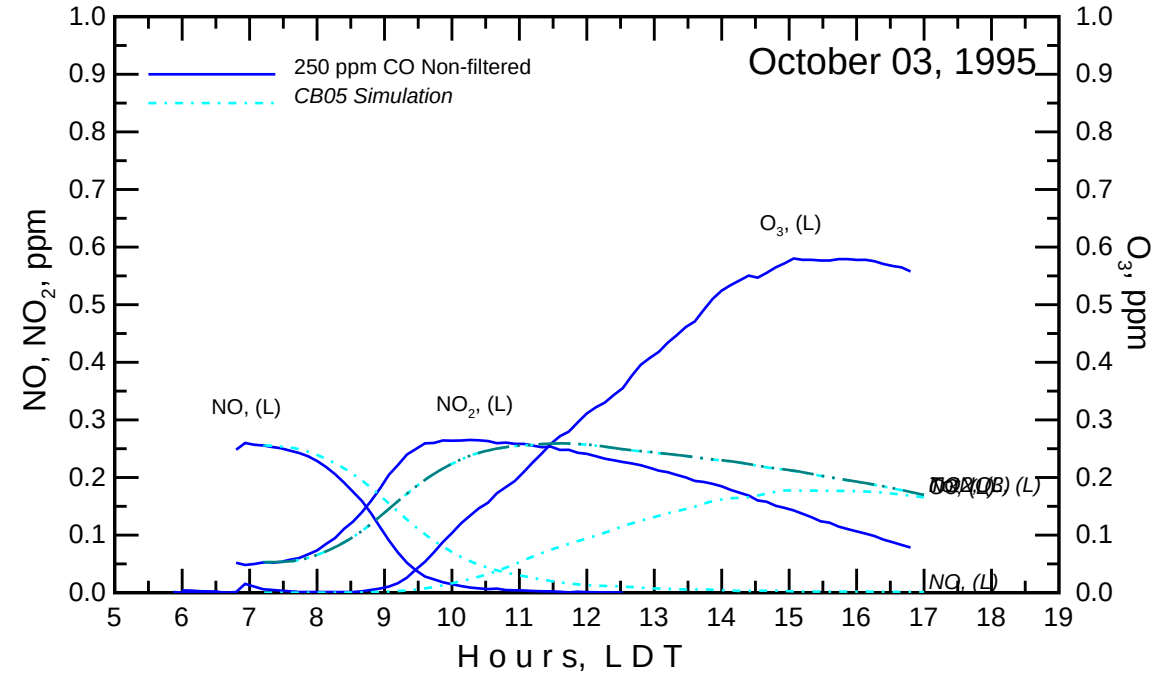


500 vs 250 ppm CO; matched 0.33 NOx

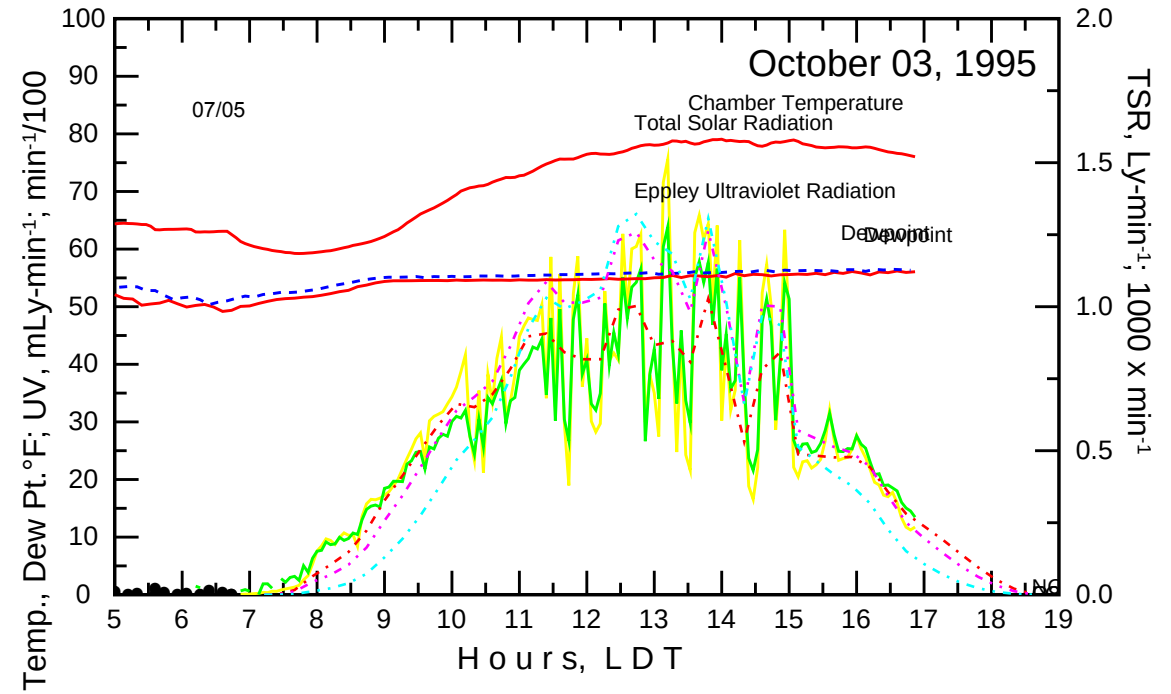

Sep 20, 2000
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

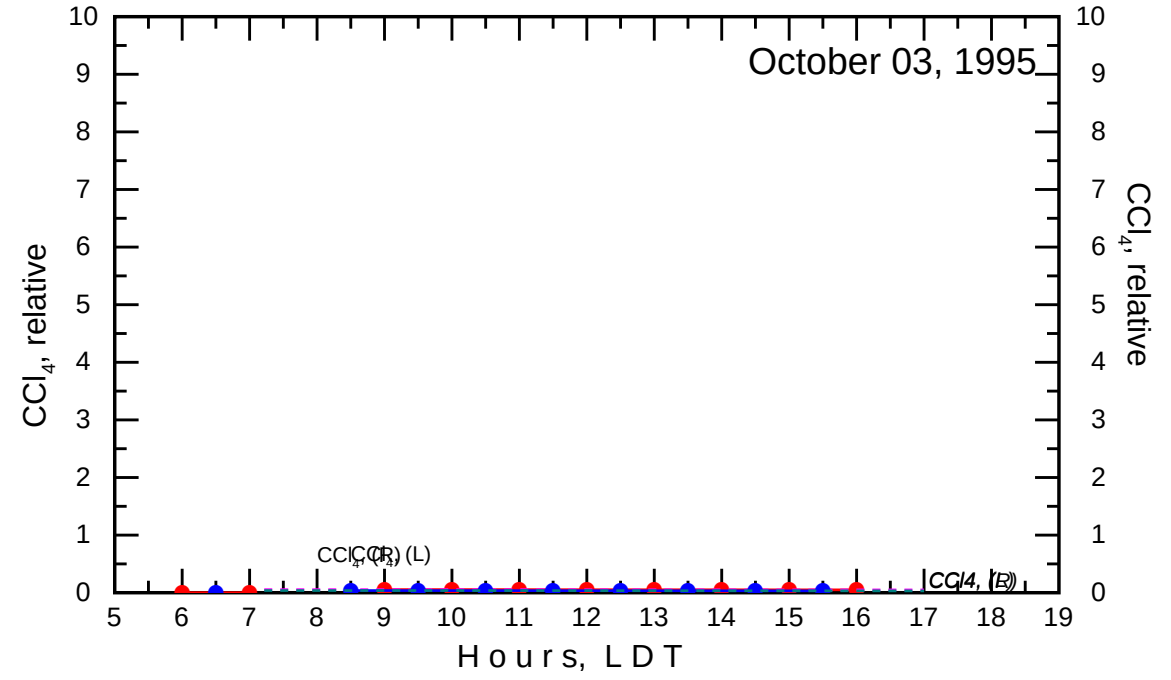

Sep 20, 2000
CCl4, (L)
CCl4, (R)
CCl4, relative
Hours, LDT

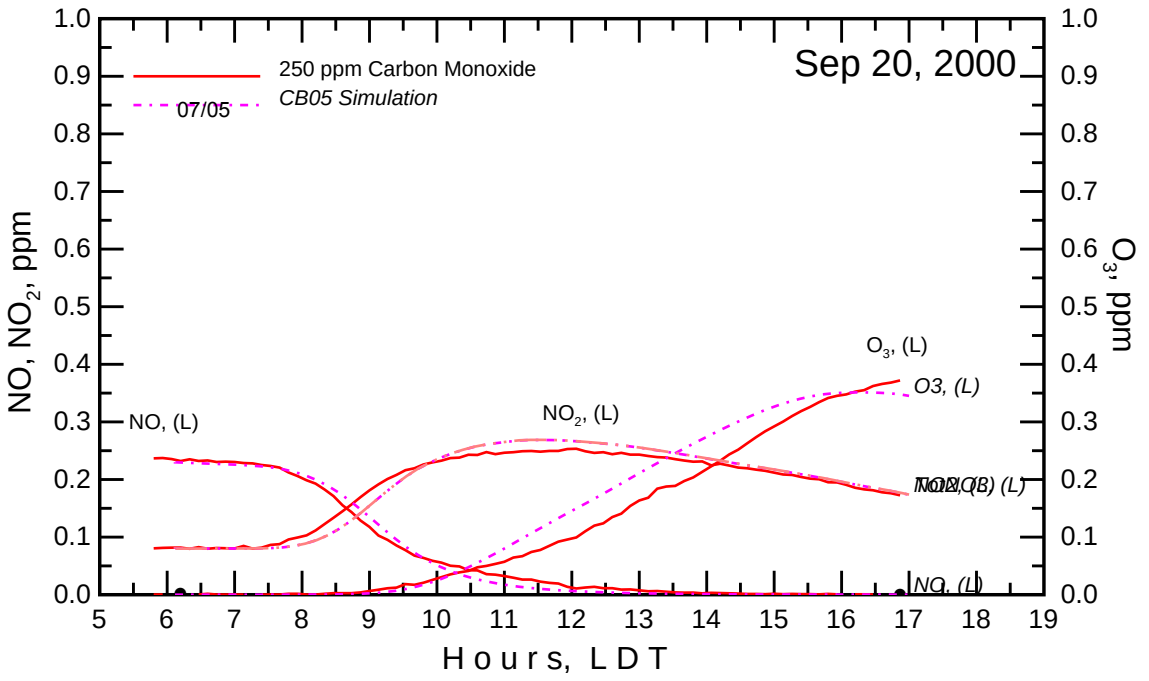


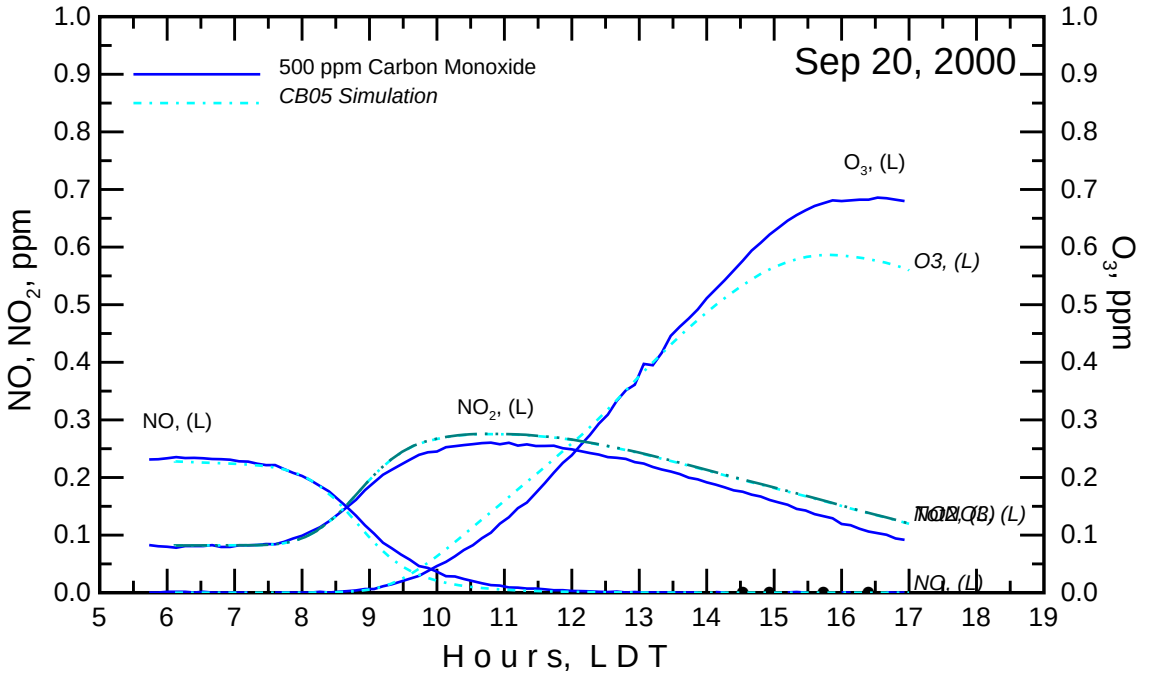


Matched CO and NOx; BLUE CO filtered with 13x Molesieve [15]

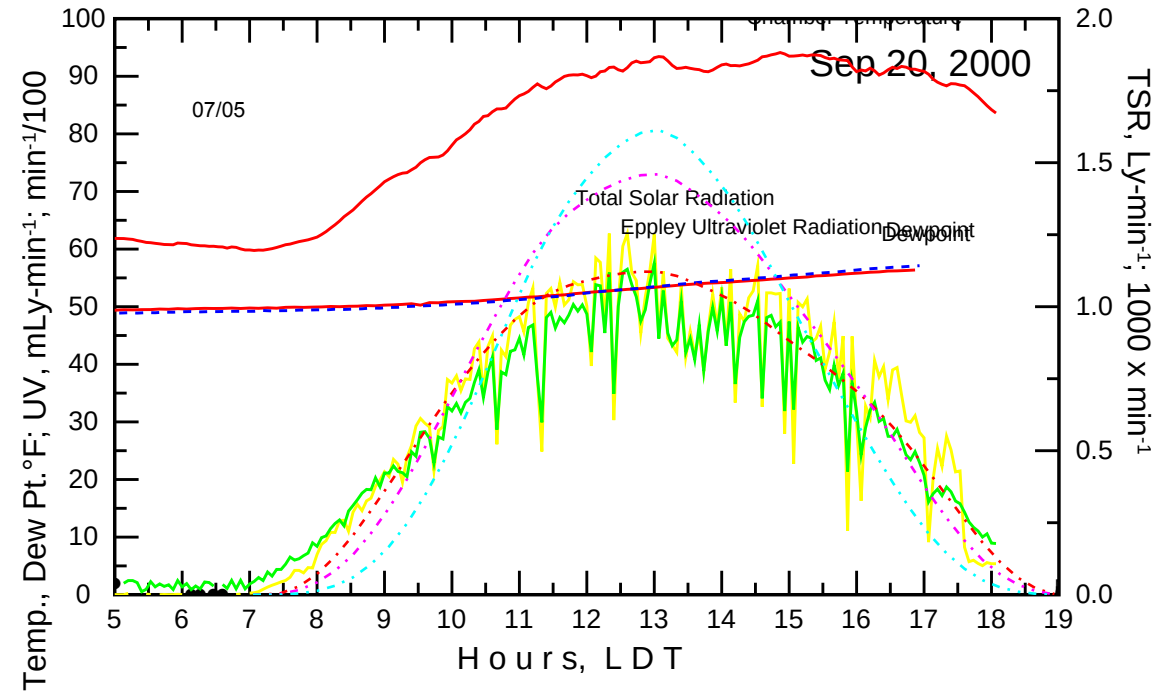

October 03, 1995
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

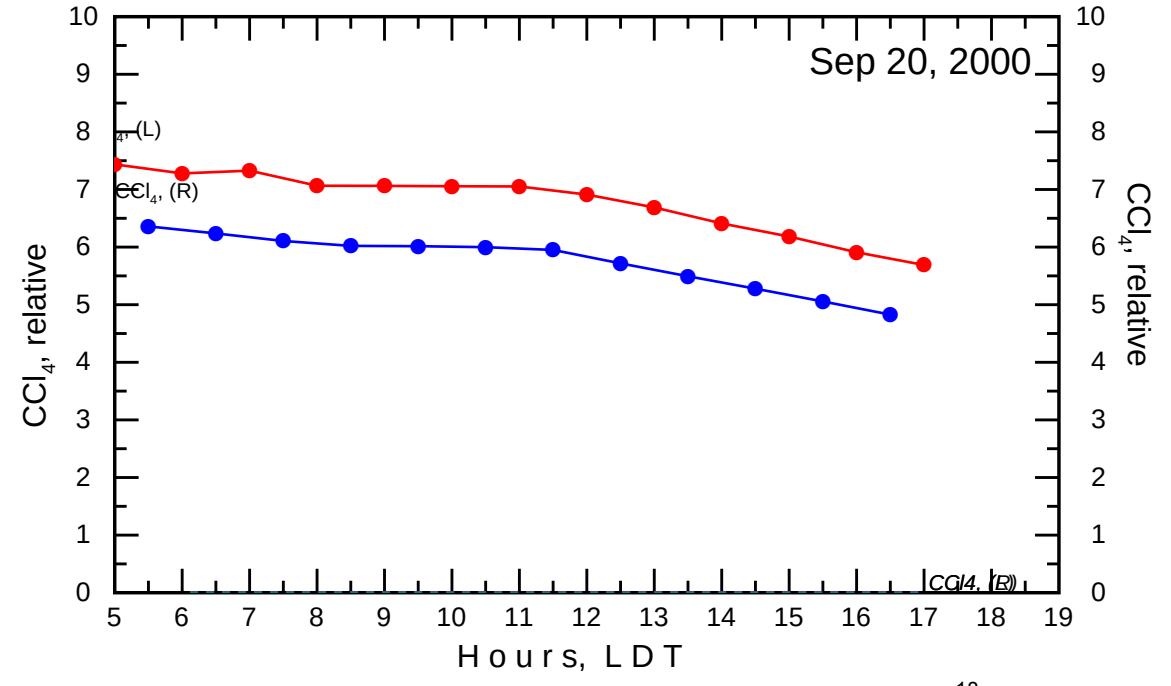

October 03, 1995
CCl4, relative
CCl4, relative
CCl4 (R) (L)
CCl4, (E)
Hours, LDT





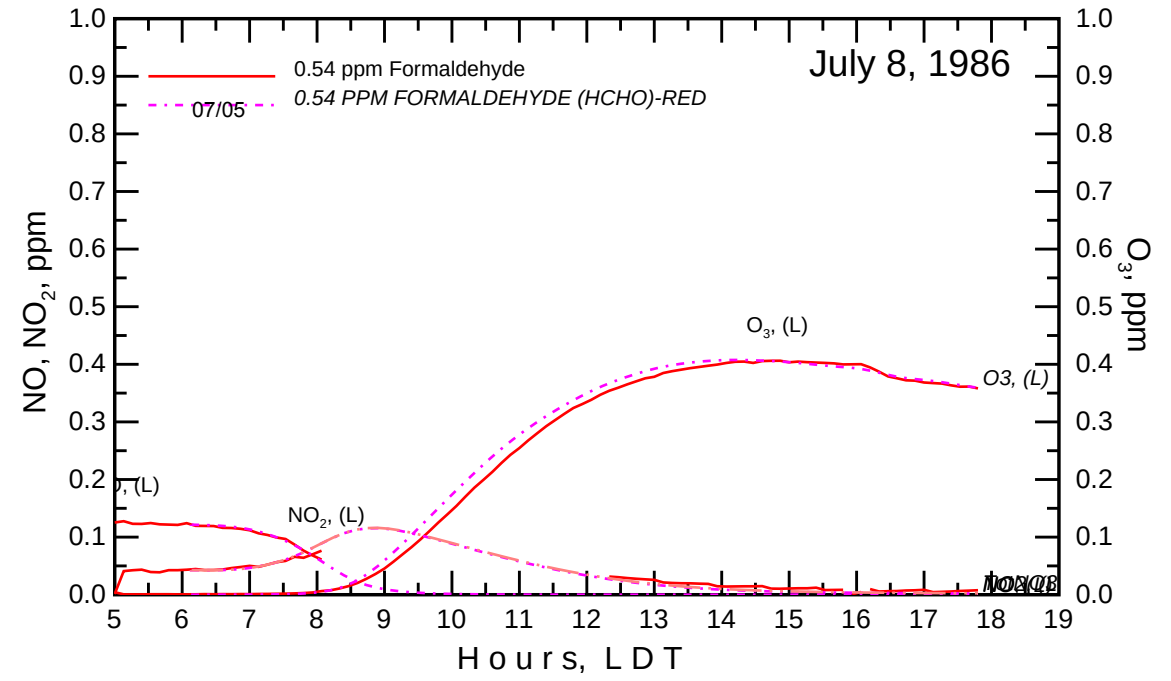
500 vs 250 ppm CO; matched 0.33 NOx

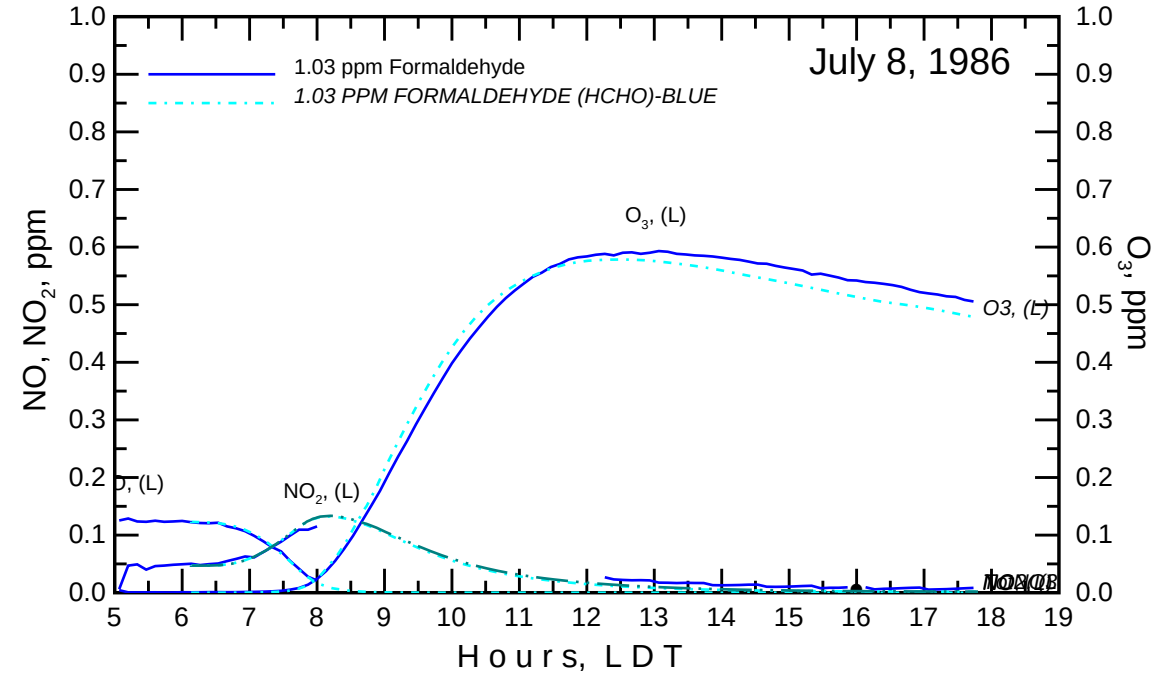

Sep 20, 2000
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


Sep 20, 2000
CCl4, (L)
CCl4, (R)
CCl4, relative
Hours, LDT

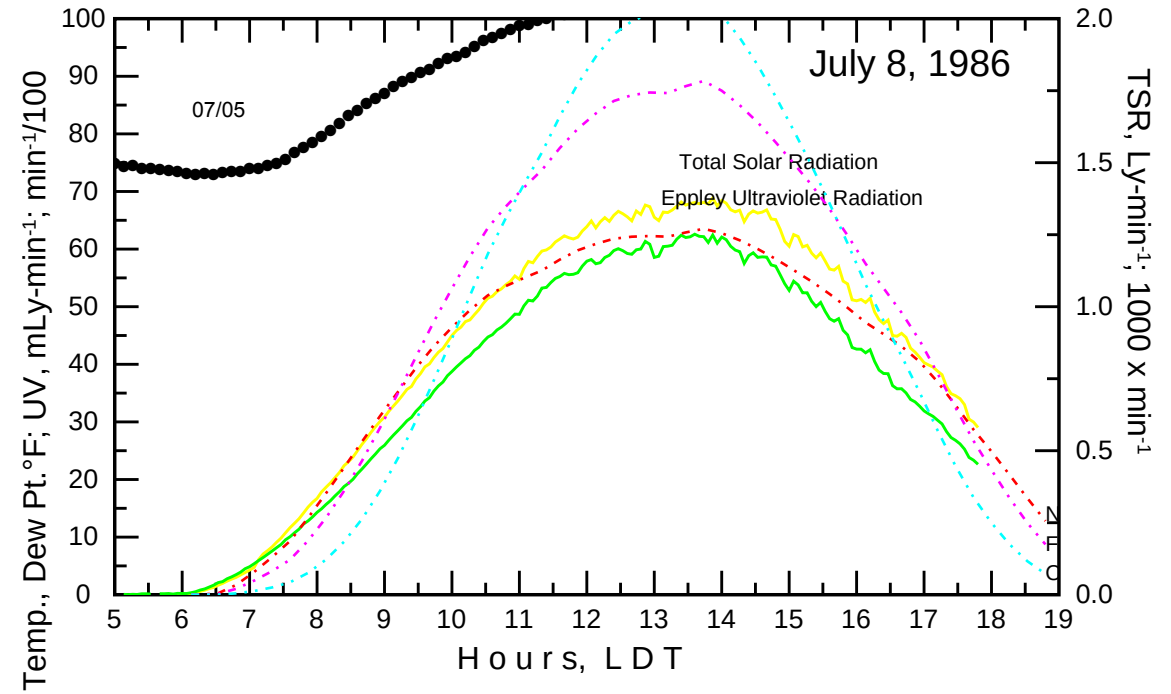
Formaldehyde (FORM)

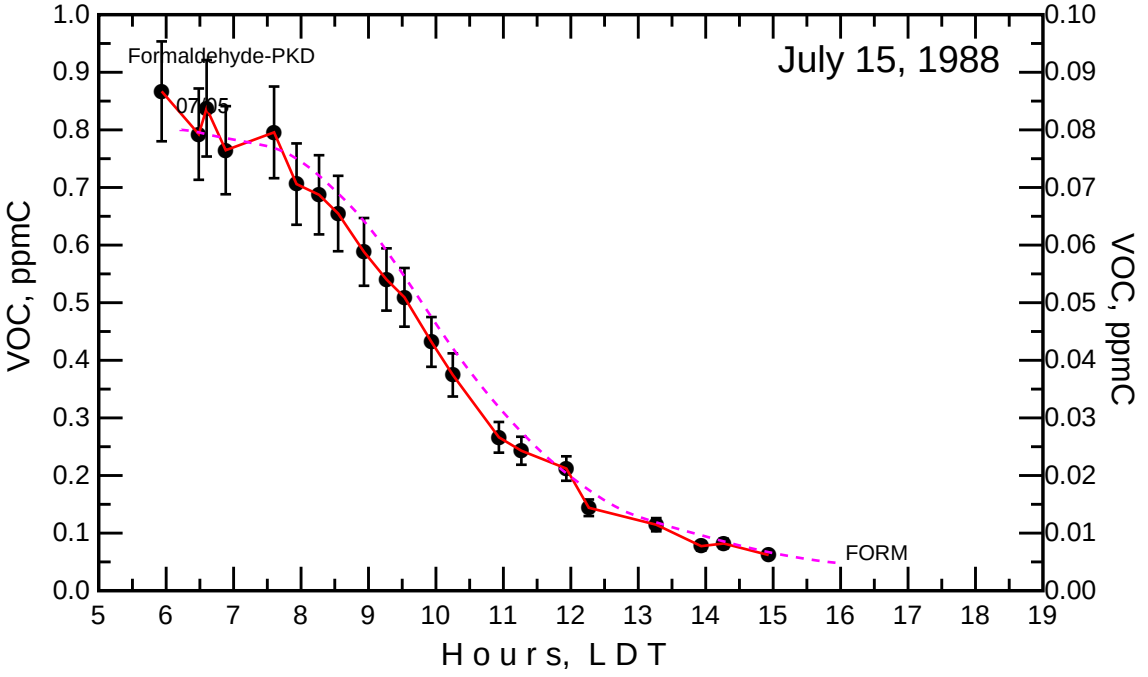
JL 08 86
JL 15 88
ST 23 97
ST 30 97

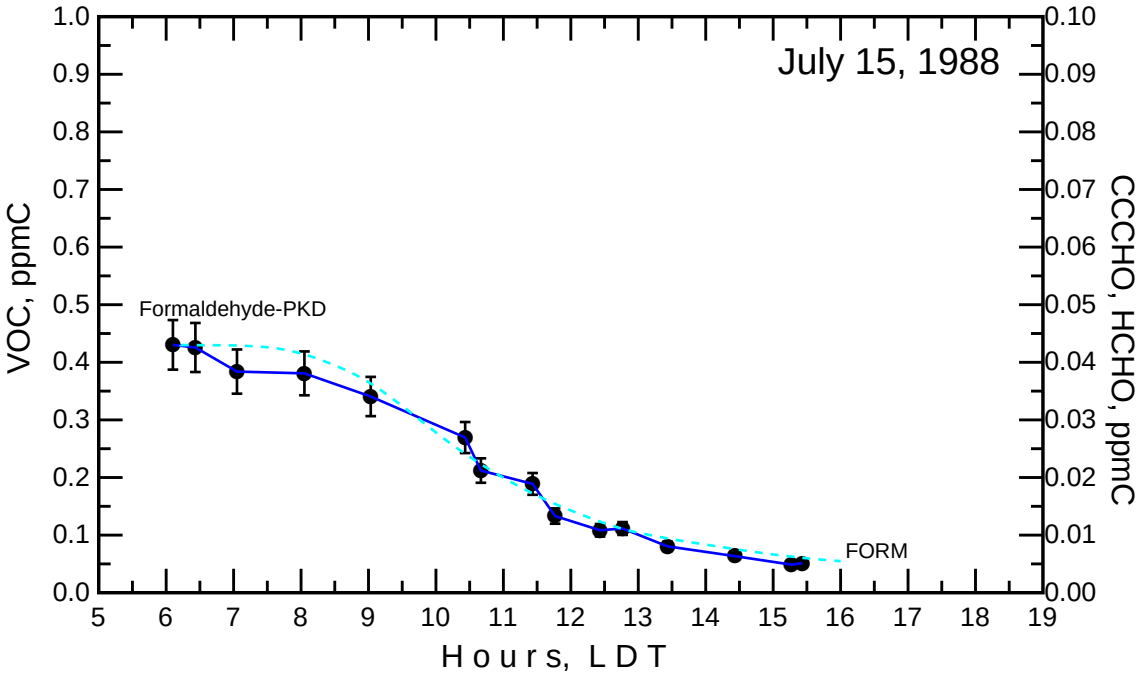


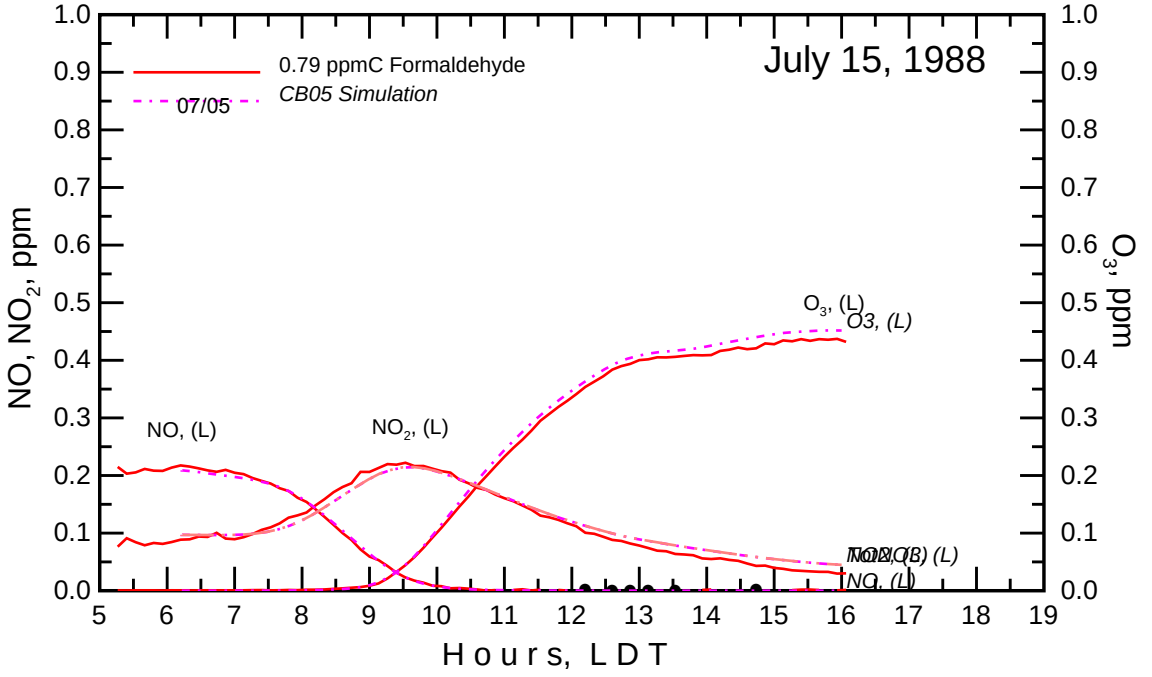


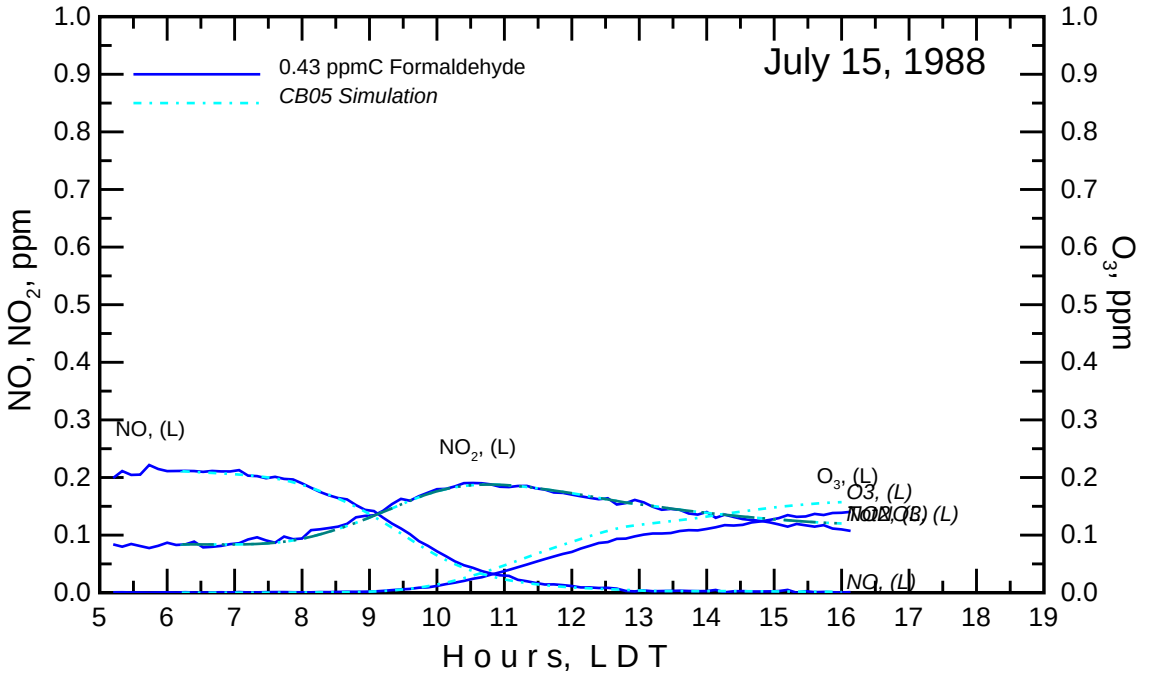
Delta HCHO at 0.17 NO_x


July 8, 1986
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

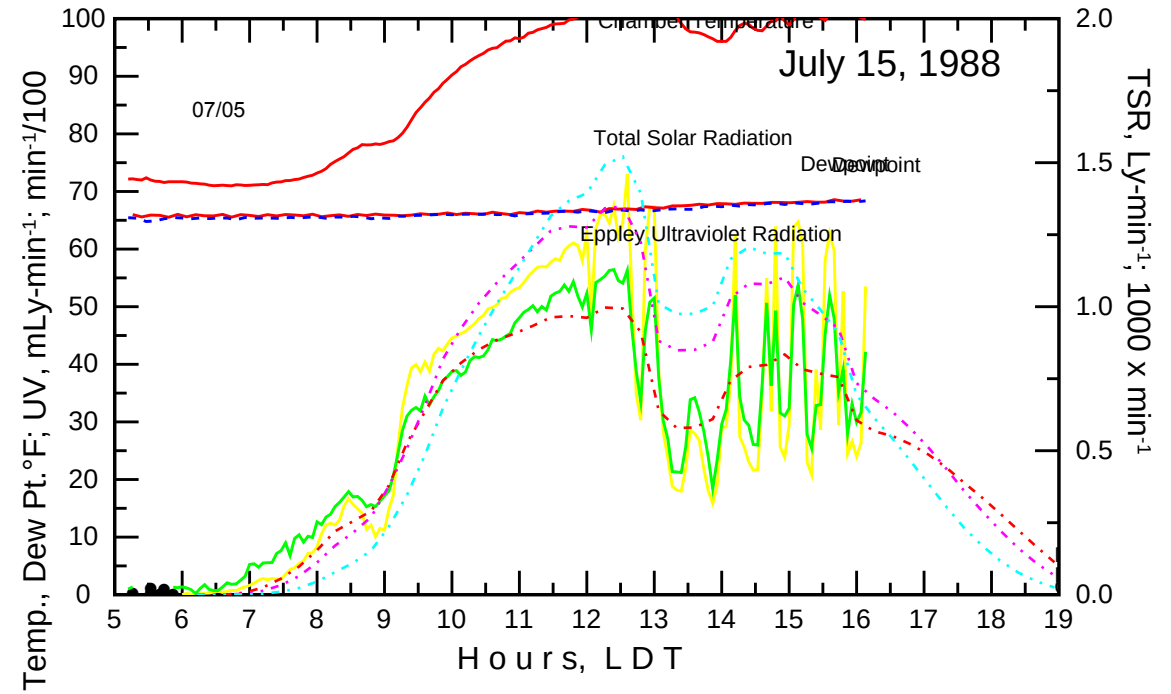

Formaldehyde-PKD
July 15, 1988
07/05
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT

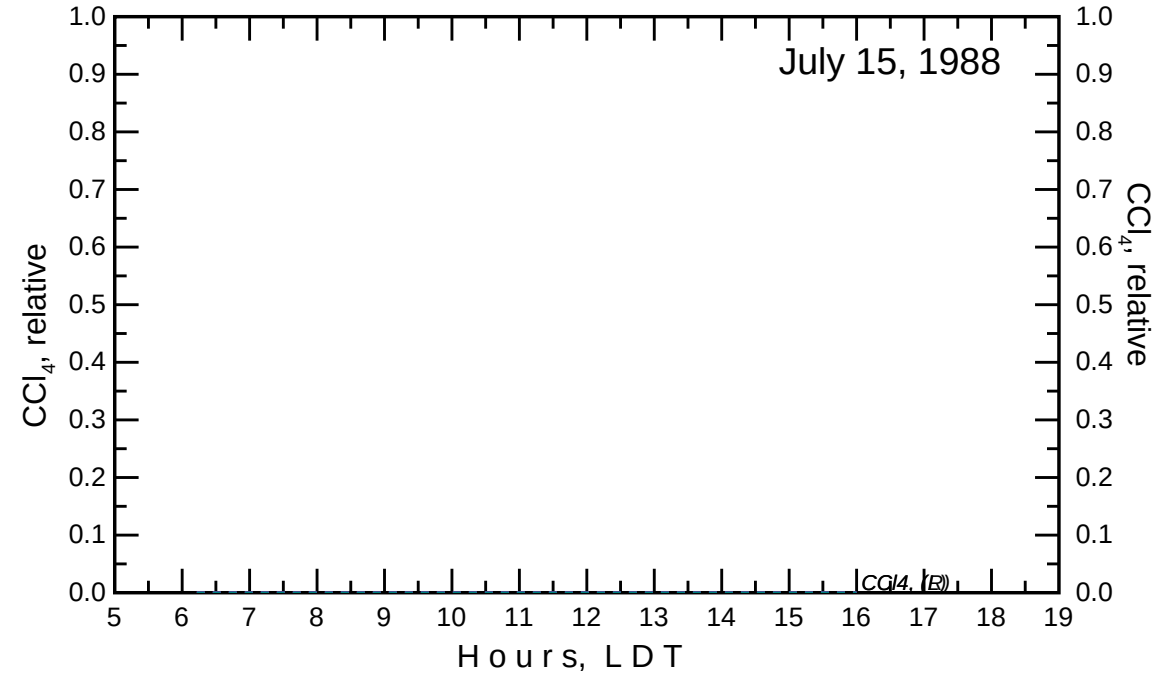

July 15, 1988
Formaldehyde-PKD
FORM
VOC, ppmC
CCCHO, HCHO, ppmC
Hours, LDT

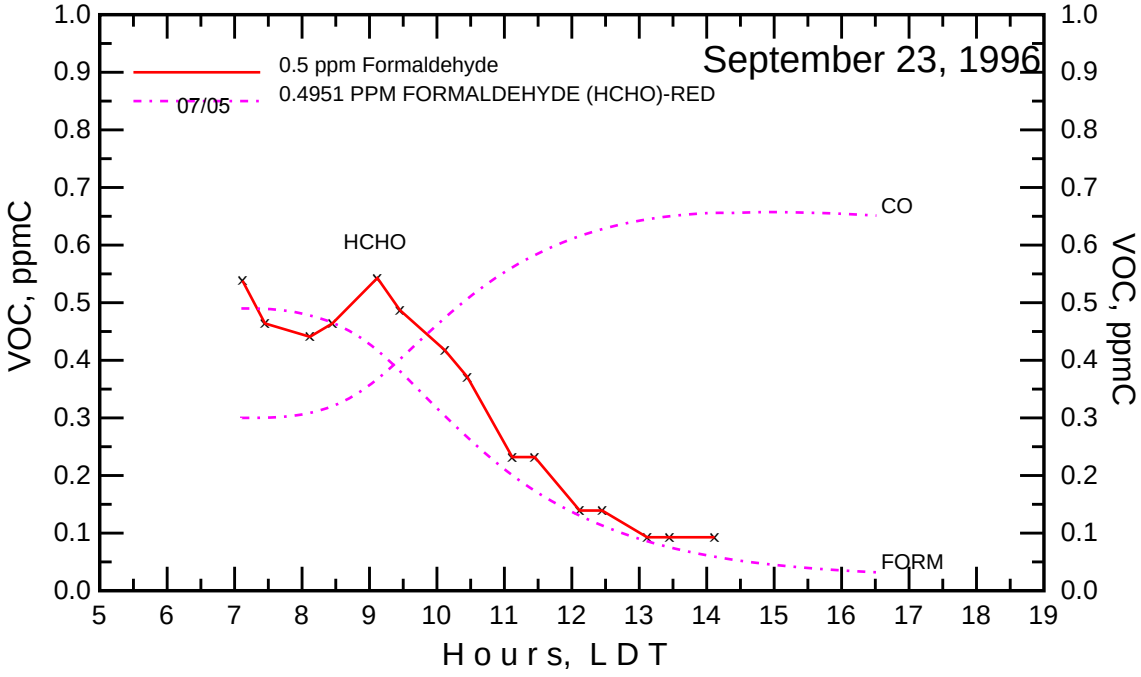


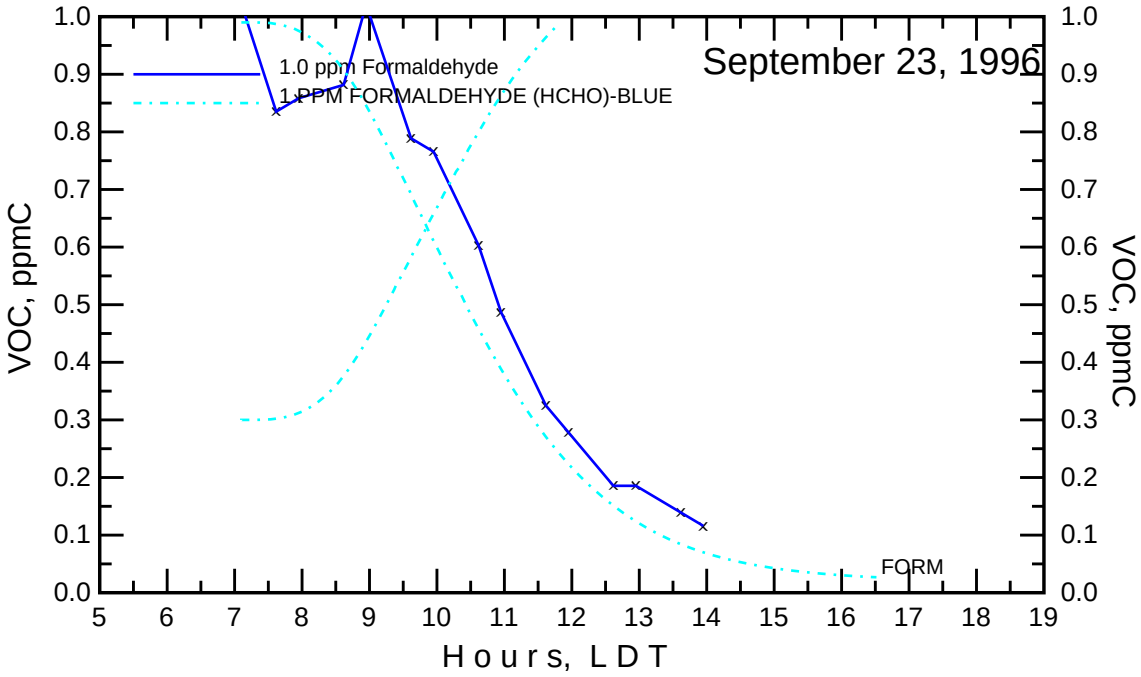


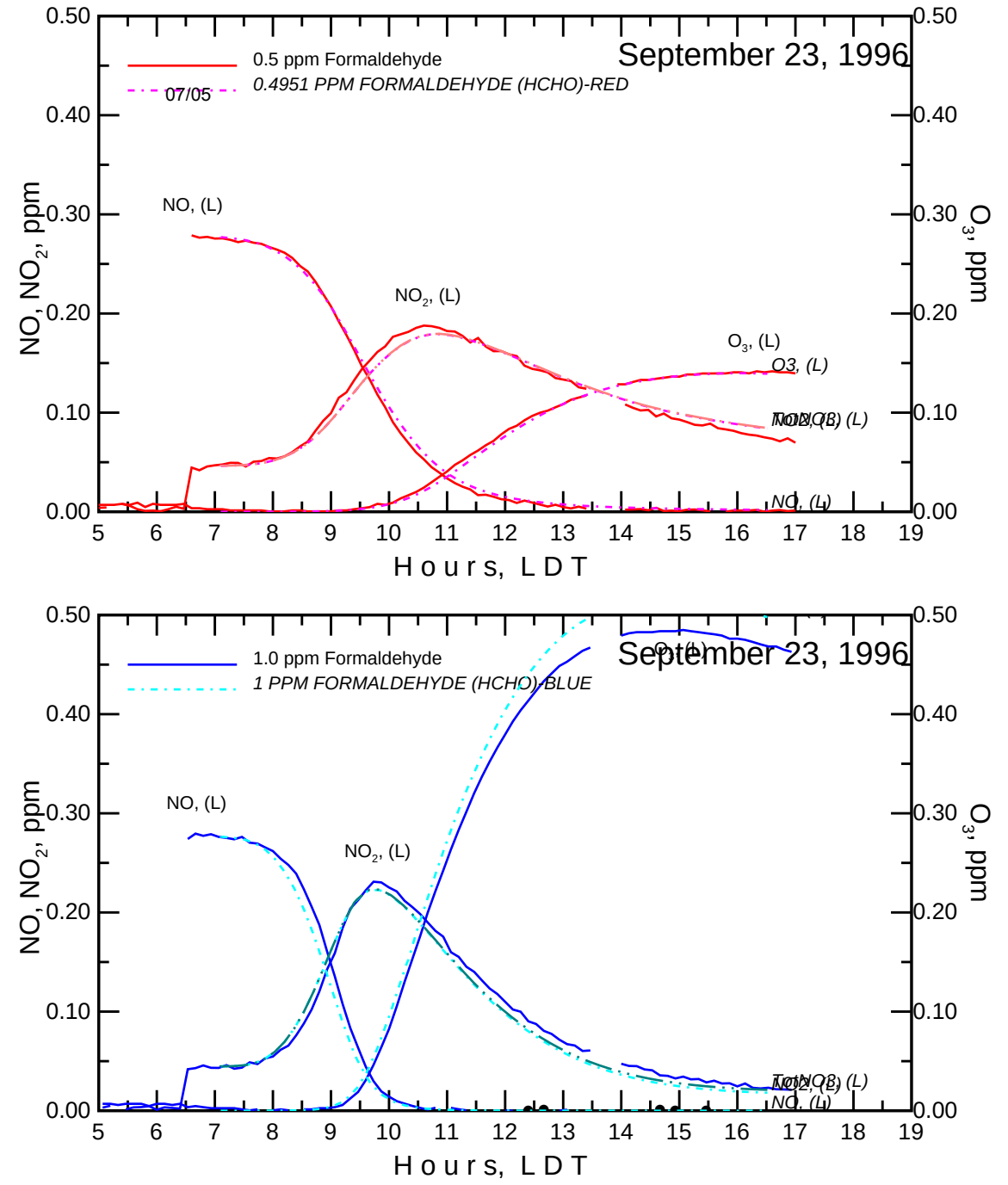
Delta HCHO at 0.3 ppm NO_x


July 15, 1988
07/05
Total Solar Radiation
Dewpoint
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

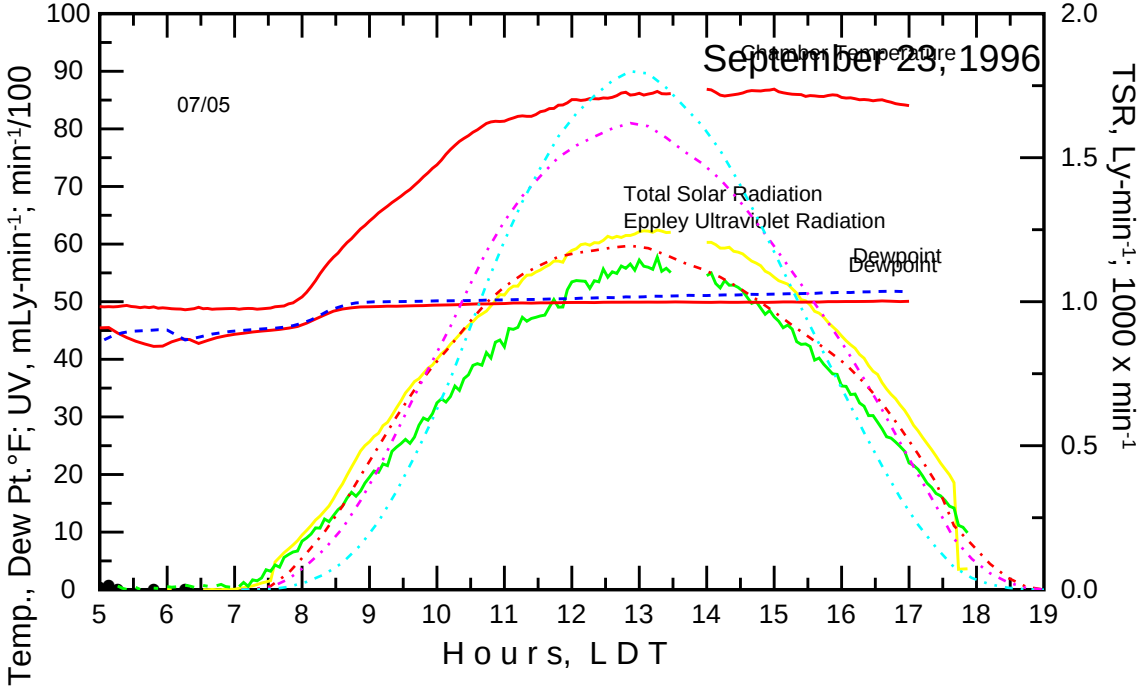

July 15, 1988
CCl4, relative
CCl4, relative
CCl4 (B)
Hours, LDT

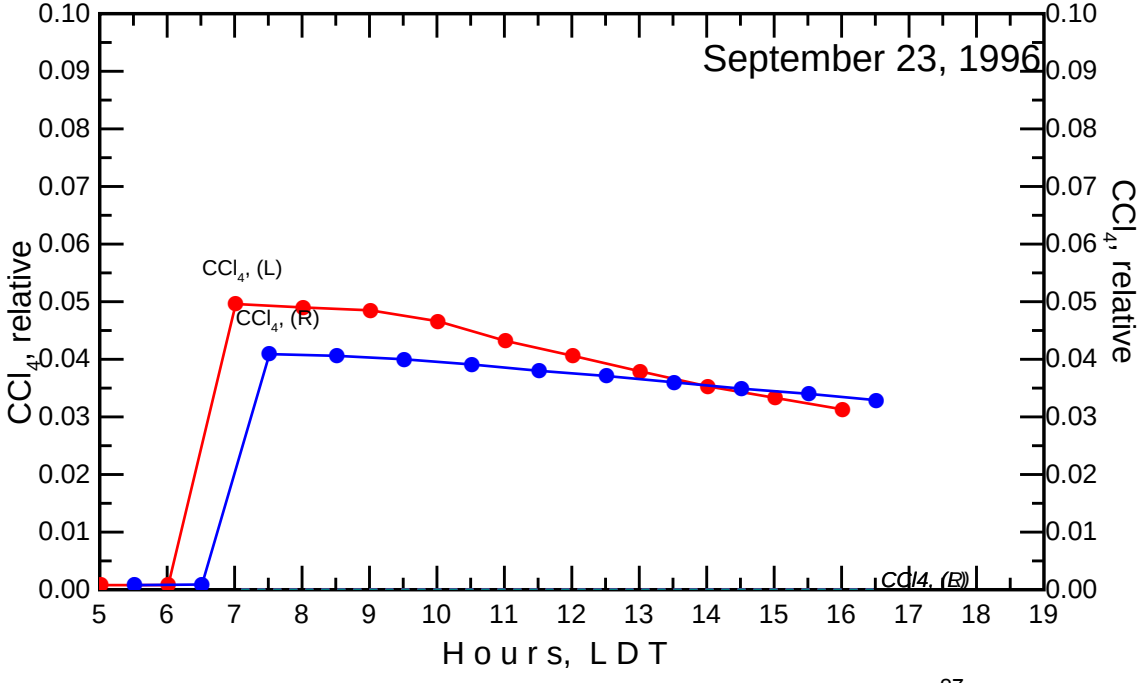

September 23, 1996
0.5 ppm Formaldehyde
0.4951 PPM FORMALDEHYDE (HCHO)-RED
07/05
HCHO
CO
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT

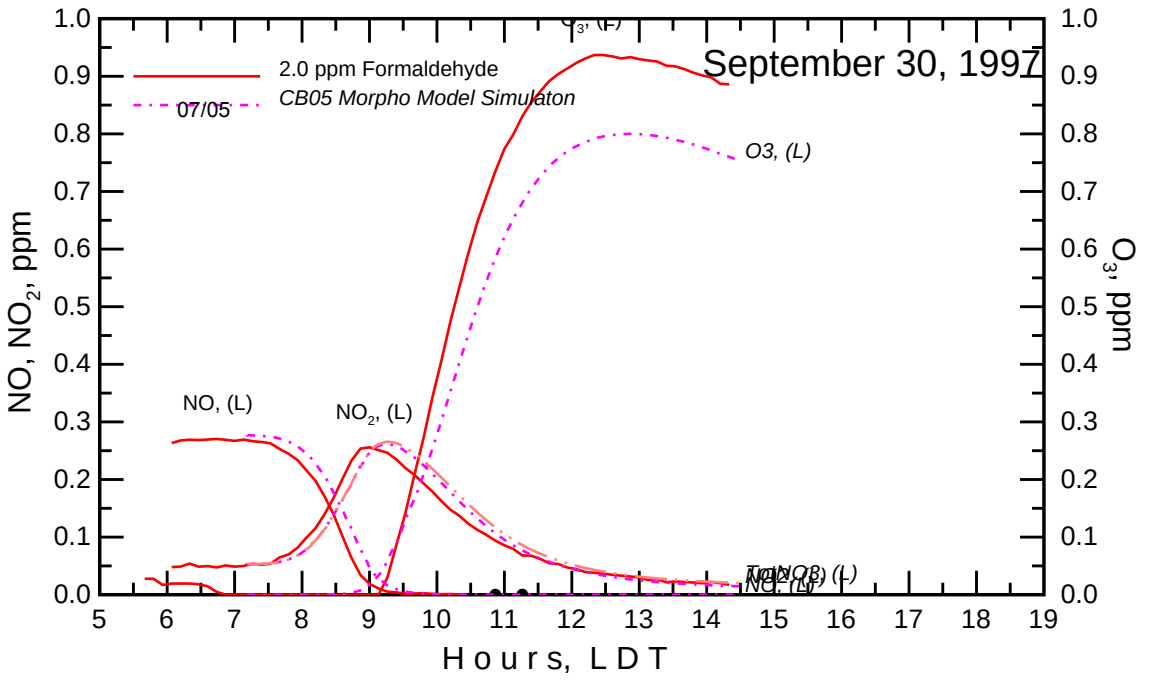

September 23, 1996
1.0 ppm Formaldehyde
1.1 PPM FORMALDEHYDE (HCHO)-BLUE
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT

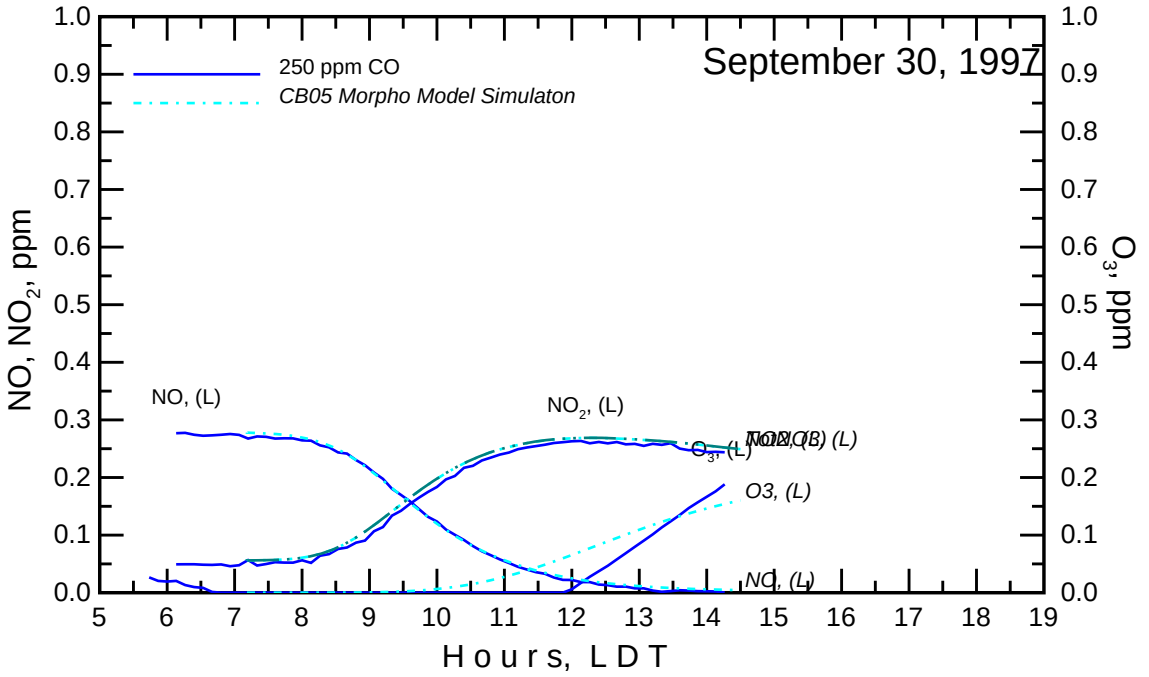


Delta Formaldehyde

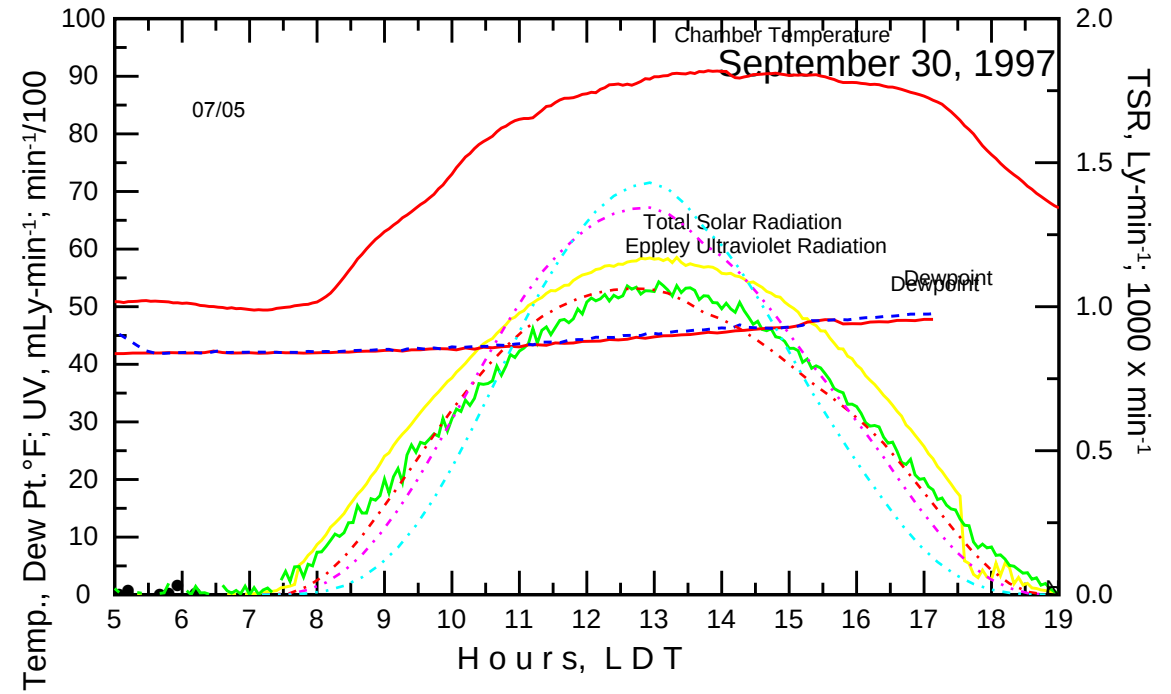

September 23, 1996
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

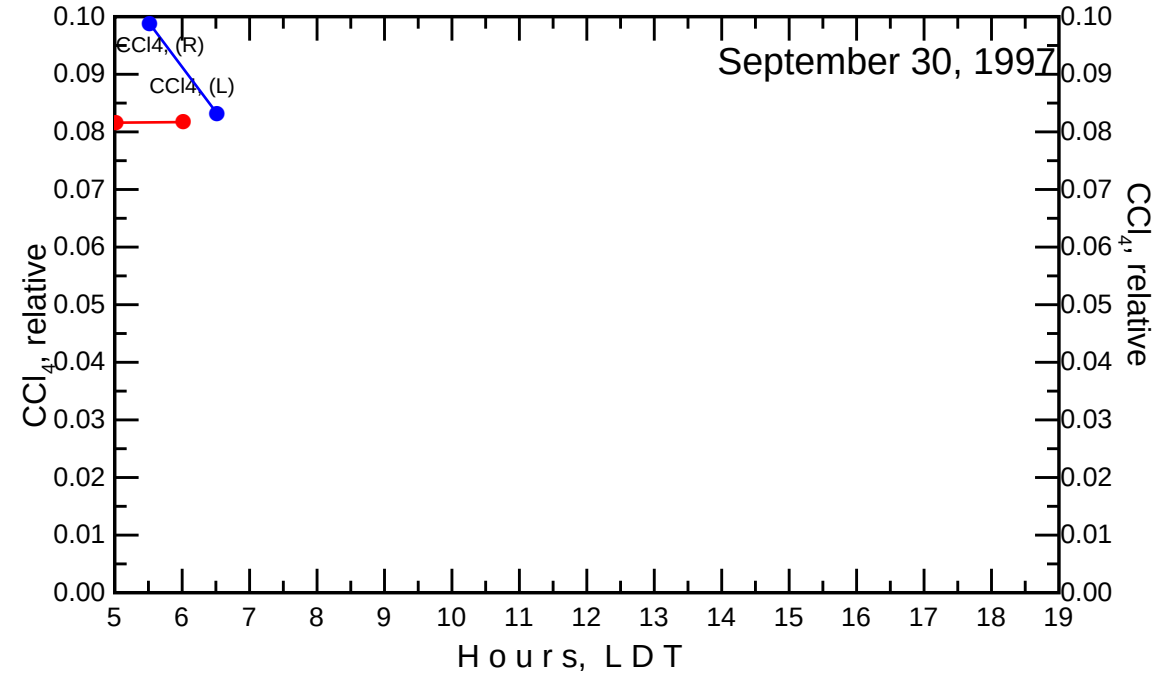

September 23, 1996
CCl4, (L)
CCl4, (R)
CCl4, (R)
CCl4, relative
CCl4, relative
Hours, LDT





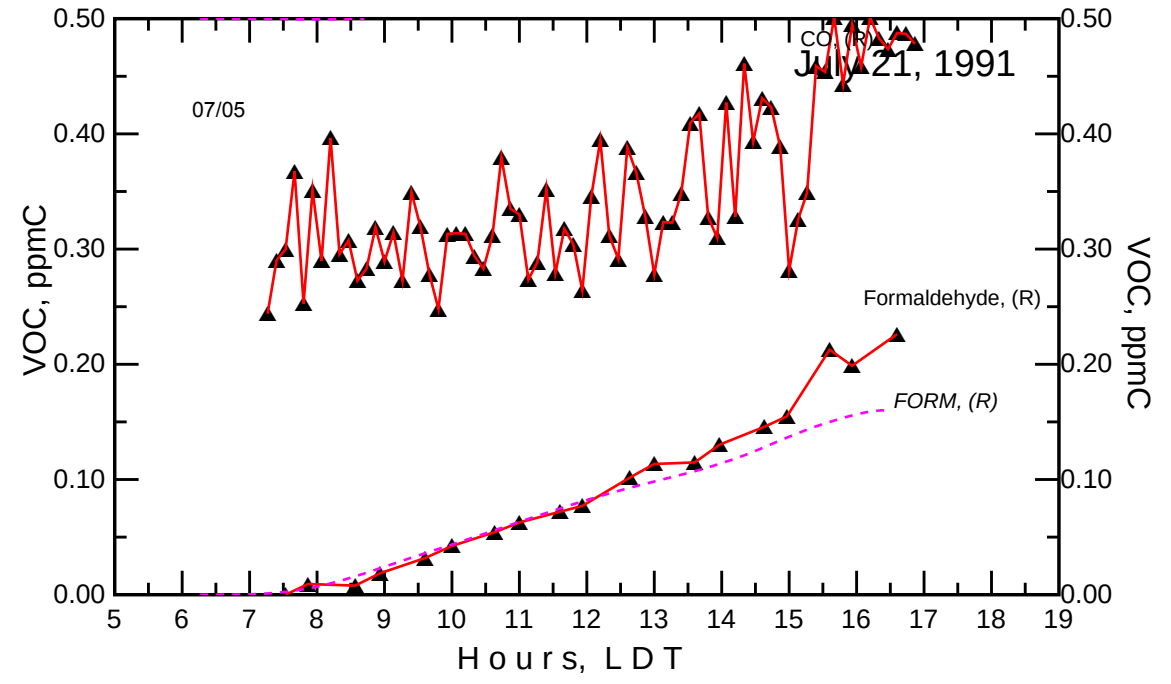
Characterization: Formaldehyde vs CO; matched NOx

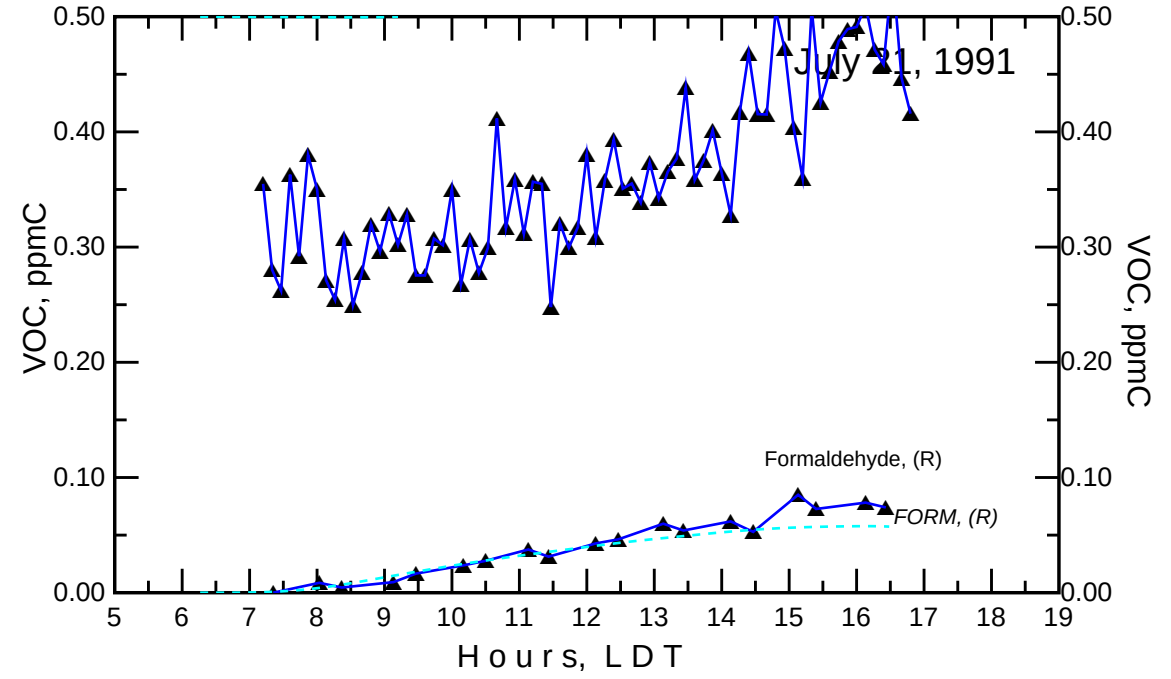

Chamber Temperature
September 30, 1997
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

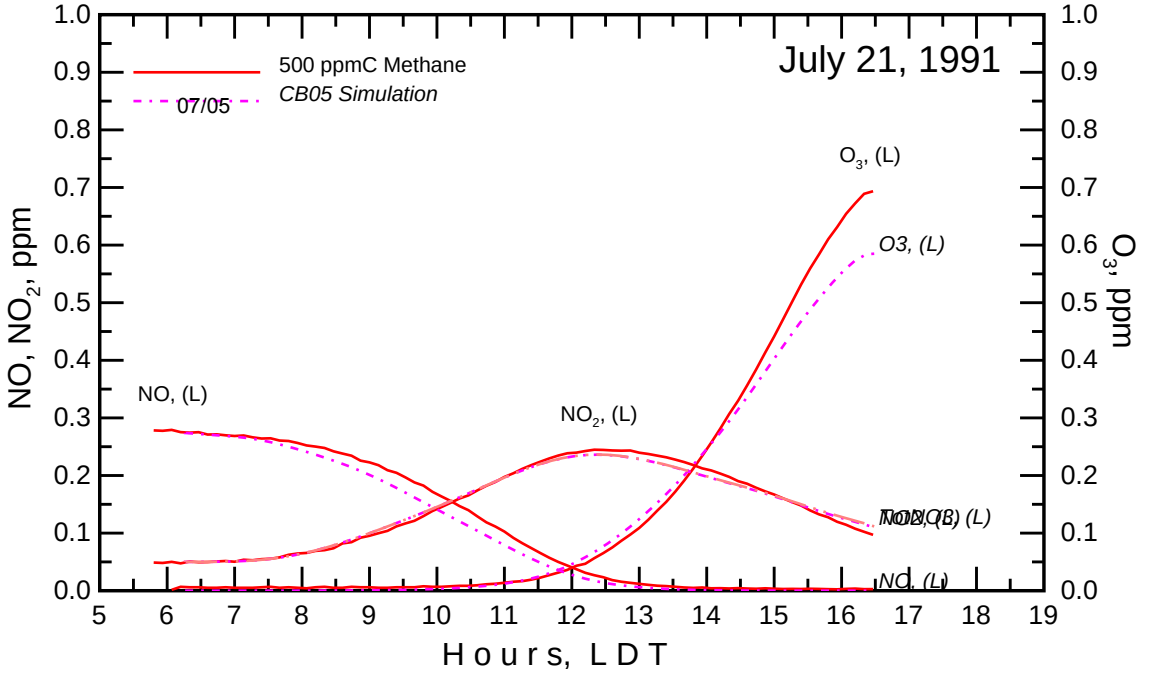

CCl4, (R)
CCl4, (L)
September 30, 1997
CCl4, relative
CCl4, relative
Hours, LDT

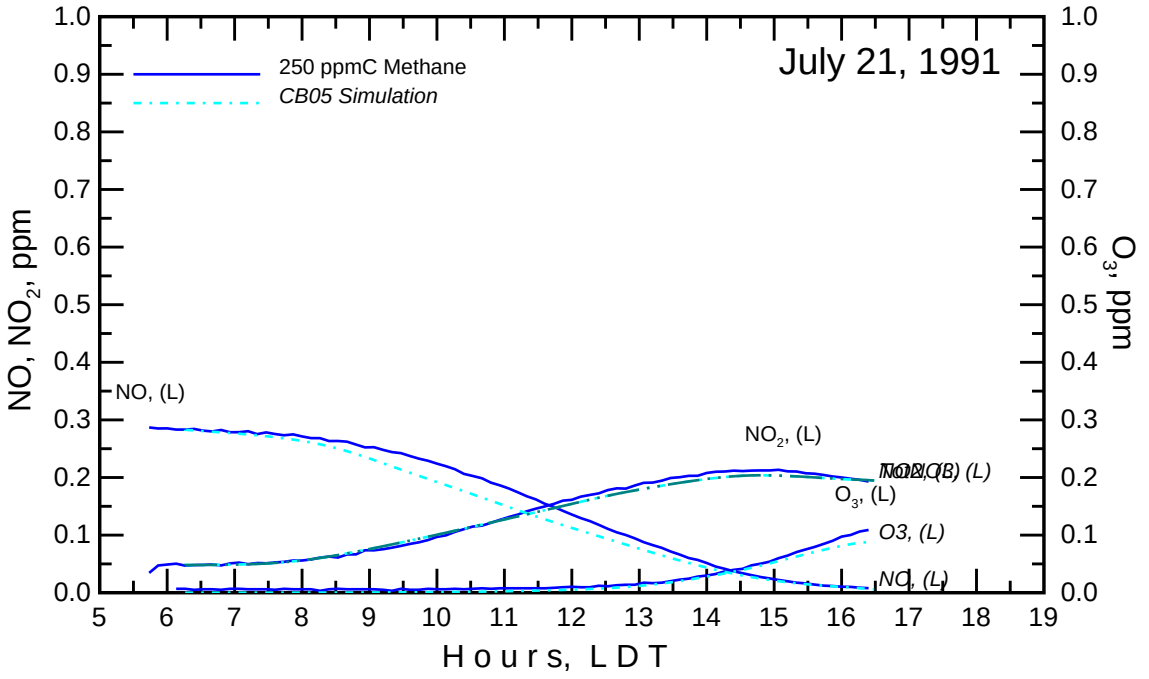
Methane (CH4)

JL 21 91
AU 01 97
AU10 92
ST 07 90
ST 19 96
ST 20 93

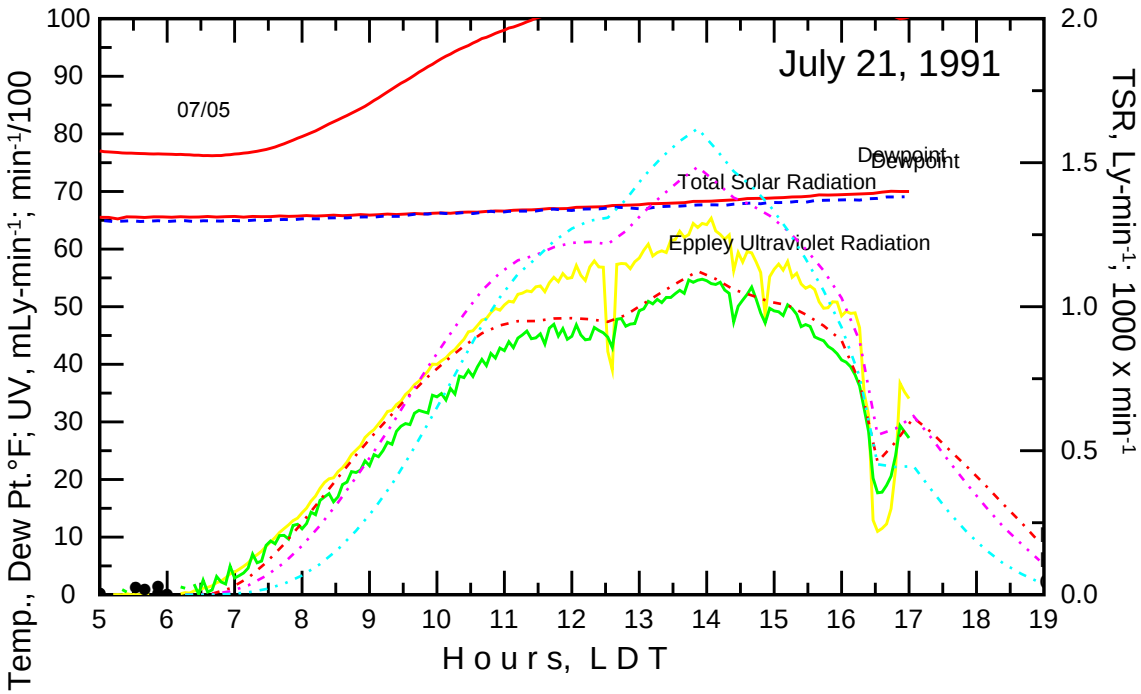

July 21, 1991
07/05
Formaldehyde, (R)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

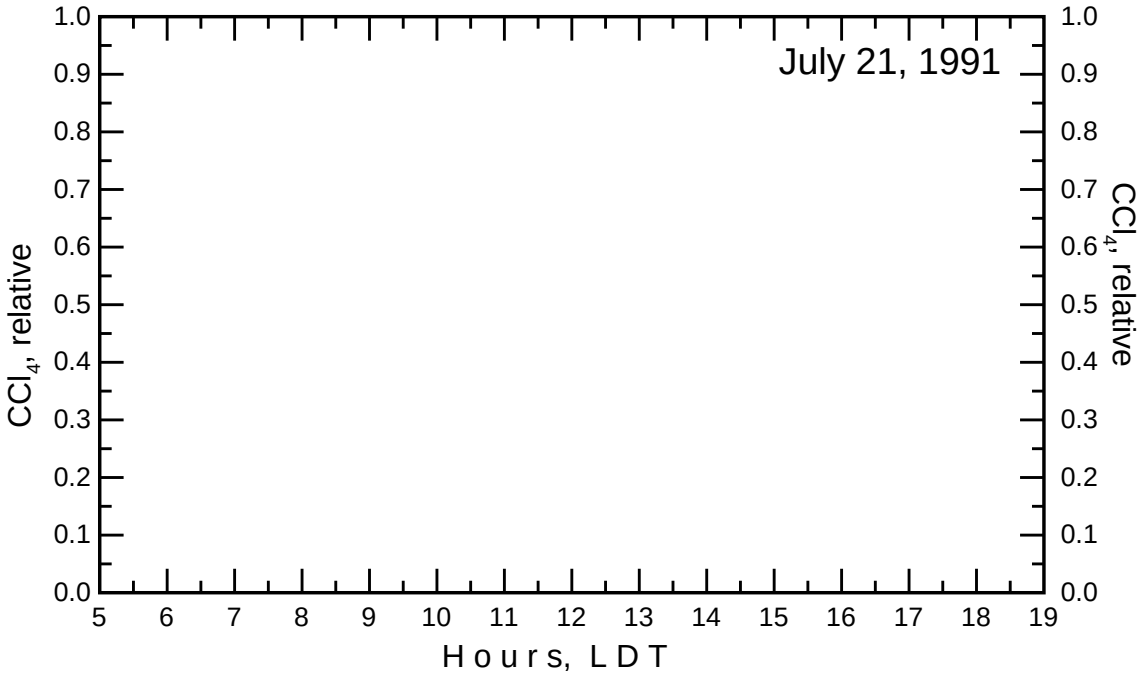

July 21, 1991
Formaldehyde, (R)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

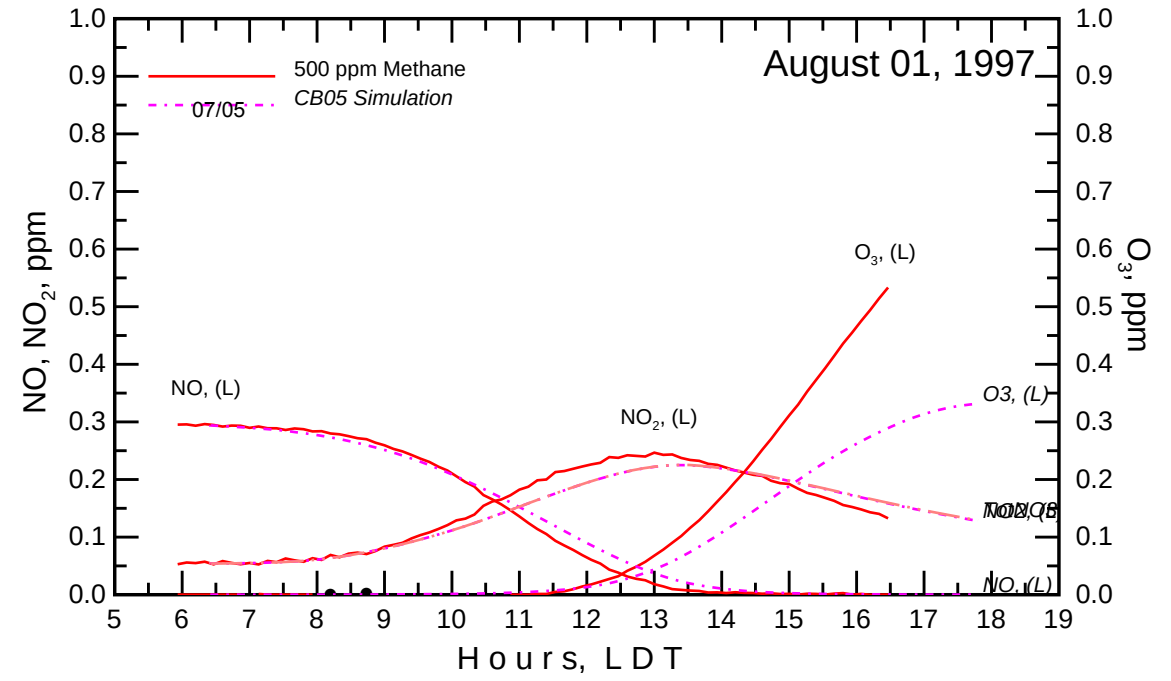


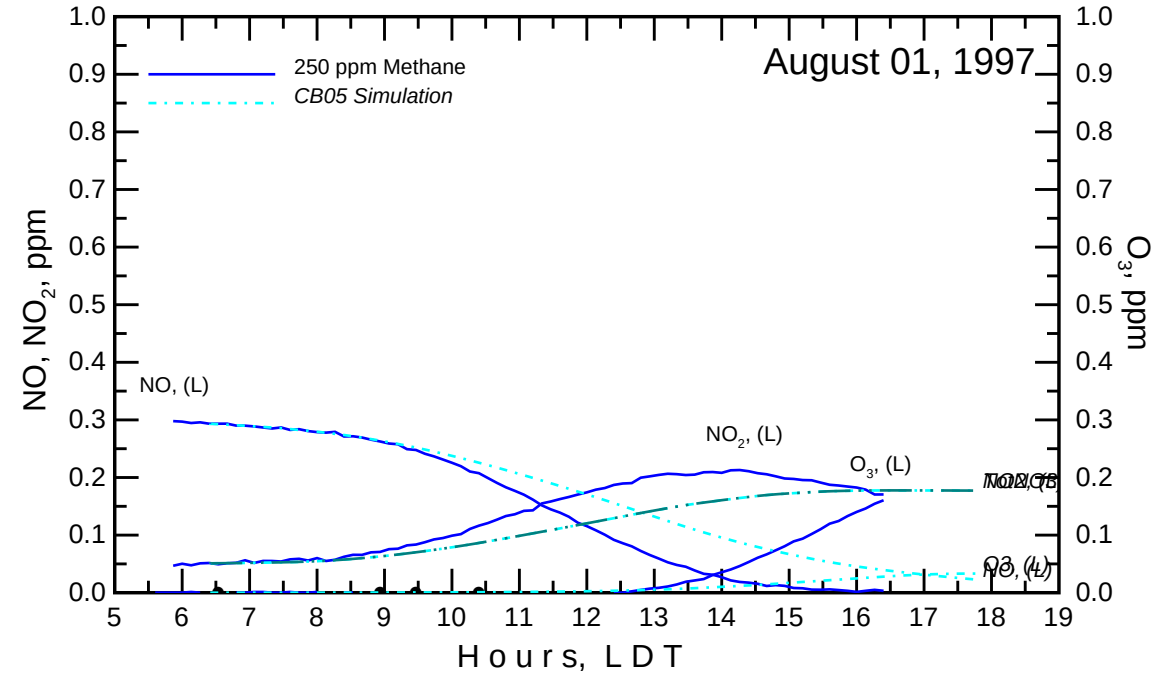


Run C1-- Delta Methane

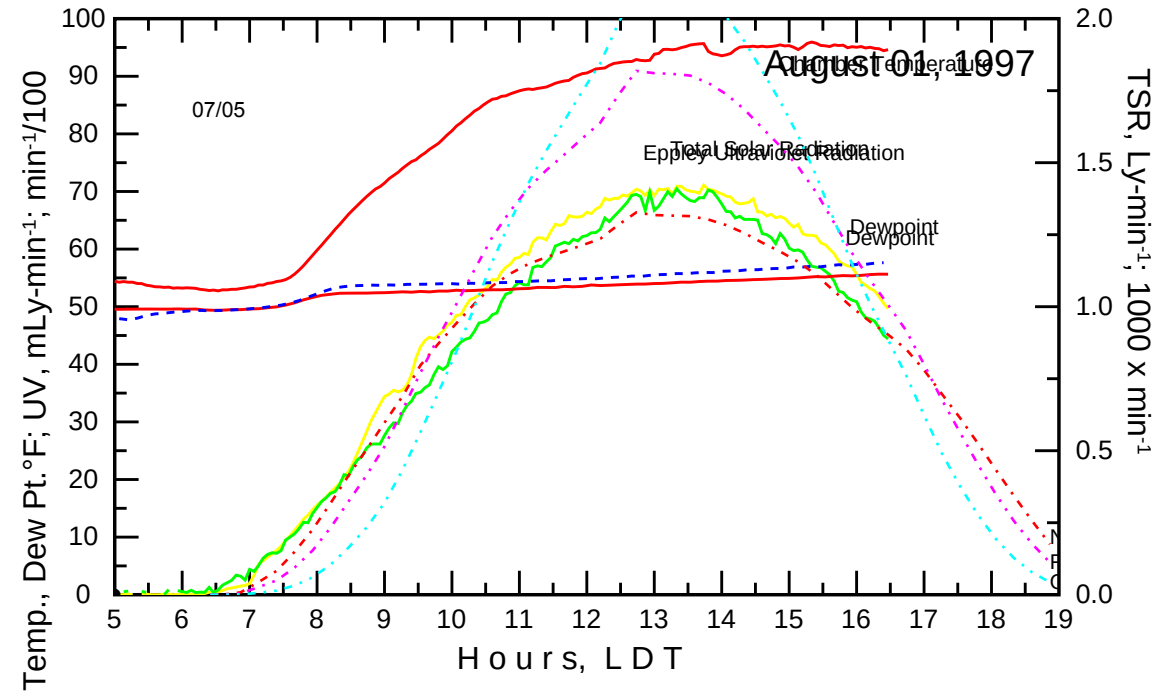

July 21, 1991
07/05
Dewpoint
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

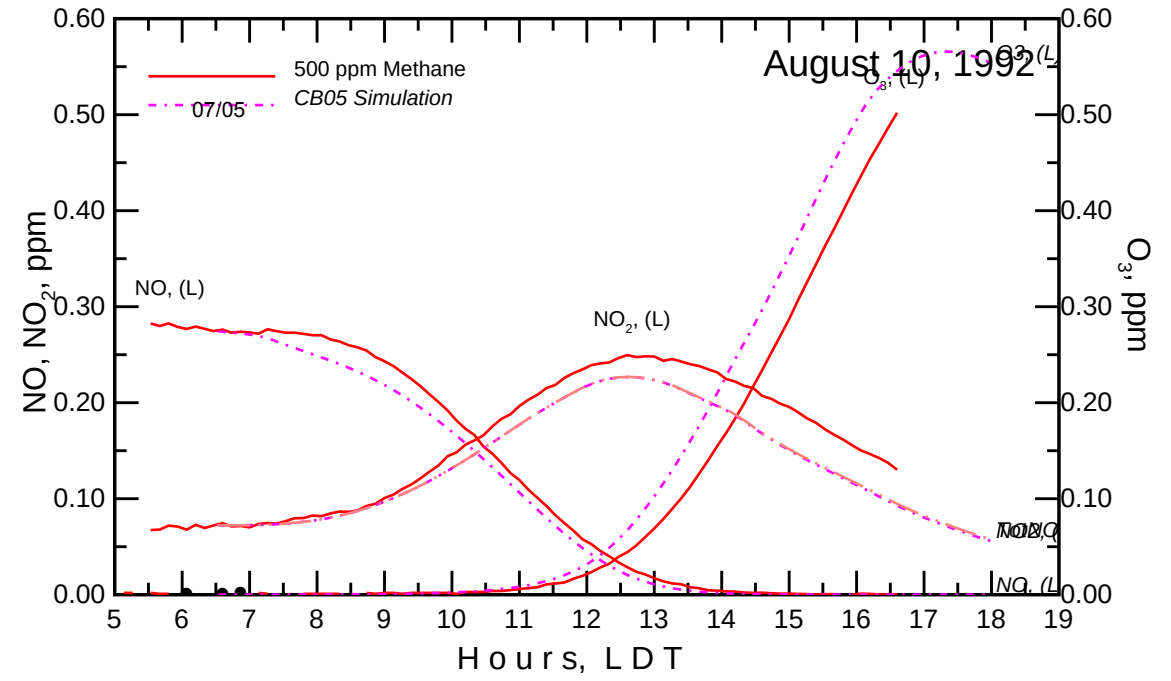

July 21, 1991
CCl4, relative
CCl4, relative
Hours, LDT

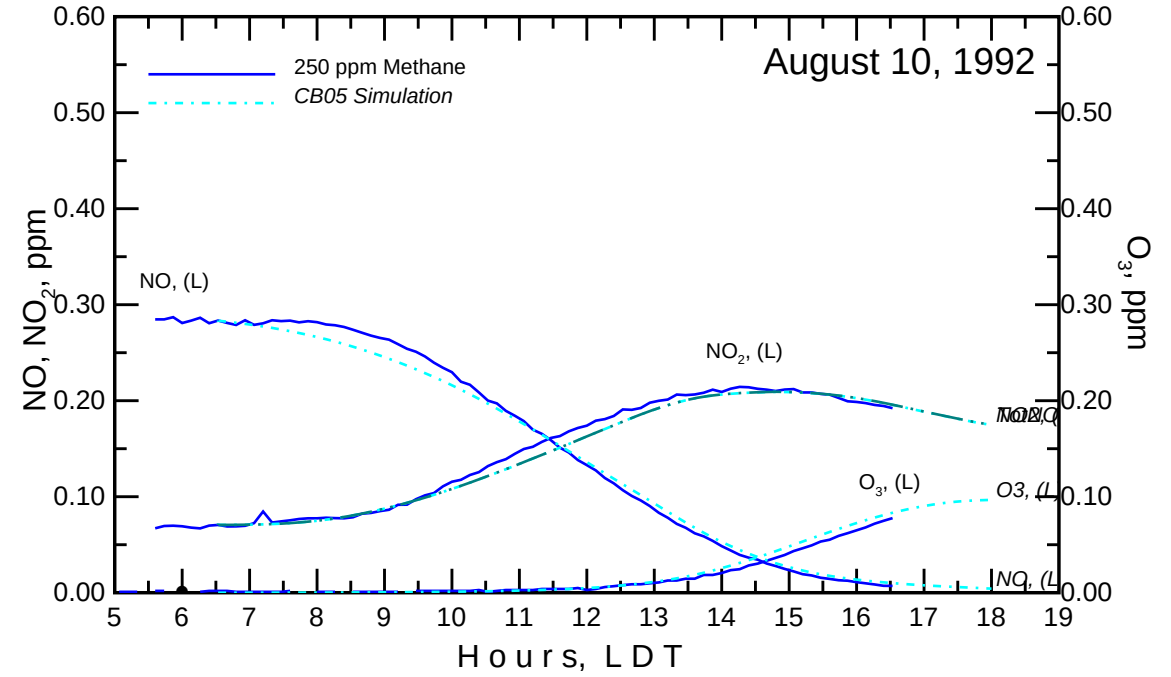


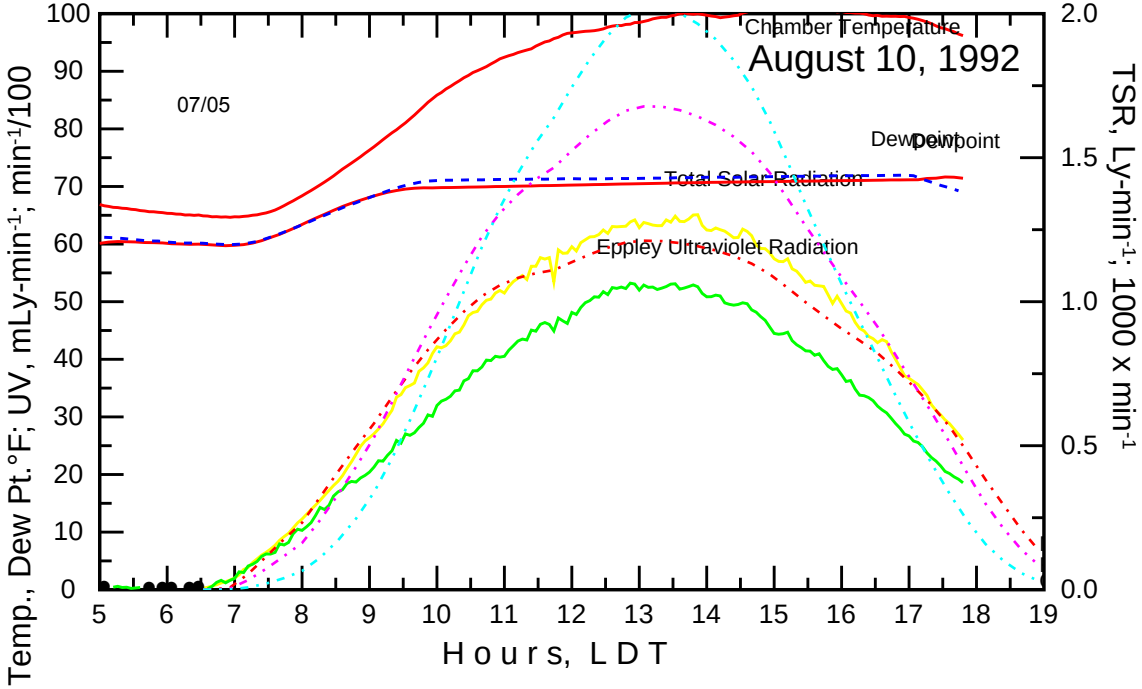


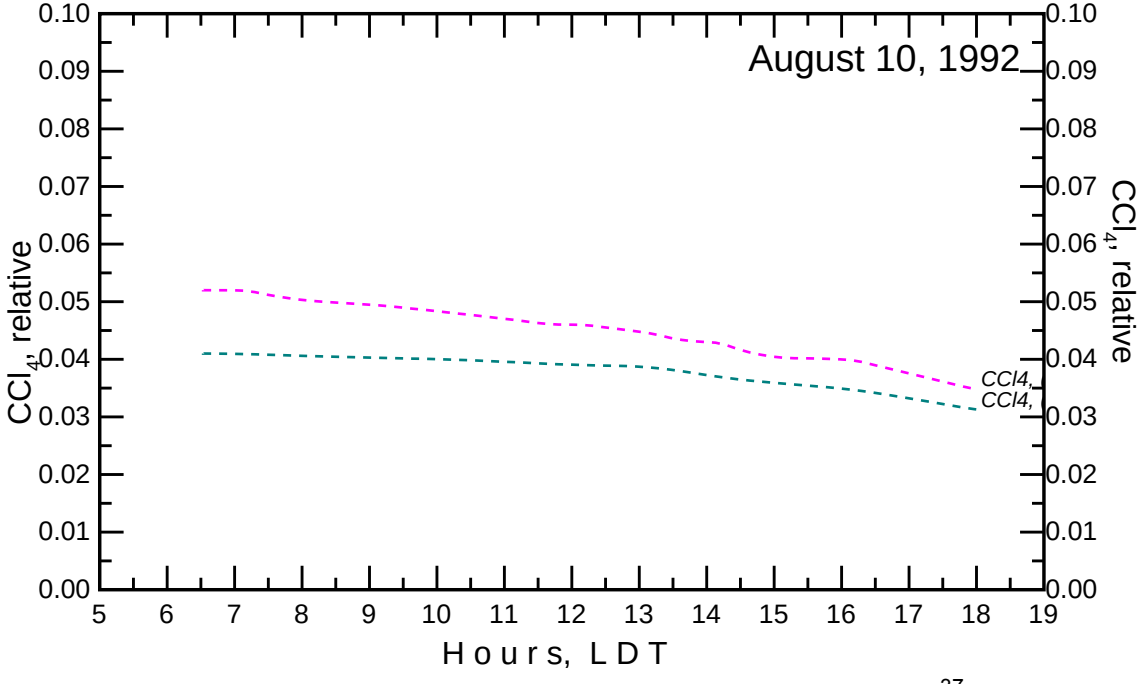
250 vs 500 ppm Methane; 0.35 NOx

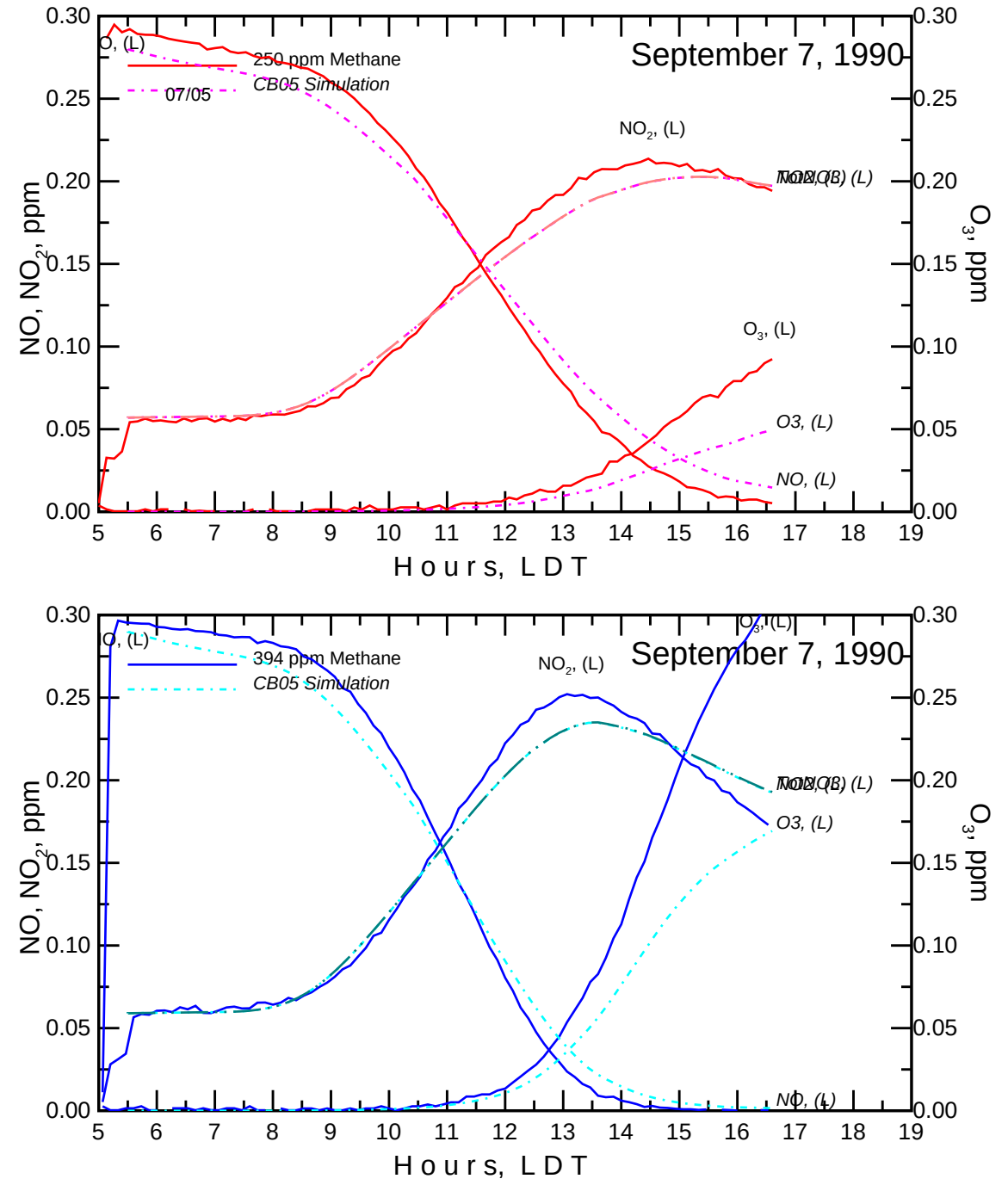

August 01, 1997
07/05
Ambient Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19


August 10, 1992
500 ppm Methane
CB05 Simulation
07/05
NO, (L)
NO2, (L)
O3, (L)
NO, NO2, ppm
O3, ppm
Hours, LDT

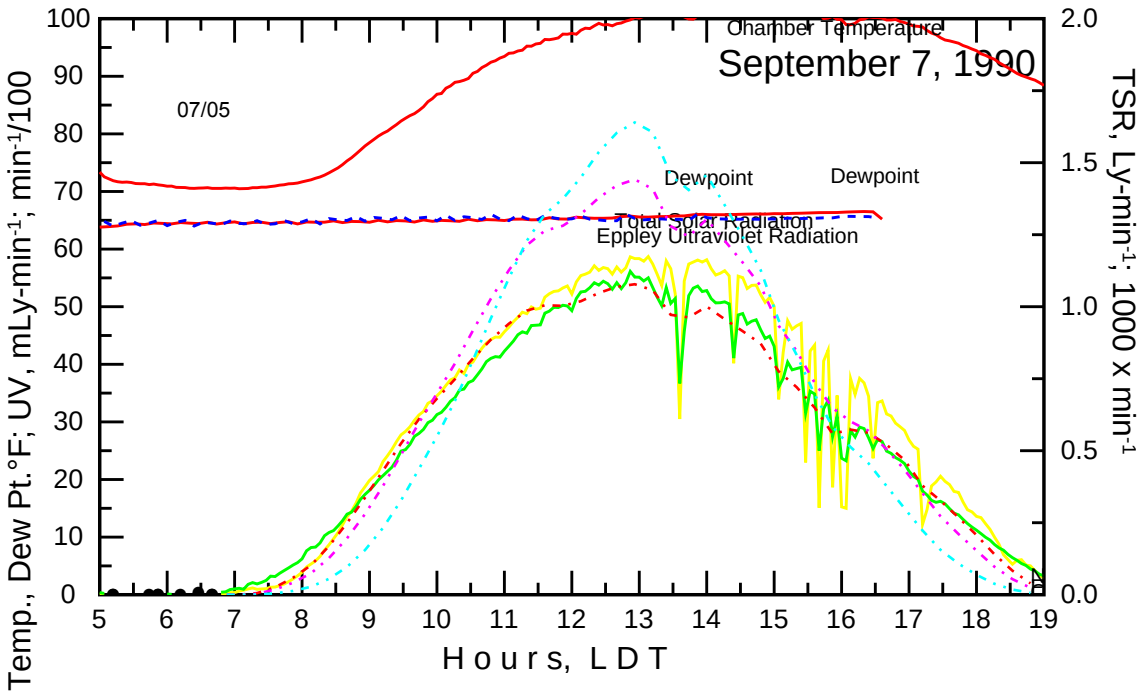

August 10, 1992
250 ppm Methane
CB05 Simulation
NO, (L)
NO2, (L)
O3, (L)
NO, NO2, ppm
O3, ppm
Hours, LDT

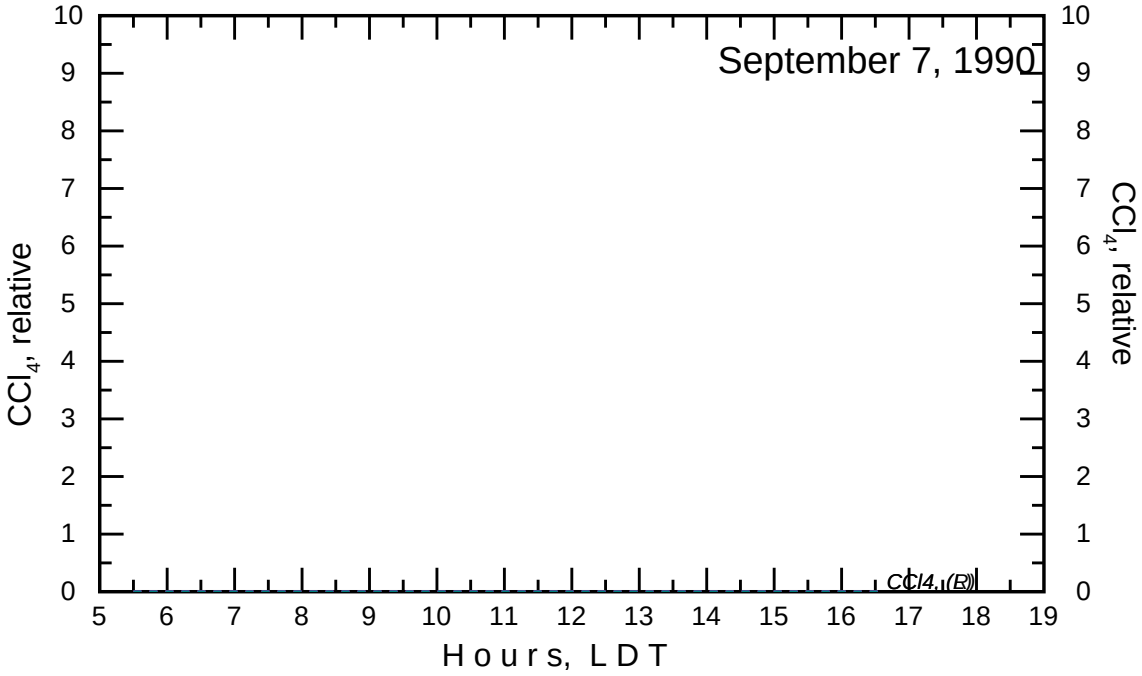

August 10, 1992
07/05
Chamber Temperature
Dewpoint
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

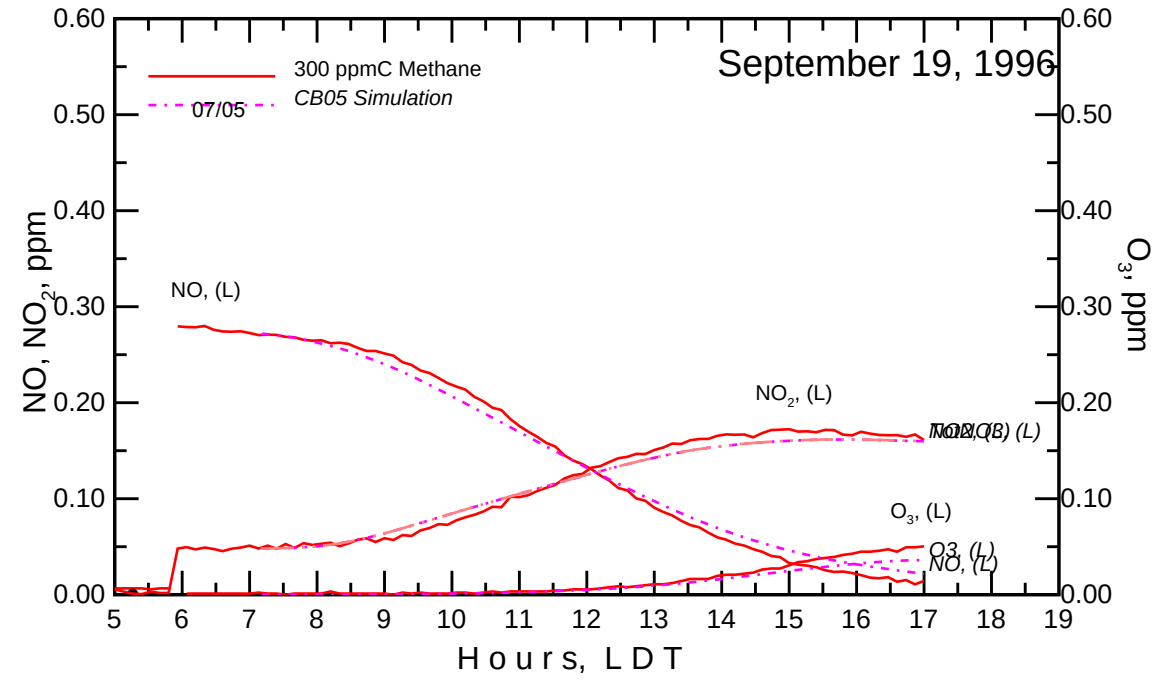

August 10, 1992
CCl4, relative
CCl4, relative
CCl4,
CCl4,
Hours, LDT

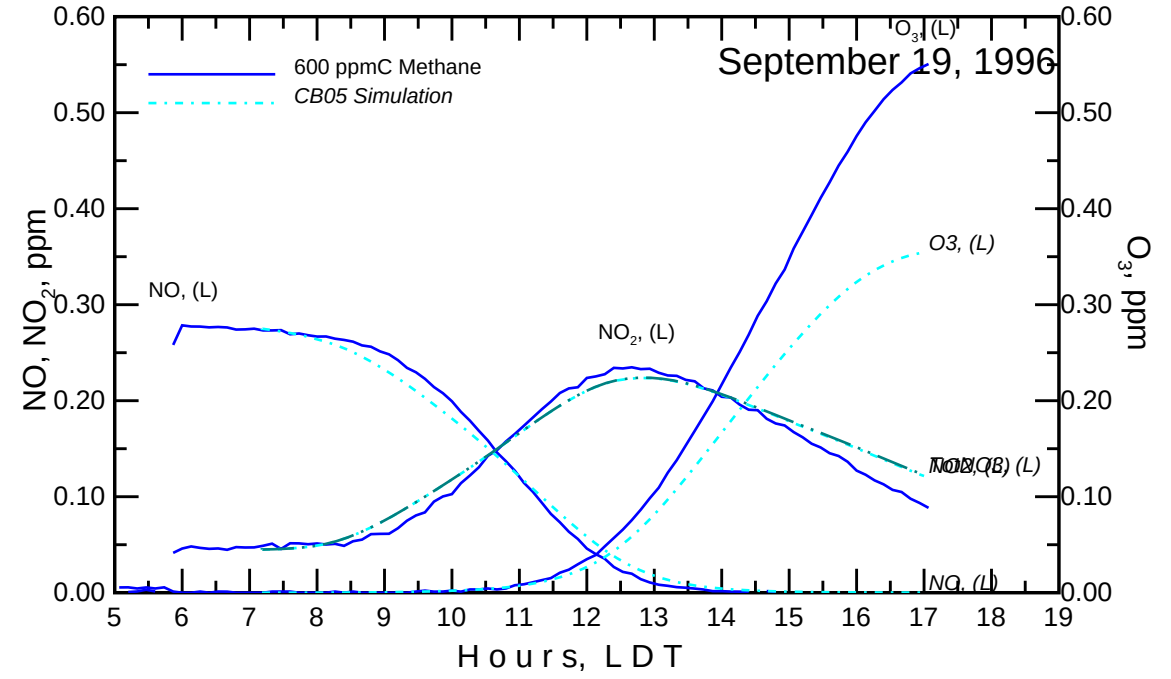


Matched Methane

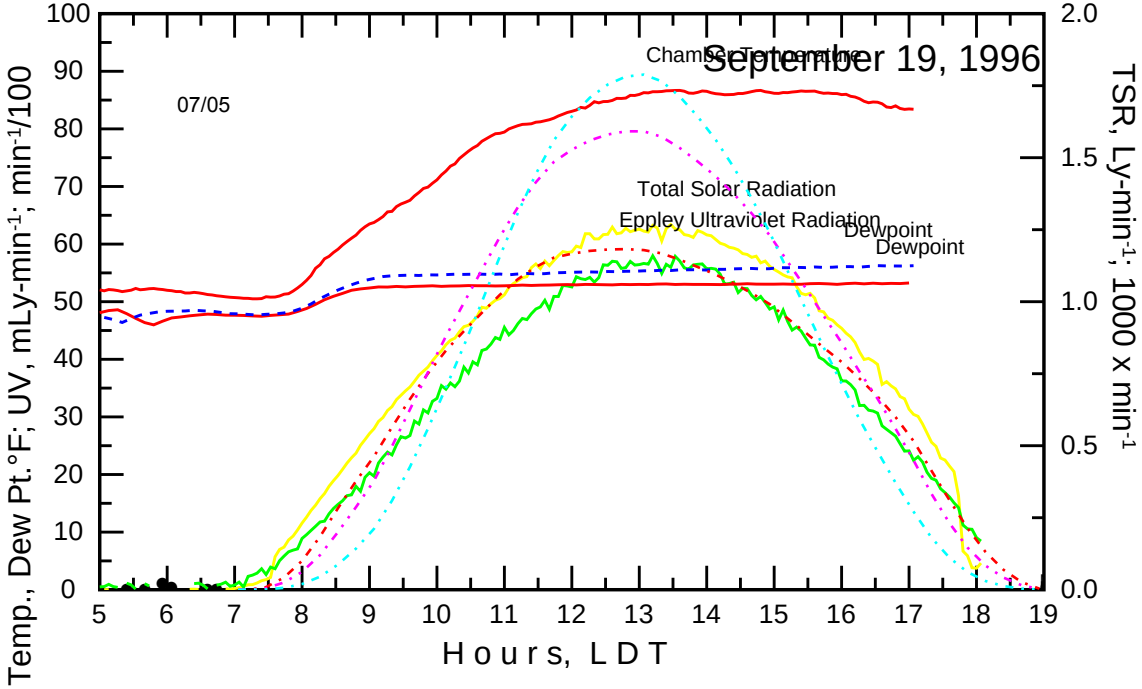

Chamber Temperature
September 7, 1990
07/05
Dewpoint
Dewpoint
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

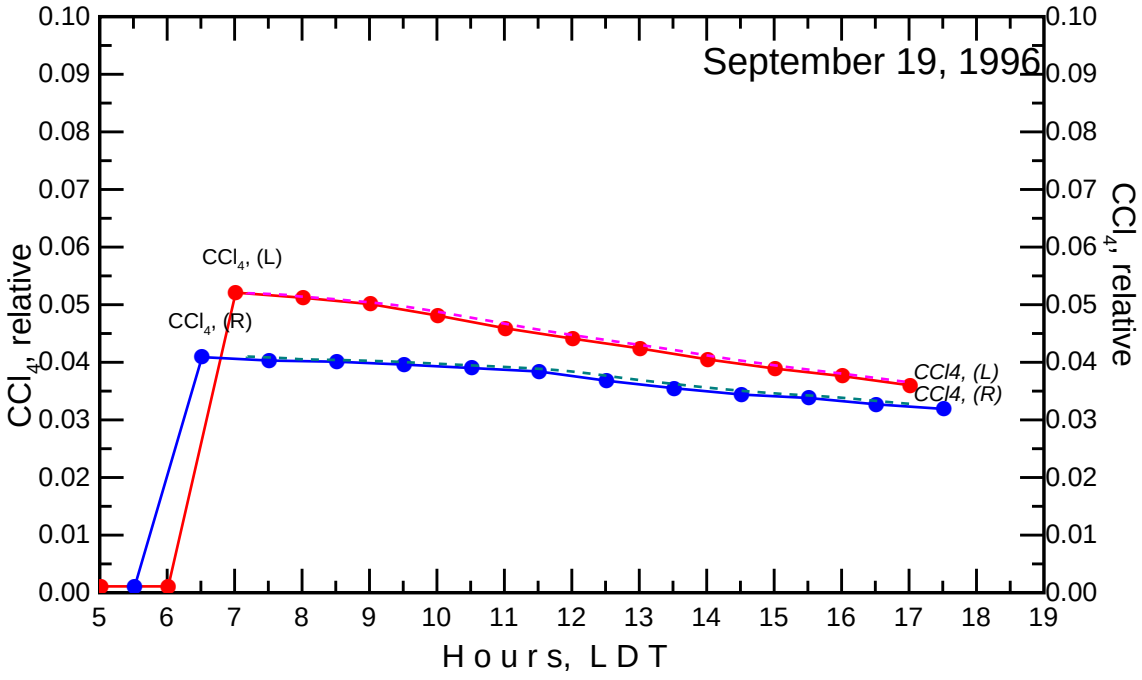

September 7, 1990
CCl4, relative
CCl4, relative
CCl4,I(B)
Hours, LDT

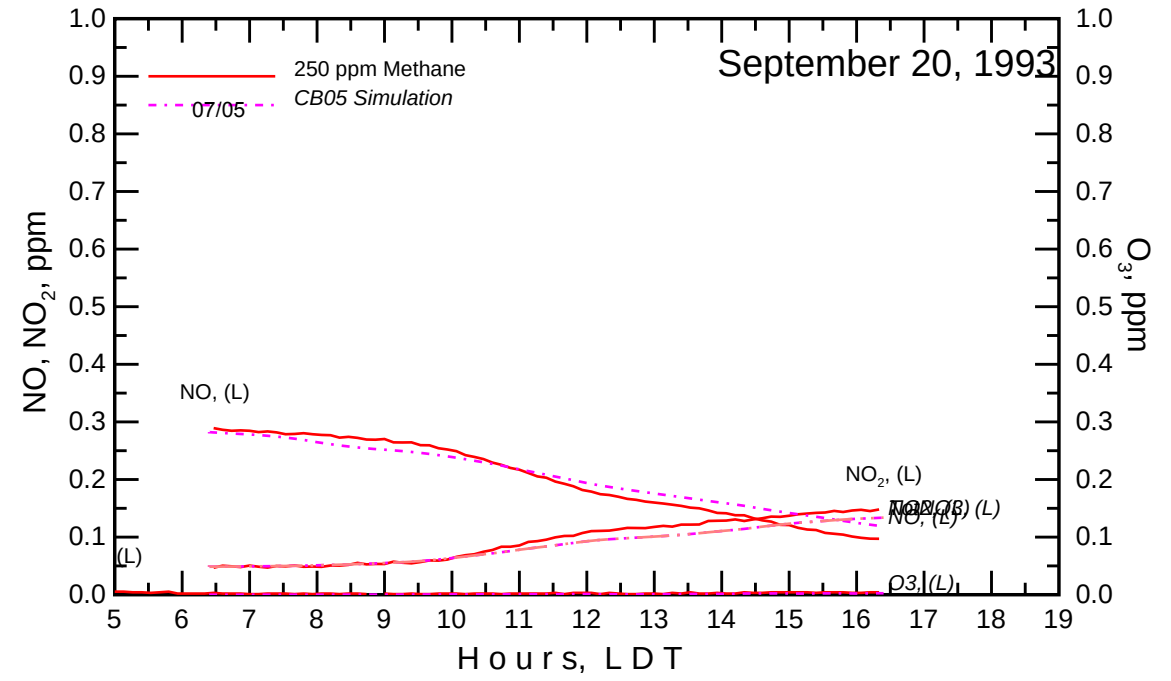


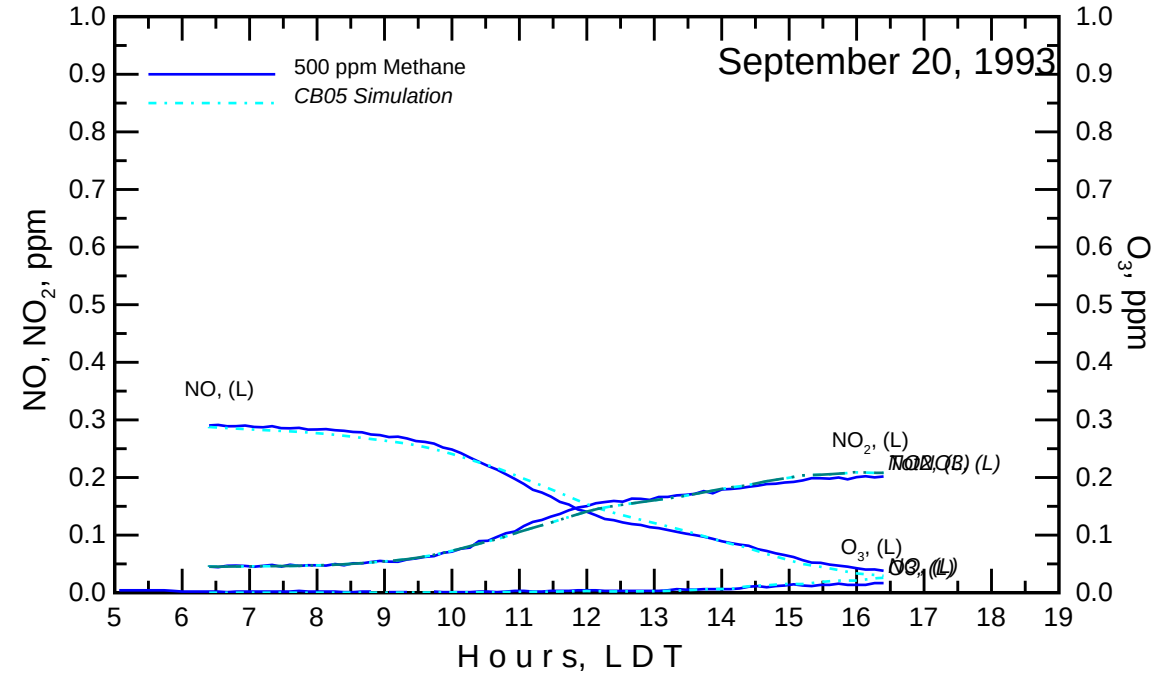


Delta Methane

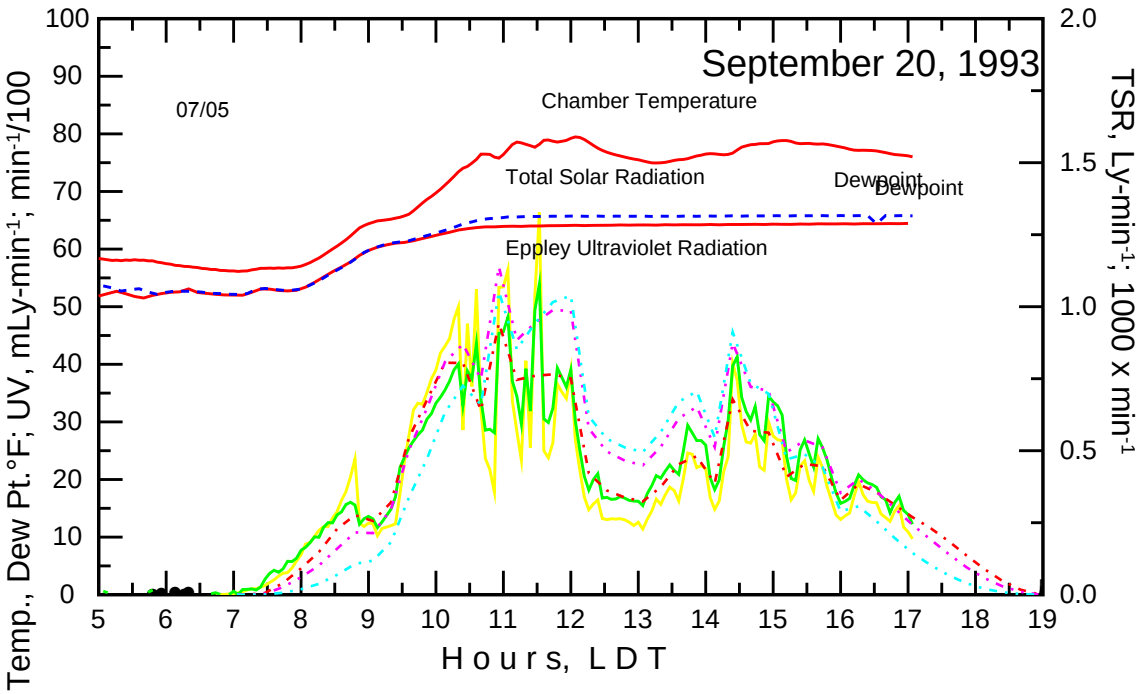

September 19, 1996
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


September 19, 1996
CCl4, (L)
CCl4, (R)
CCl4, (L)
CCl4, (R)
CCl4, relative
CCl4, relative
Hours, LDT



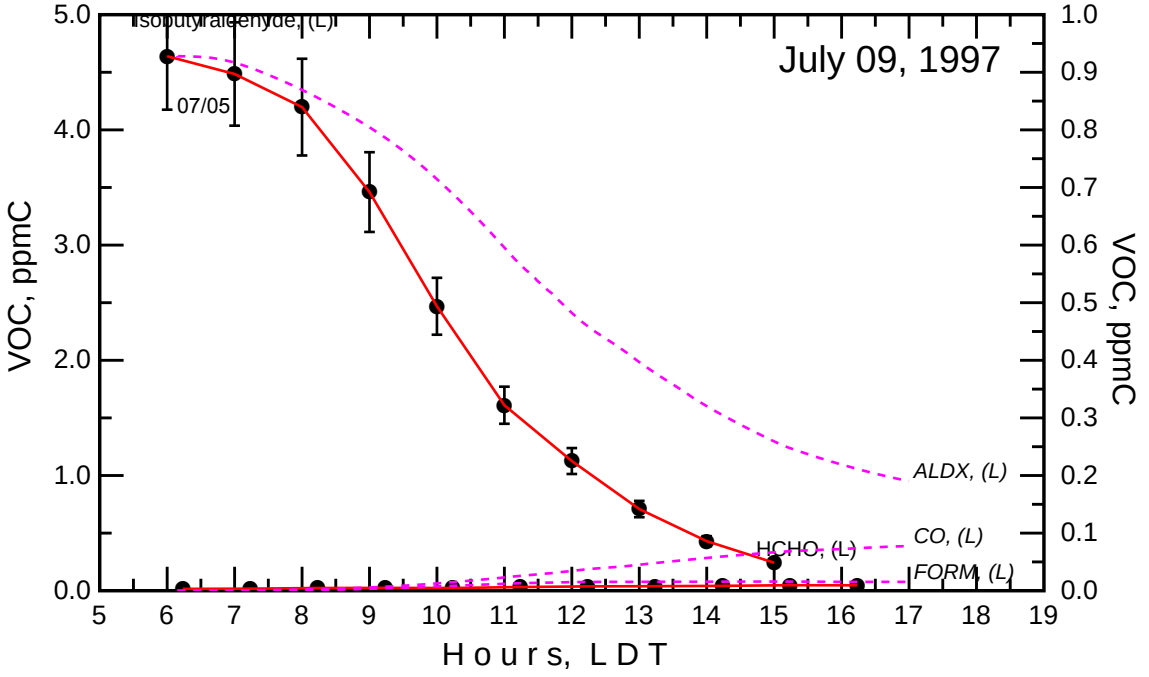


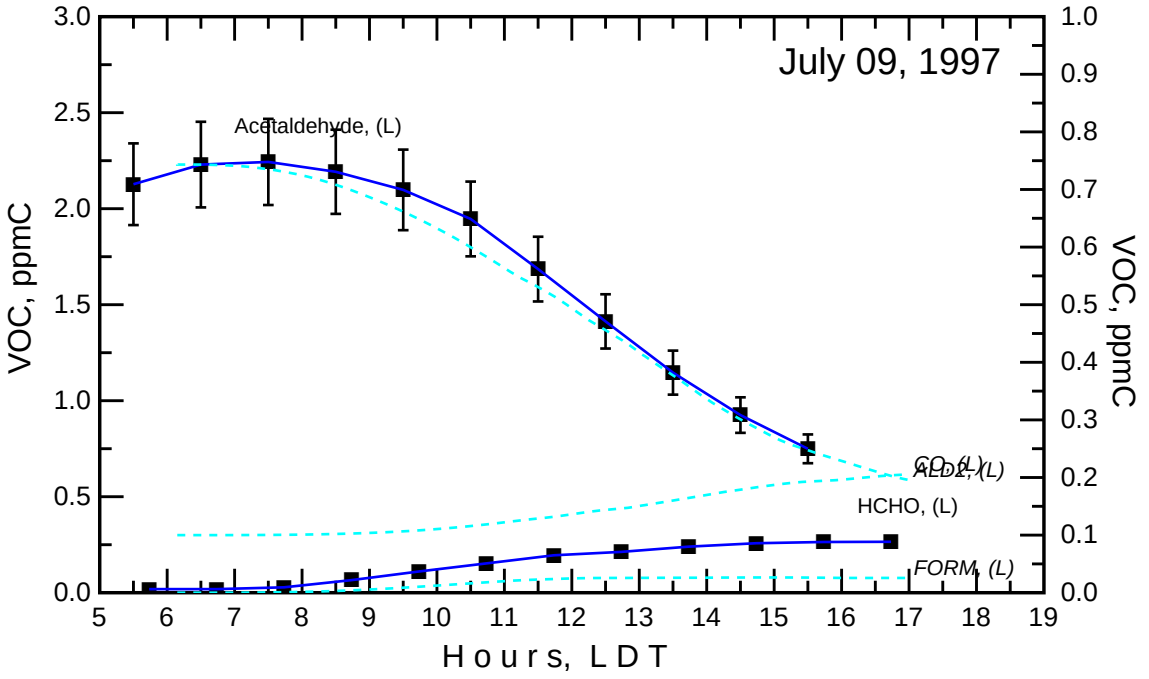
500 vs 250 Methane

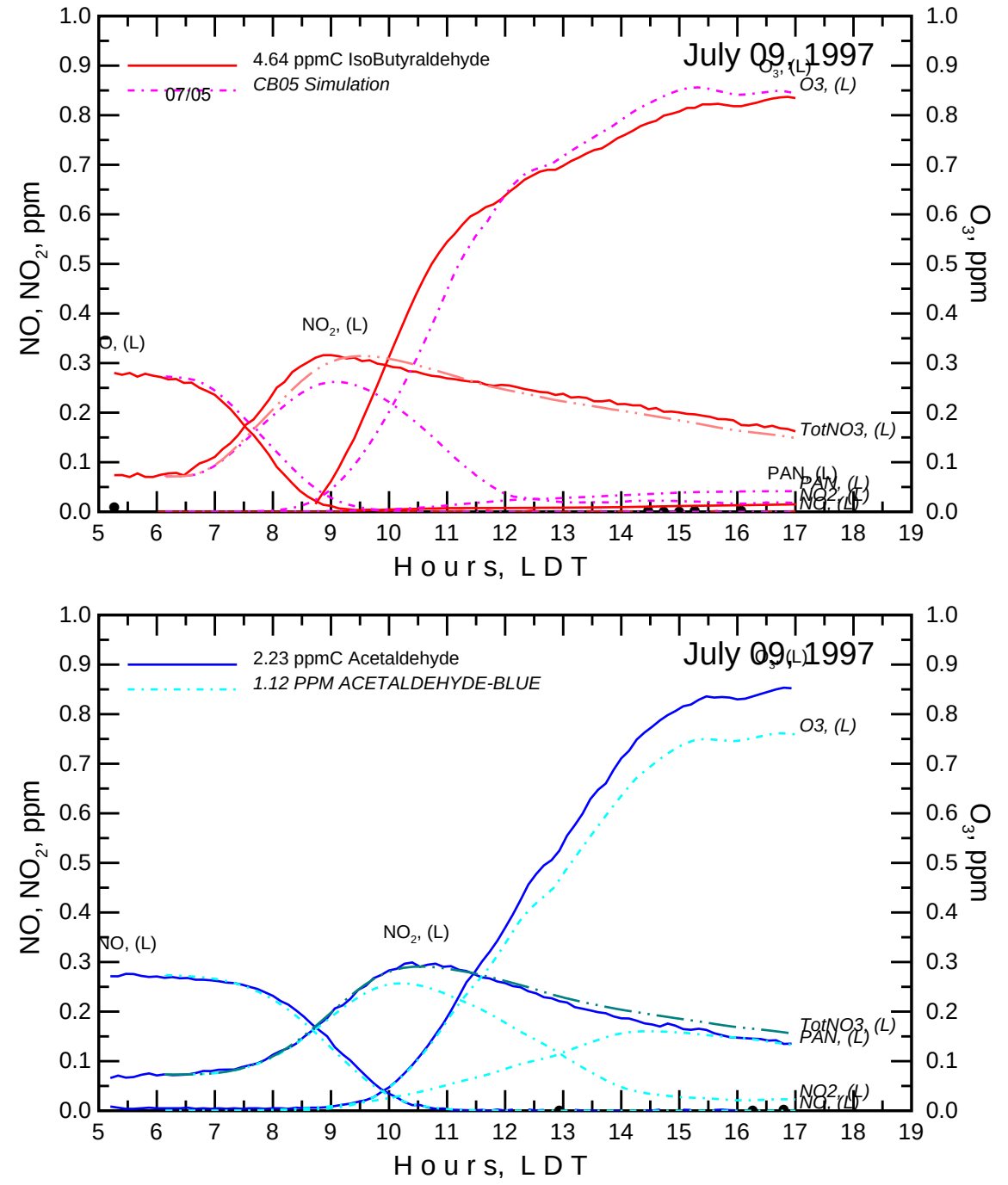

September 20, 1993
07/05
Chamber Temperature
Total Solar Radiation
Dewpoint
Dewpoint
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

Acetaldehyde (ALD2)

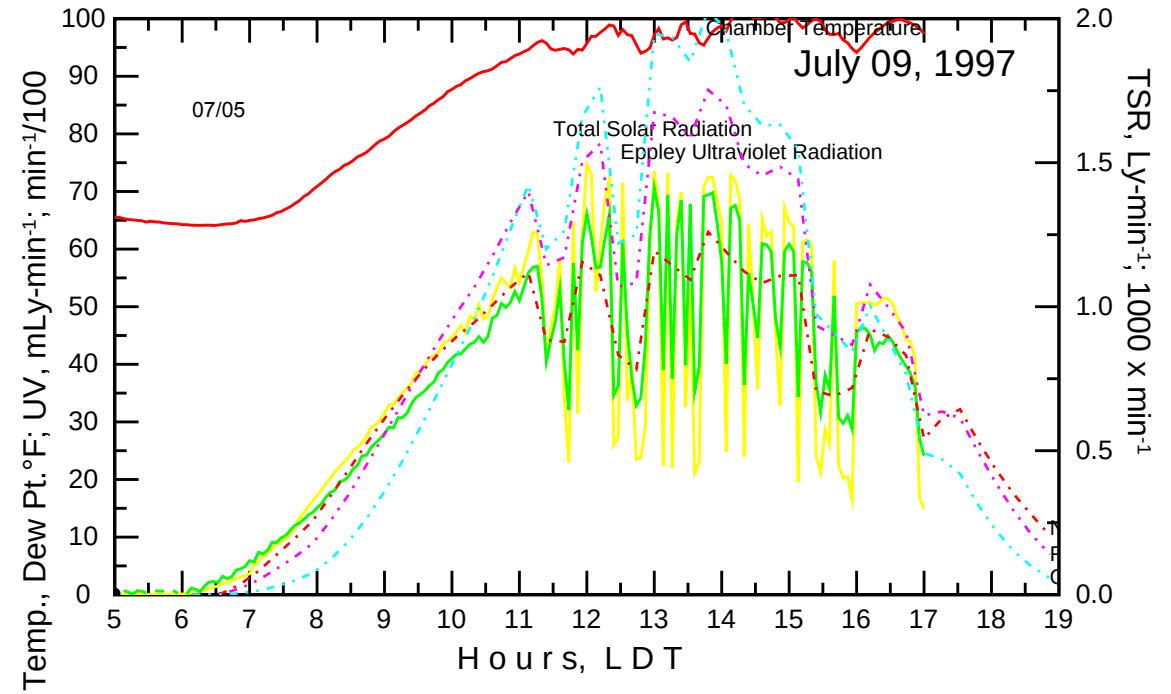
JL 09 97
JL 18 97
AU 17 78

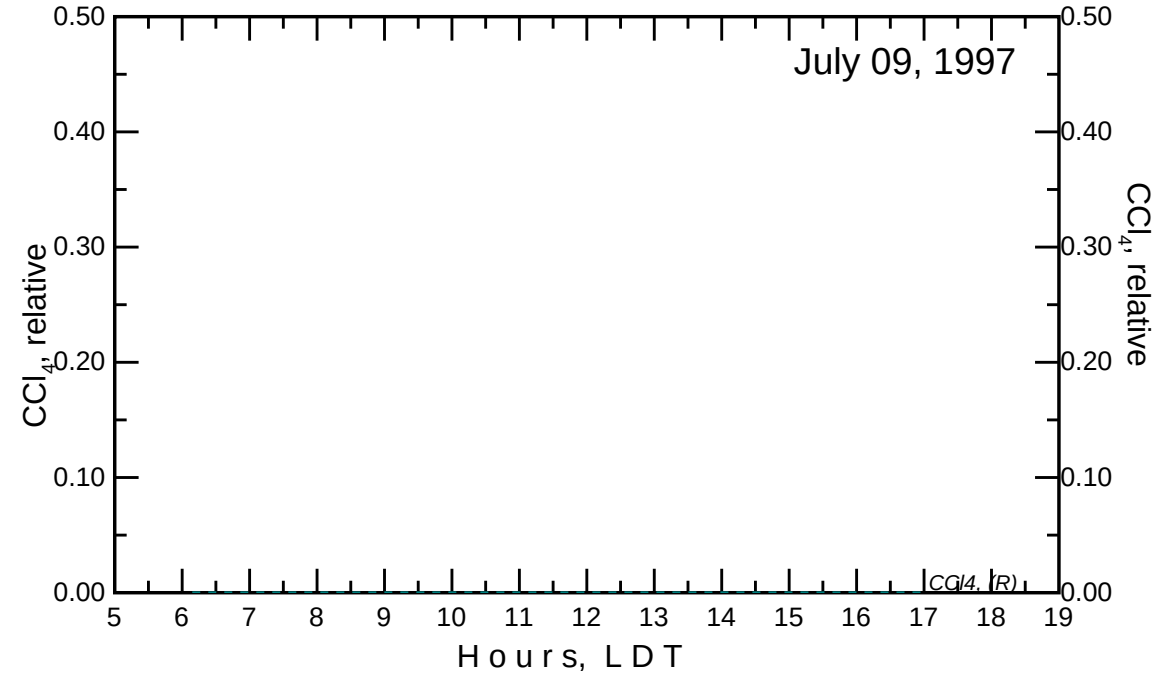

July 09, 1997
Isobutyraldehyde, (L)
07/05
ALDX, (L)
CO, (L)
HCHO, (L)
FORM, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

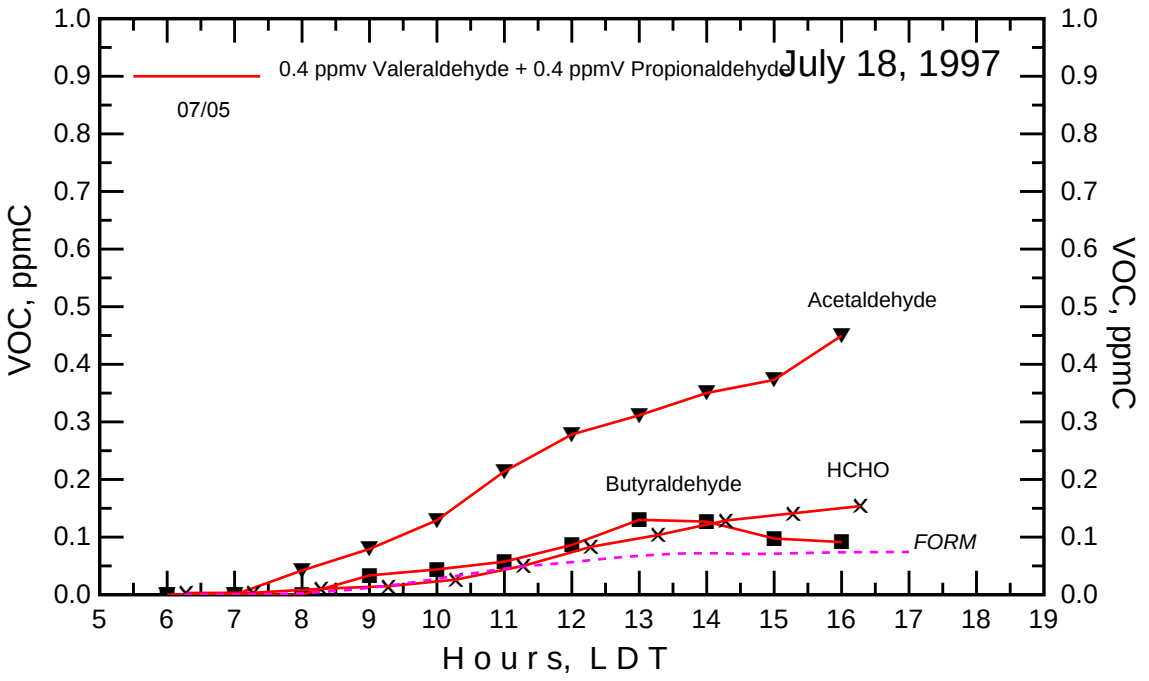

July 09, 1997
Acetaldehyde, (L)
CO, (L)
ALDX, (L)
HCHO, (L)
FORM, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

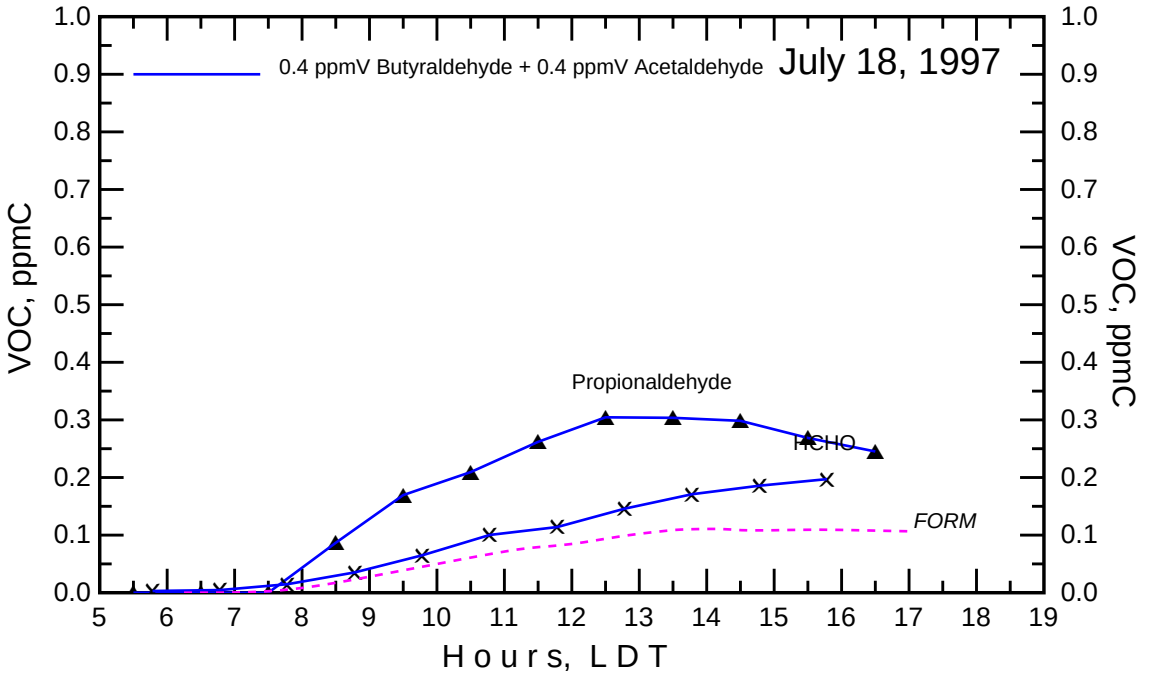


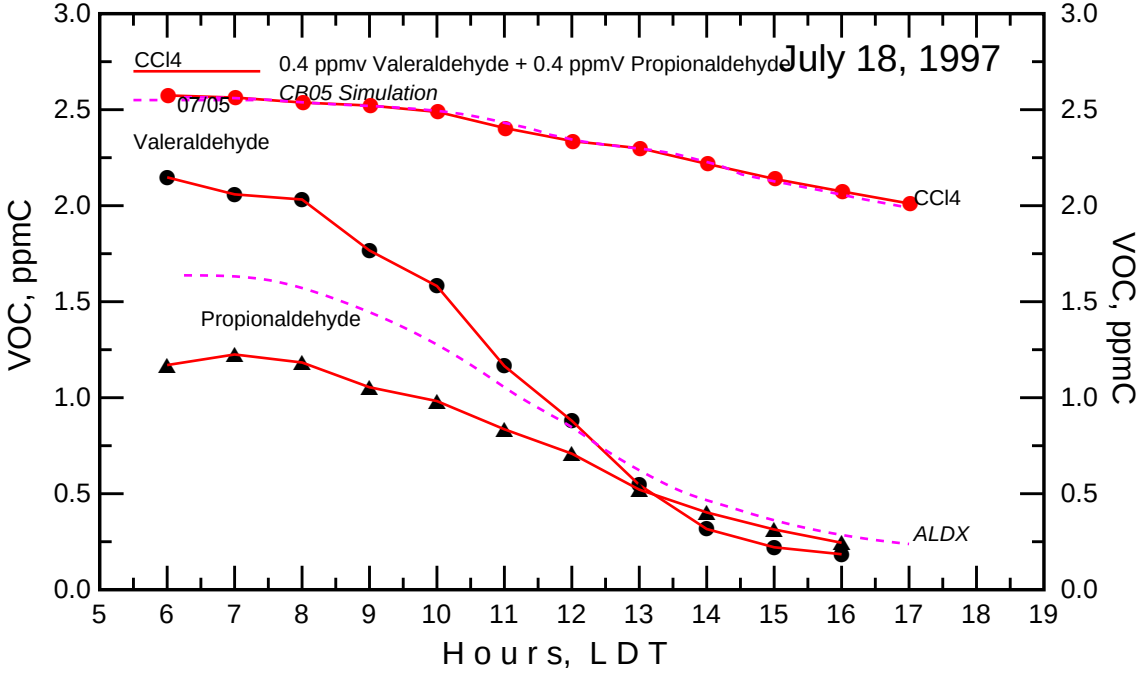
Acetaldehyde vs Isobutyraldehyde

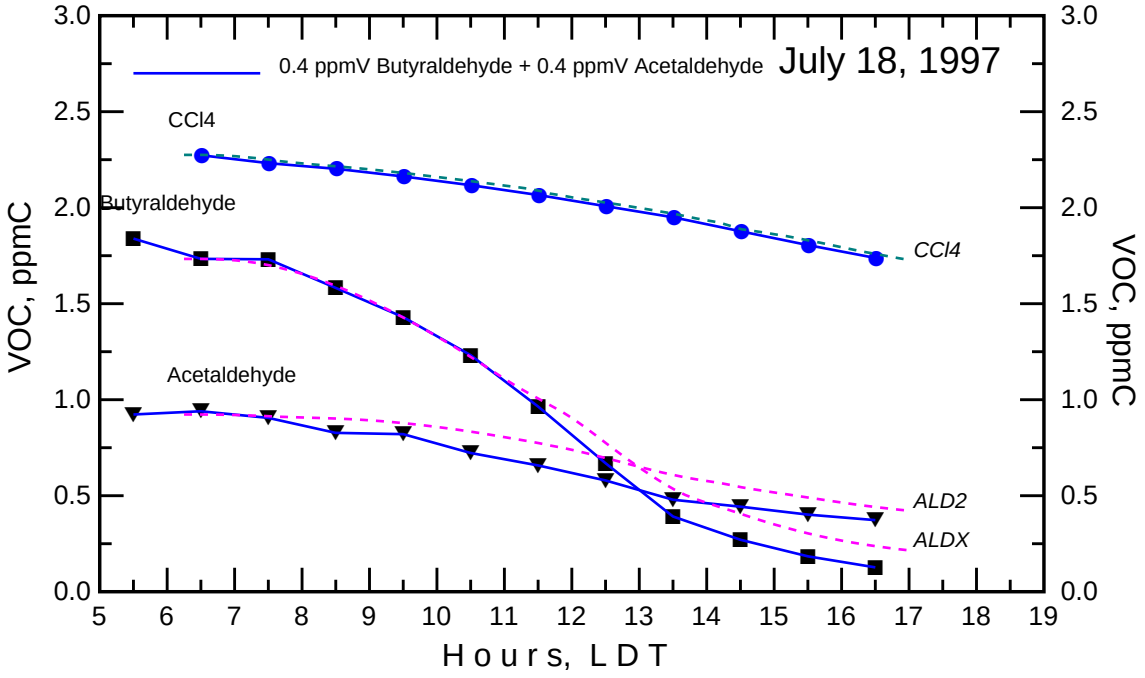

Chamber Temperature
July 09, 1997
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

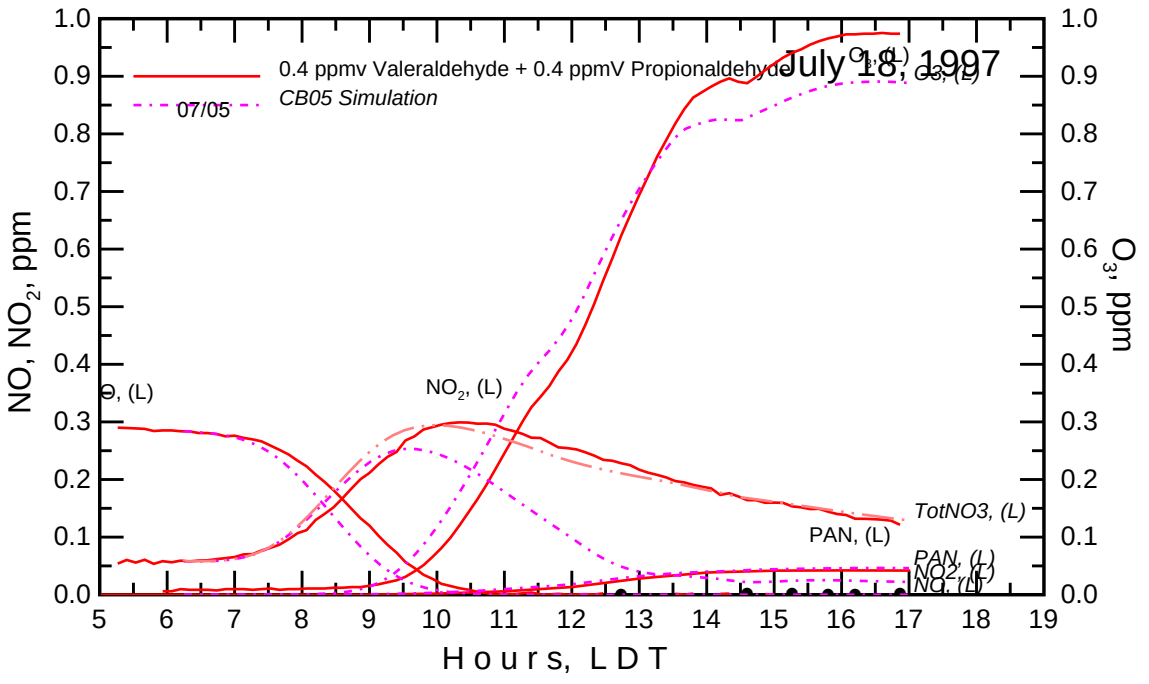

July 09, 1997
CCl4, relative
CCl4, relative
CCl4, (R)
Hours, LDT

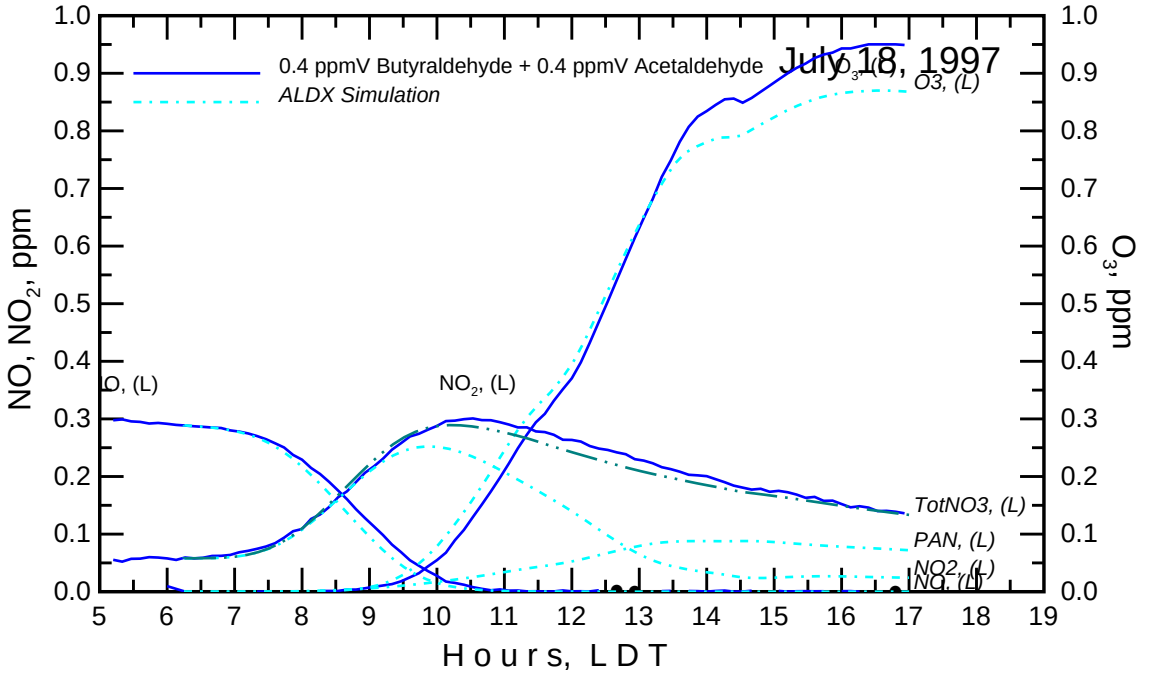

0.4 ppmv Valeraldehyde + 0.4 ppmV Propionaldehyde
July 18, 1997
07/05
Acetaldehyde
Butyraldehyde
HCHO
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT


0.4 ppmV Butyraldehyde + 0.4 ppmV Acetaldehyde
July 18, 1997
Propionaldehyde
HCHO
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT

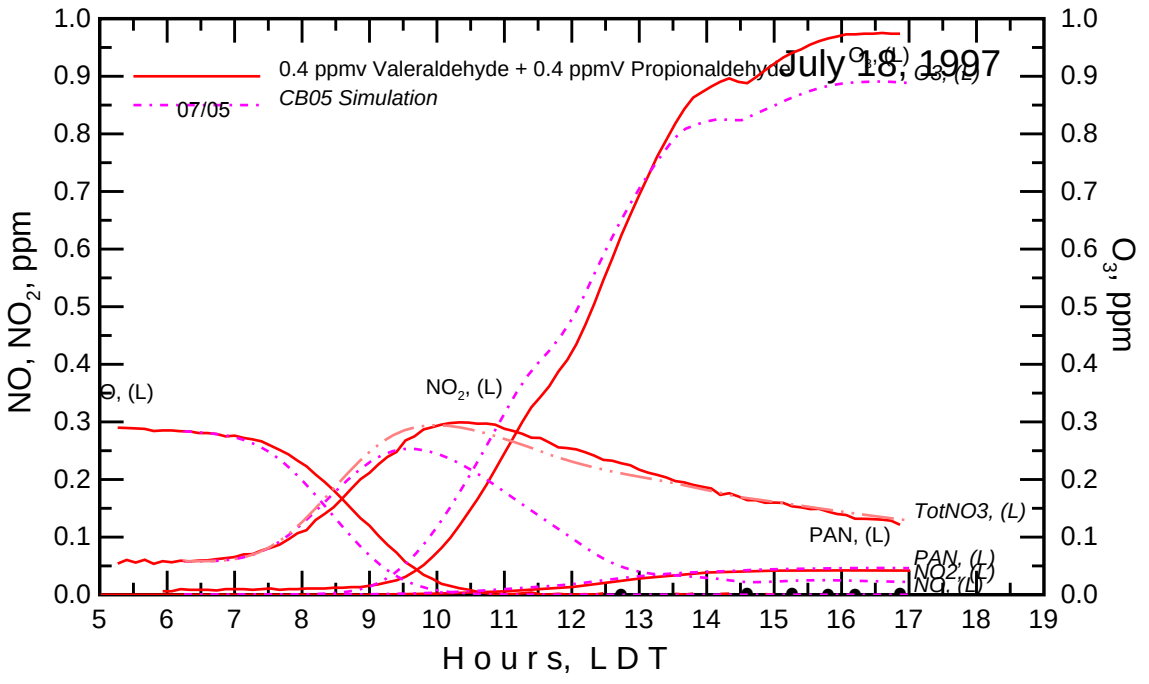

CCl4
0.4 ppmv Valeraldehyde + 0.4 ppmV Propionaldehyde
July 18, 1997
CB05 Simulation
07/05
Valeraldehyde
CCl4
Propionaldehyde
ALDX
VOC, ppmC
VOC, ppmC
Hours, LDT

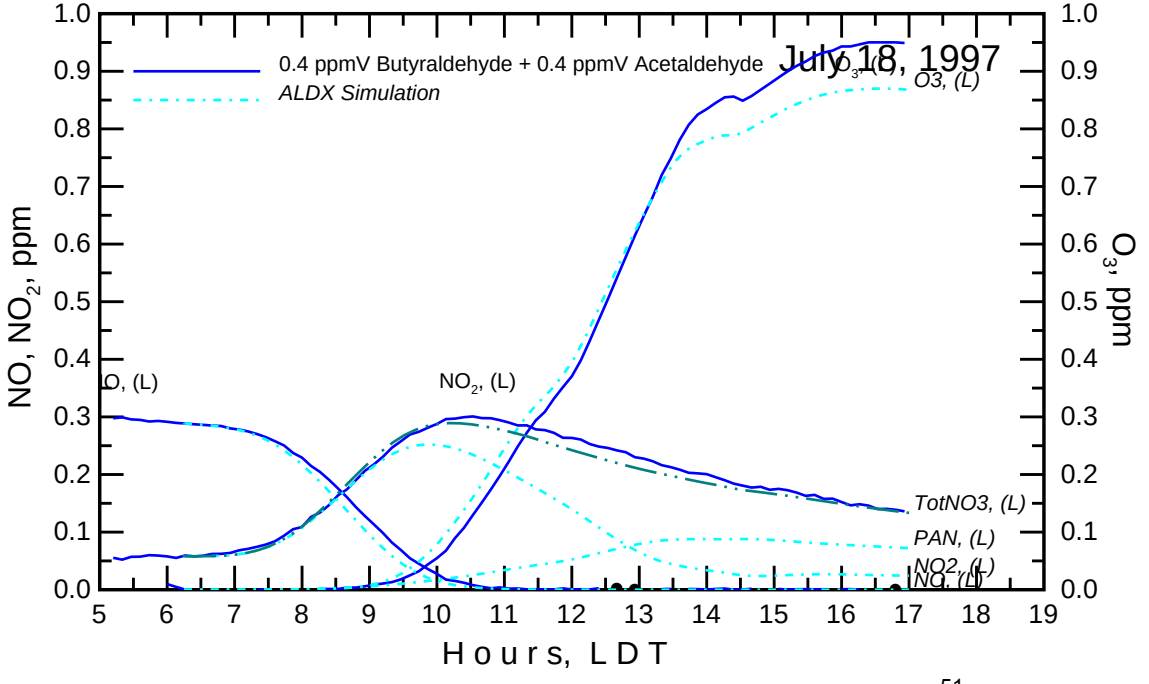

0.4 ppmV Butyraldehyde + 0.4 ppmV Acetaldehyde
July 18, 1997
CCl4
Butyraldehyde
CCl4
Acetaldehyde
ALD2
ALDX
VOC, ppmC
VOC, ppmC
Hours, LDT



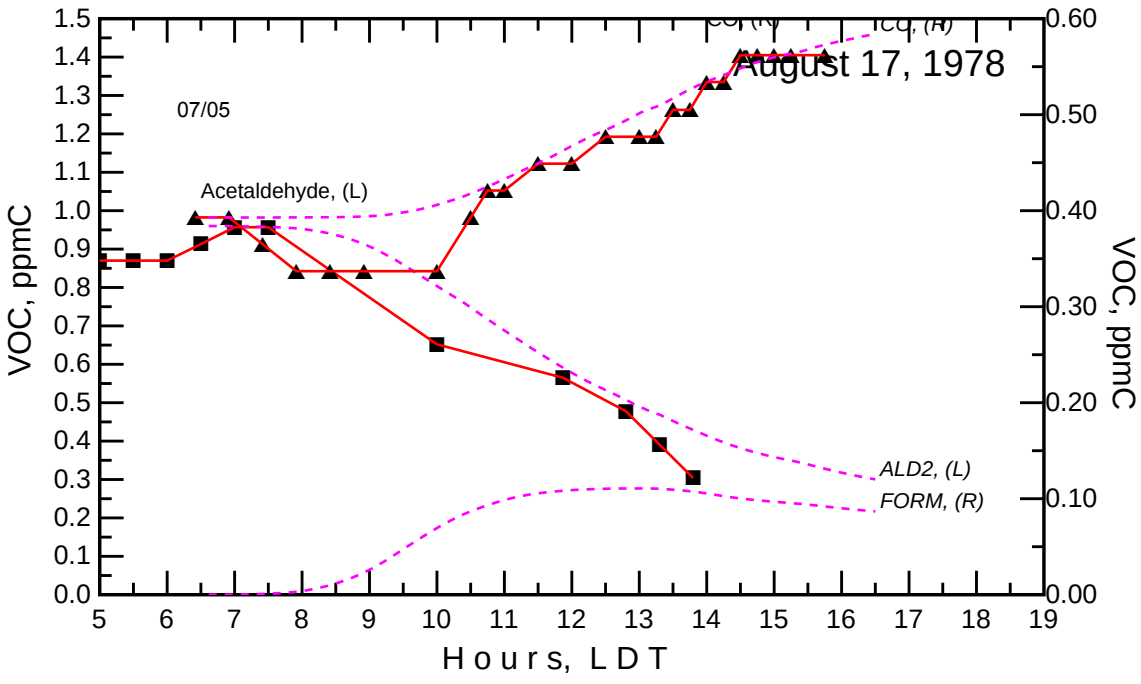


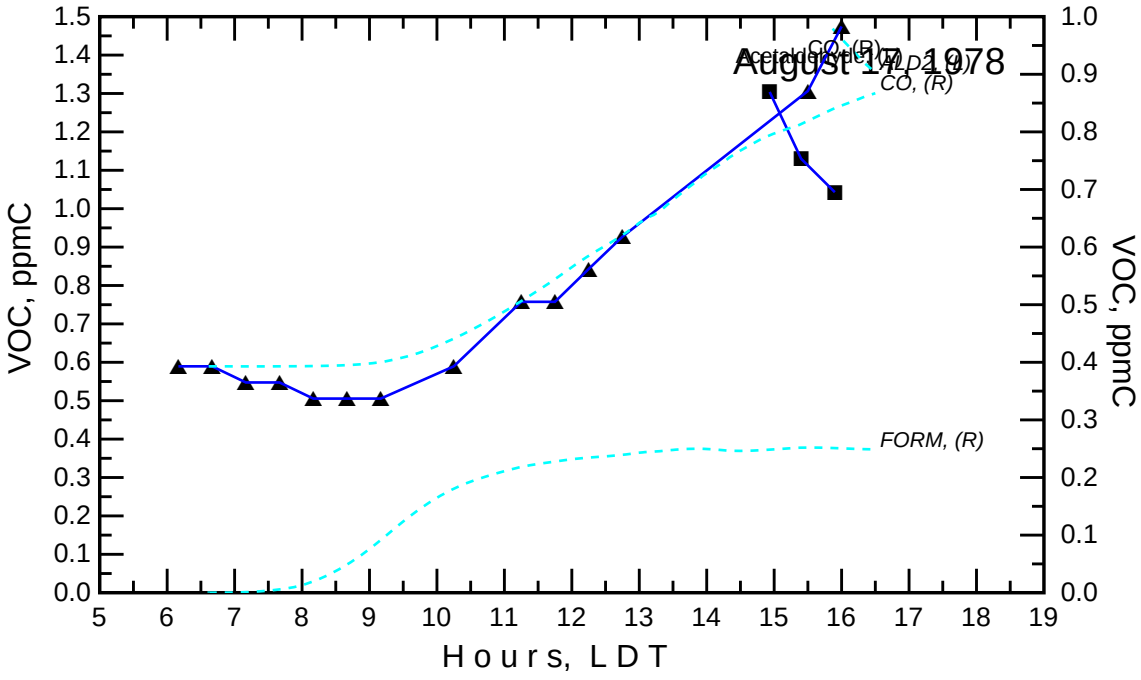
Aldehyde Mix and NOx

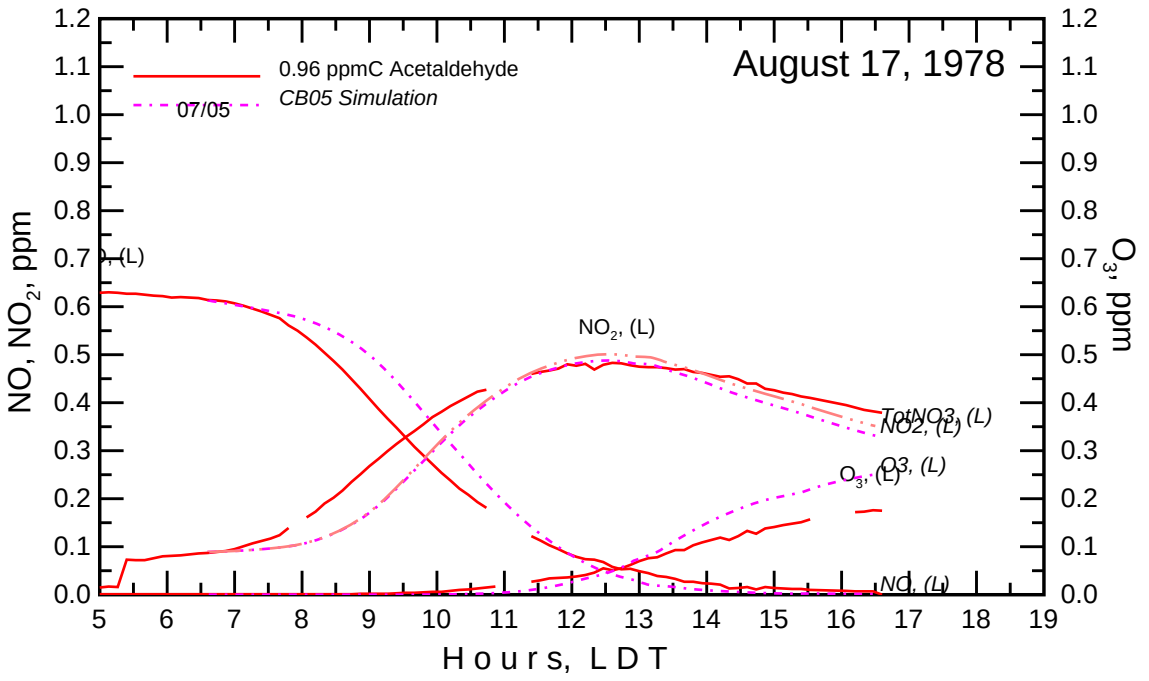


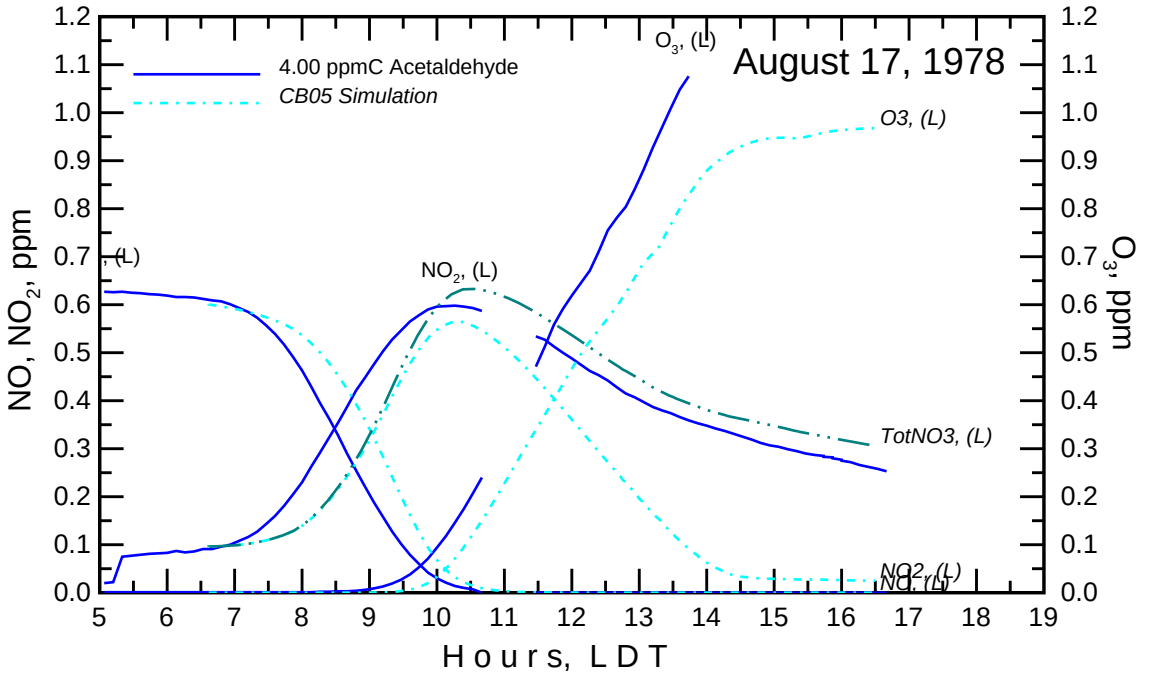


Aldehyde Mix and NOx

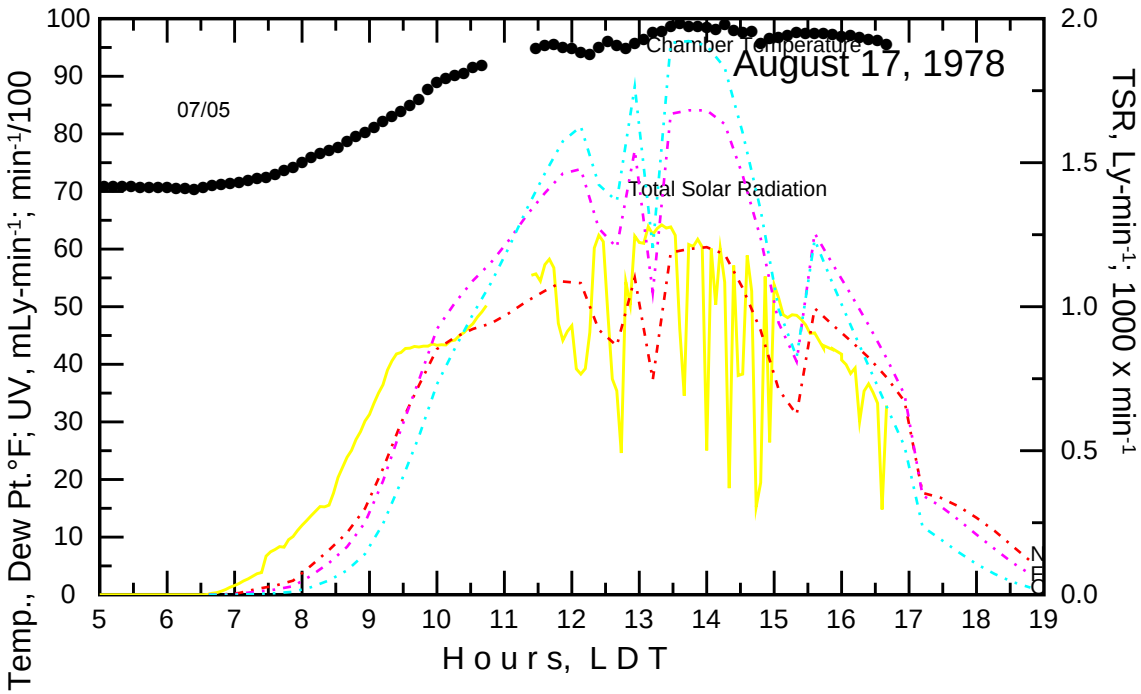

August 17, 1978
07/05
Acetaldehyde, (L)
ALD2, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

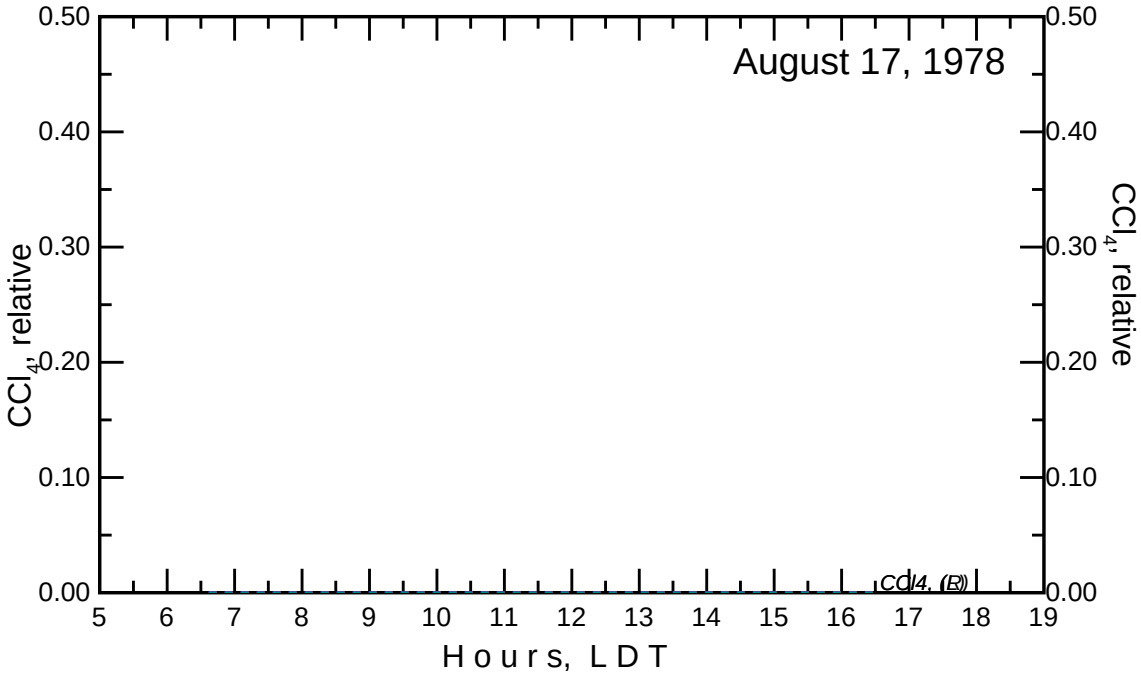

August 17, 1978
CO, (R)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT





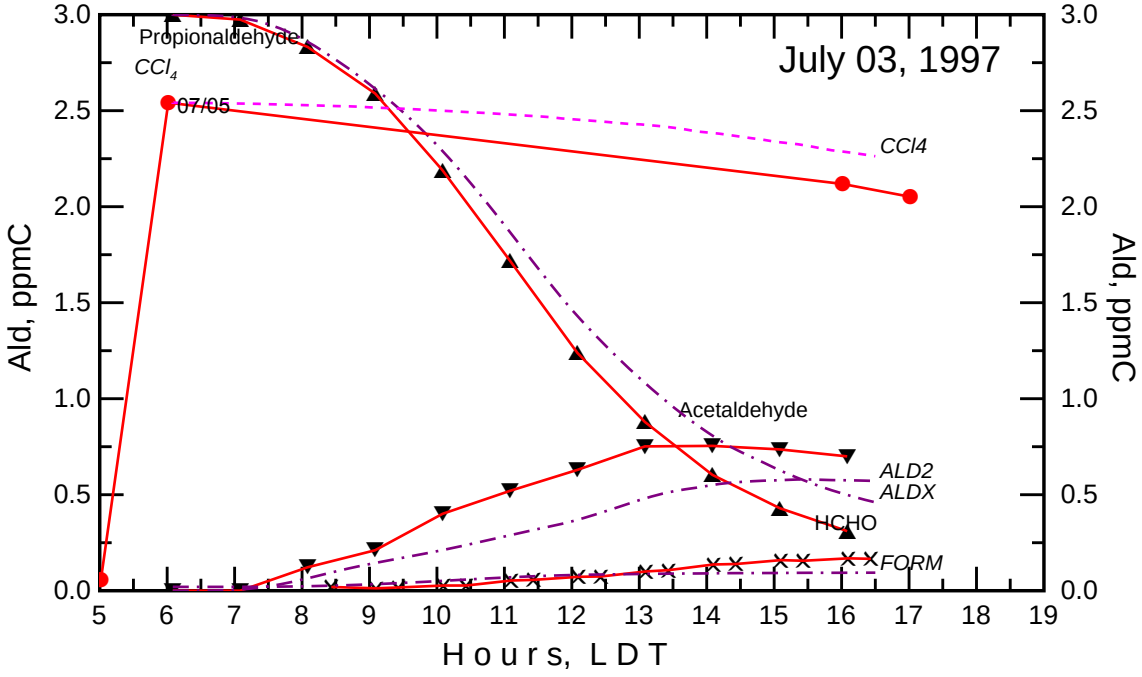
Delta HC at 0.70 ppm NO_x

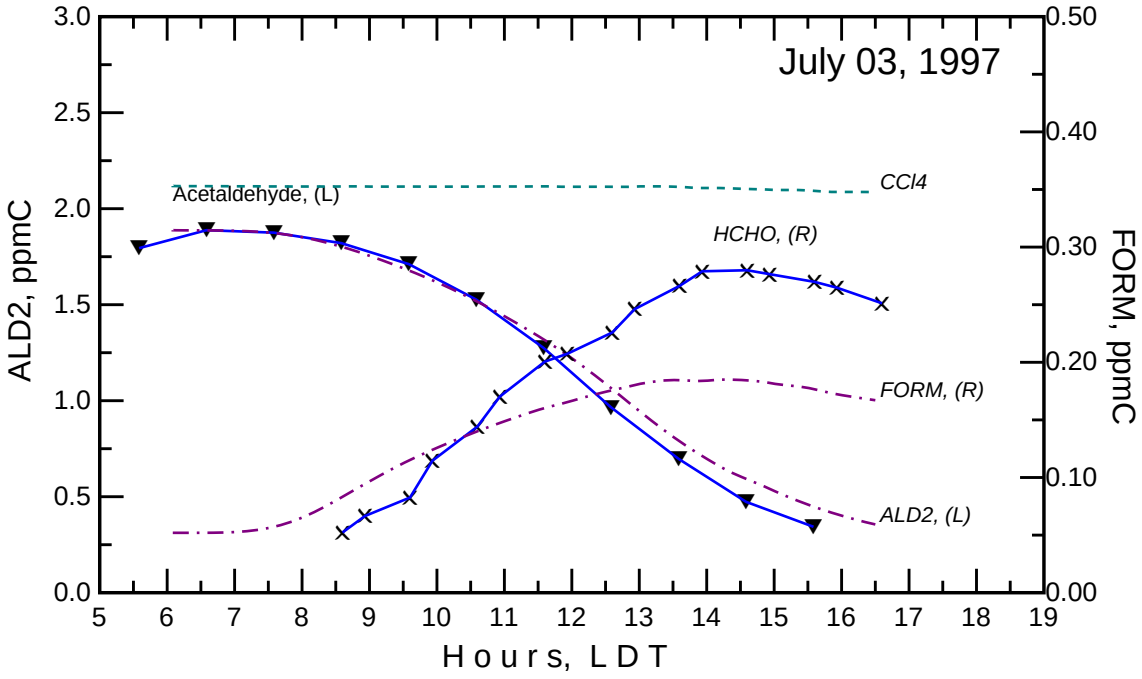

August 17, 1978
Chamber Temperature
07/05
Total Solar Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

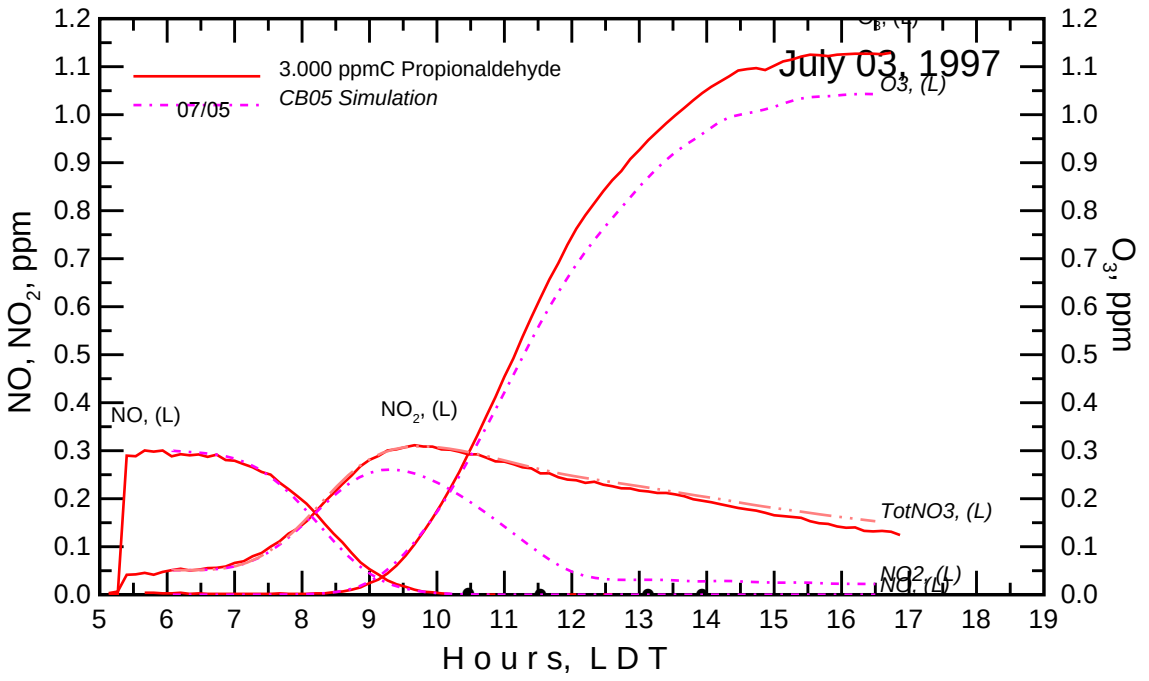

August 17, 1978
CCl4, relative
CCl4, (E)
Hours, LDT

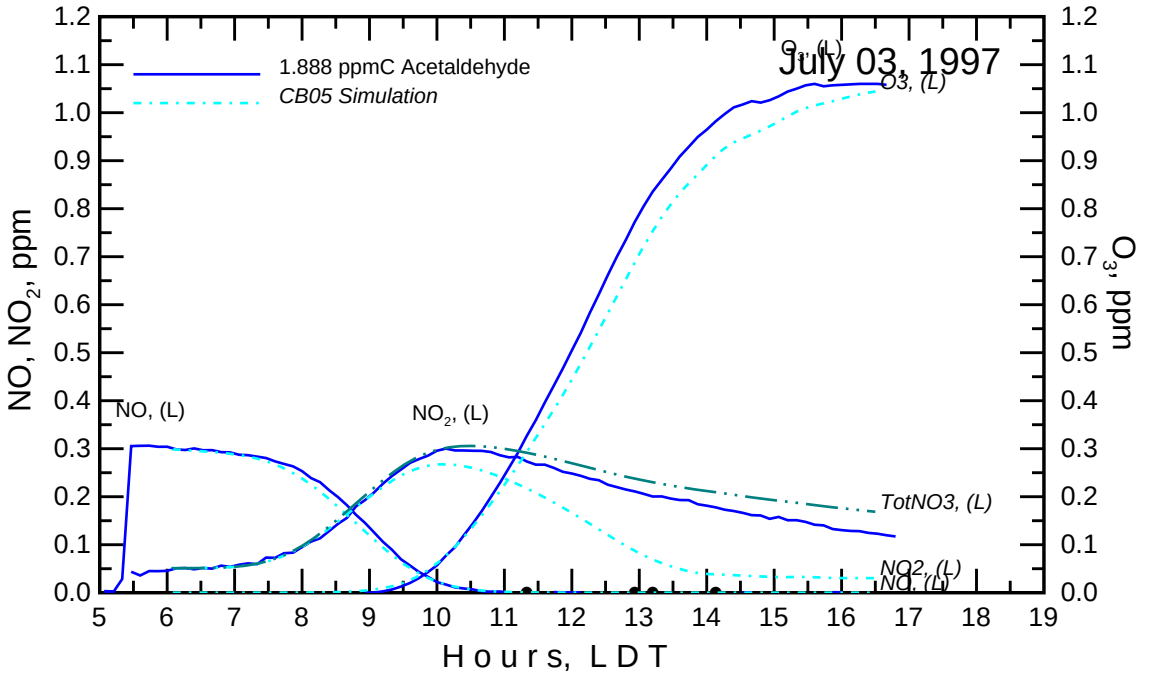
Higher Aldehydes (ALDX)

JL 03 97
AU 12 97
ST 04 97
OC 04 96

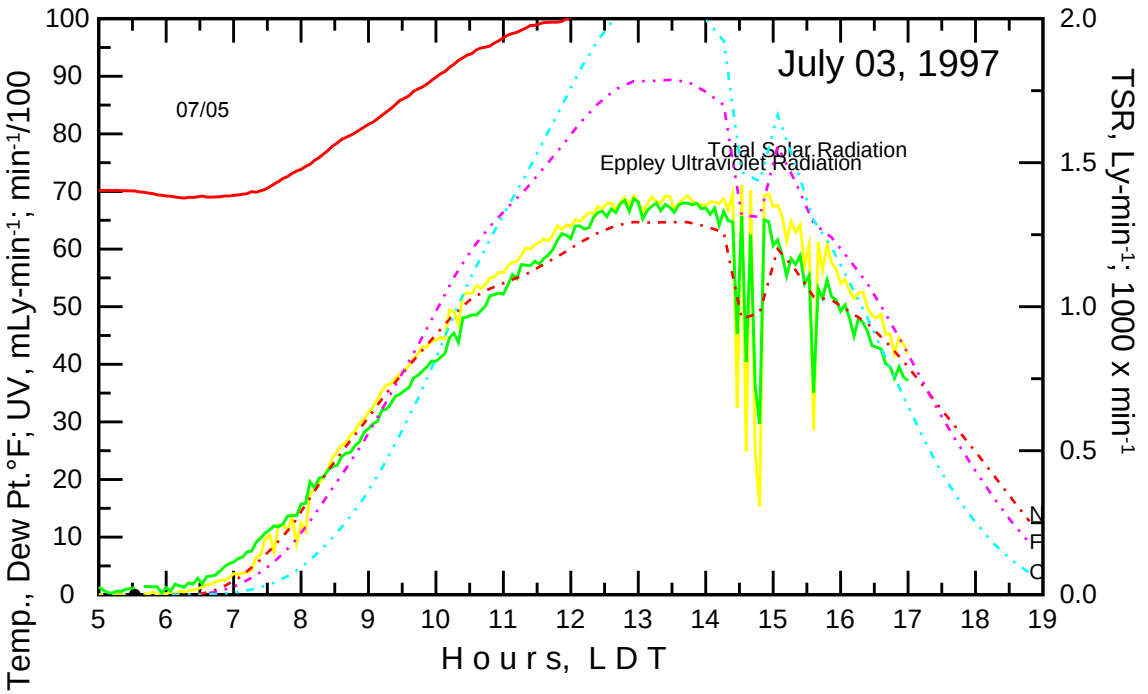

July 03, 1997
Propionaldehyde
CCl4
07/05
CCl4
Acetaldehyde
ALD2
ALDX
HCHO
FORM
Ald, ppmC
Hours, LDT

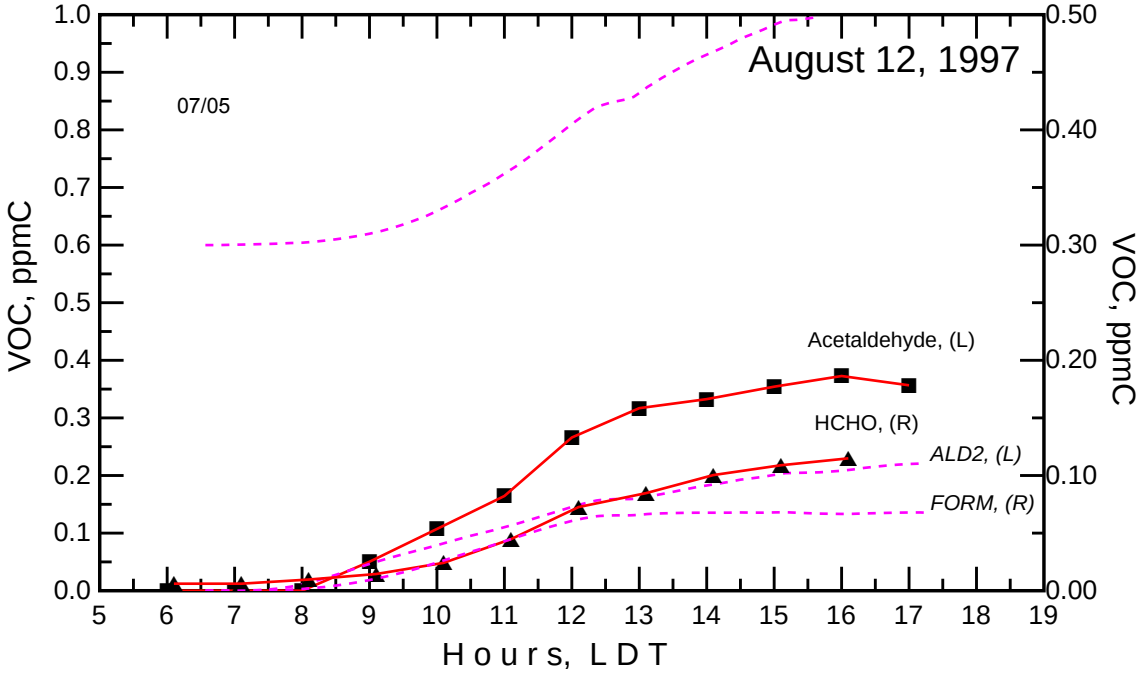

July 03, 1997
Acetaldehyde, (L)
CCl4
HCHO, (R)
FORM, (R)
ALD2, (L)
ALD2, ppmC
FORM, ppmC
Hours, LDT

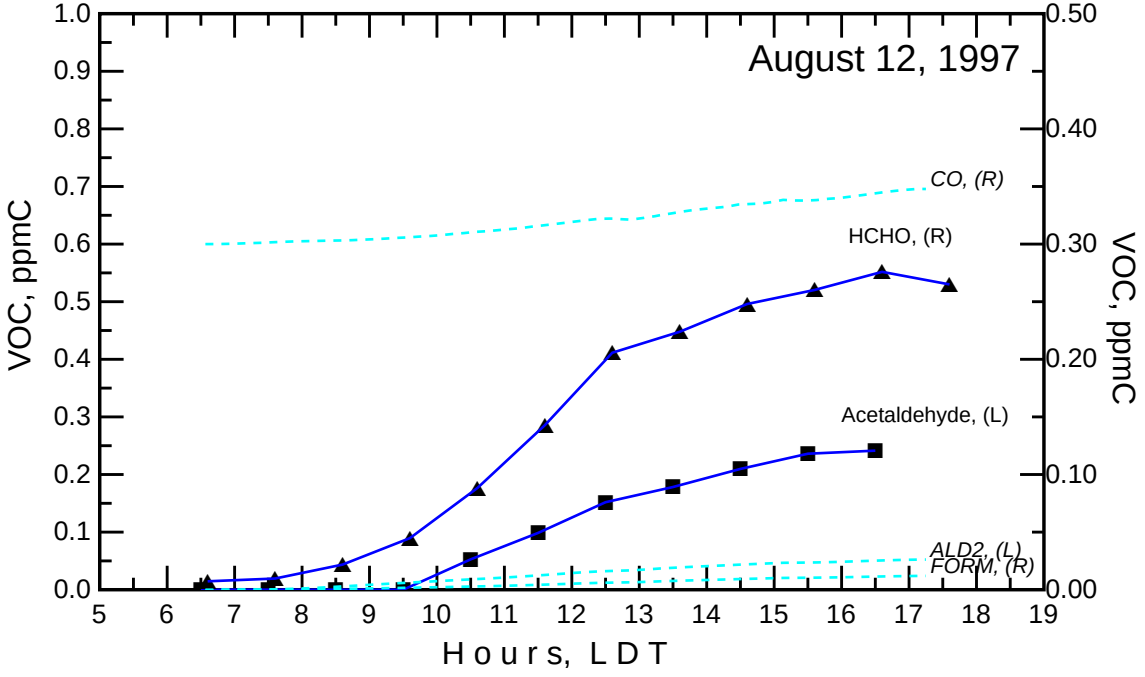


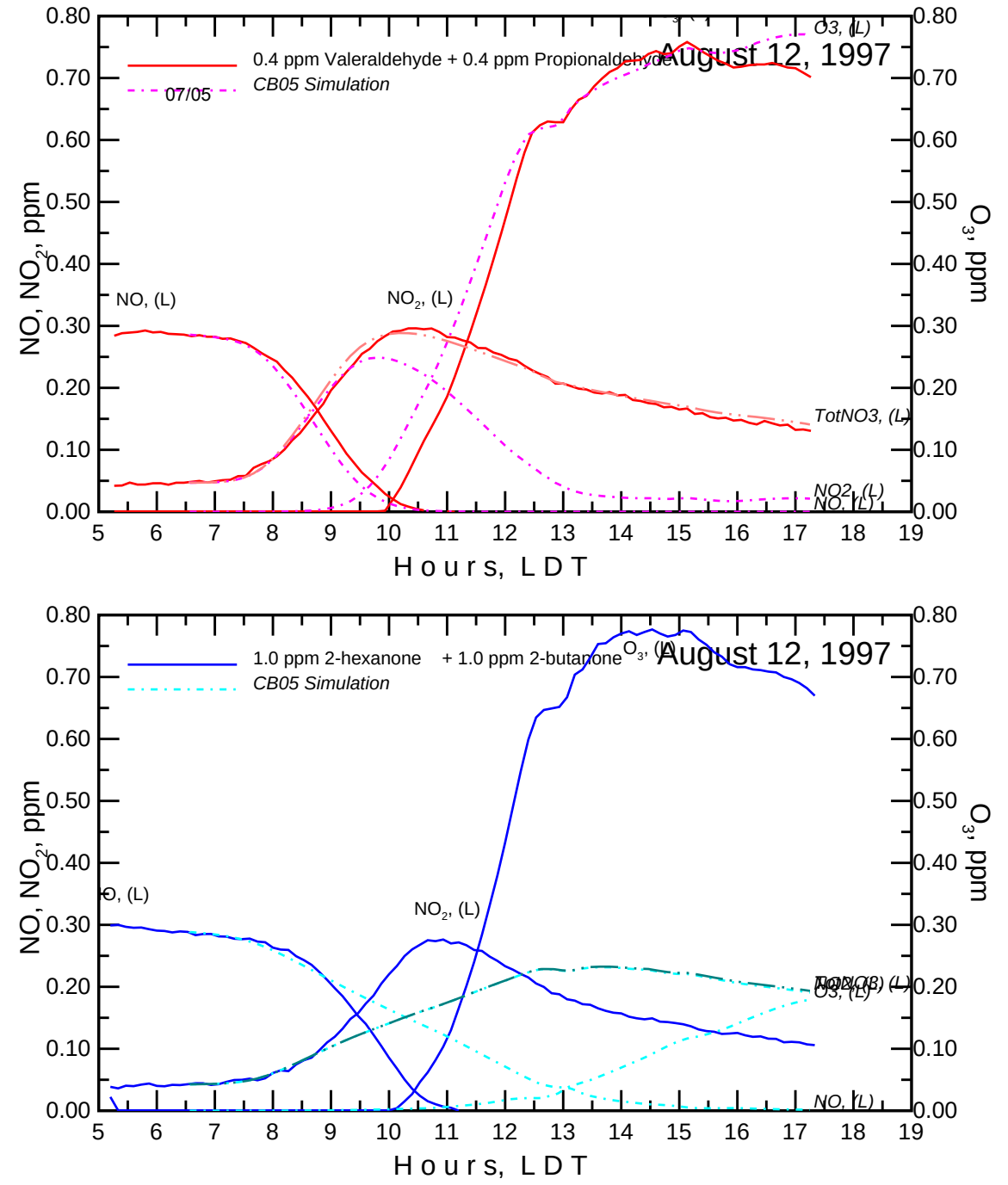


Acetaldehyde vs Propionaldehyde

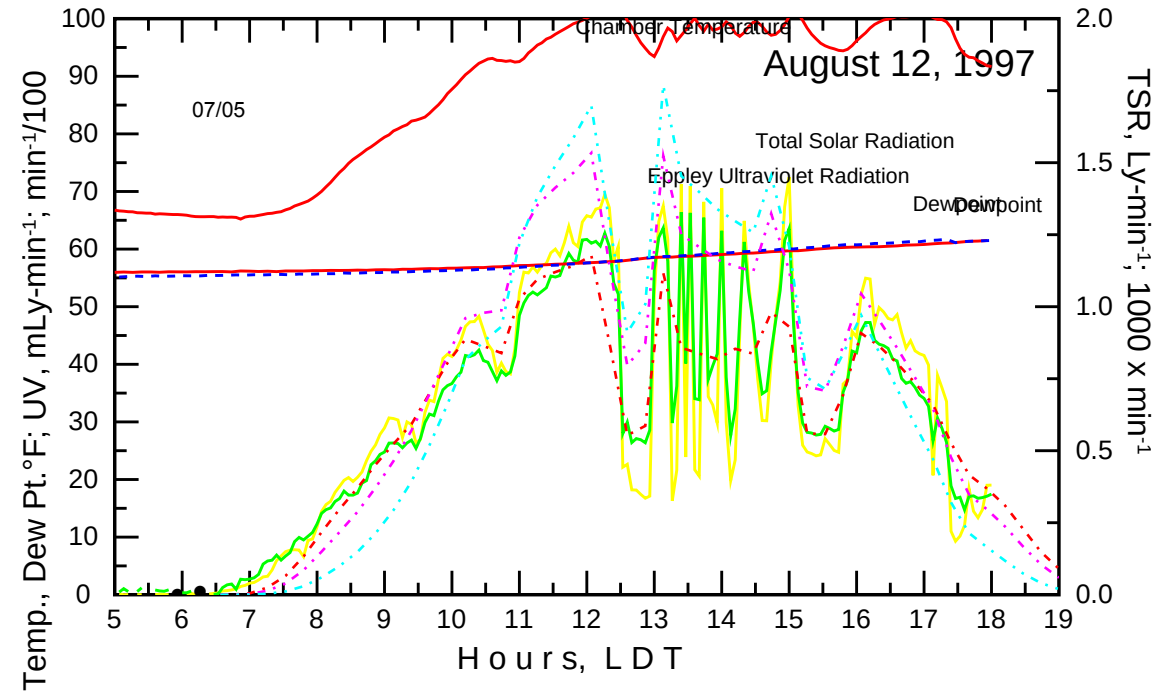

July 03, 1997
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
100
90
80
70
60
50
40
30
20
10
0
2.0
1.5
1.0
0.5
0.0
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

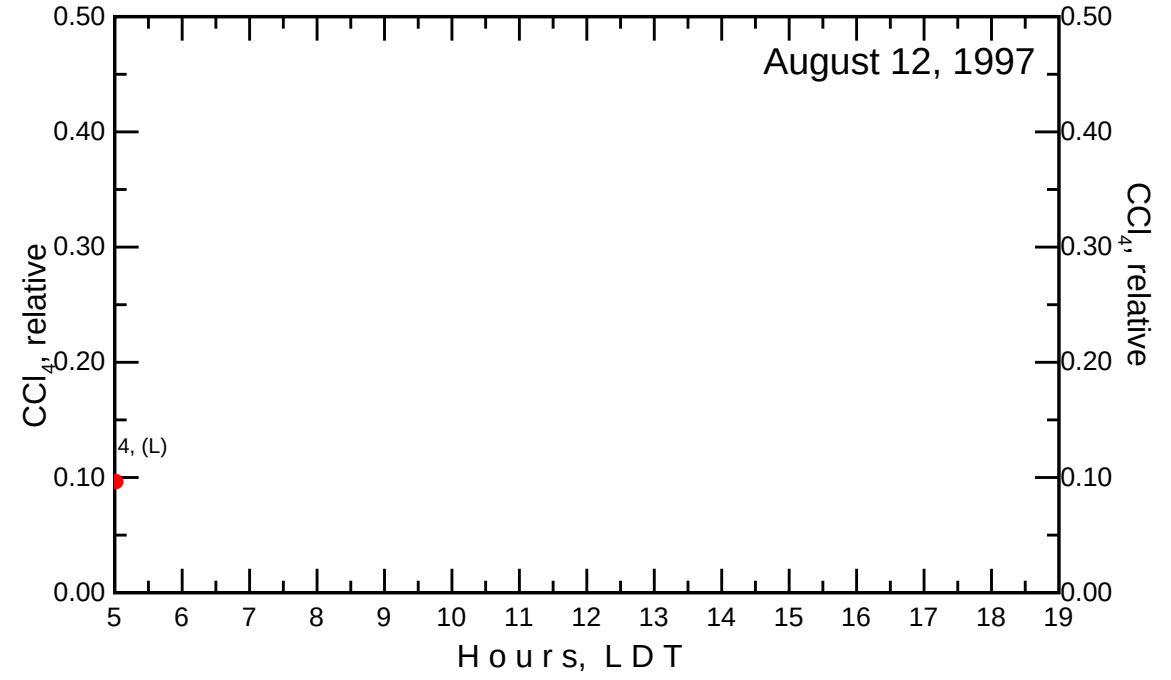

August 12, 1997
07/05
Acetaldehyde, (L)
HCHO, (R)
ALD2, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

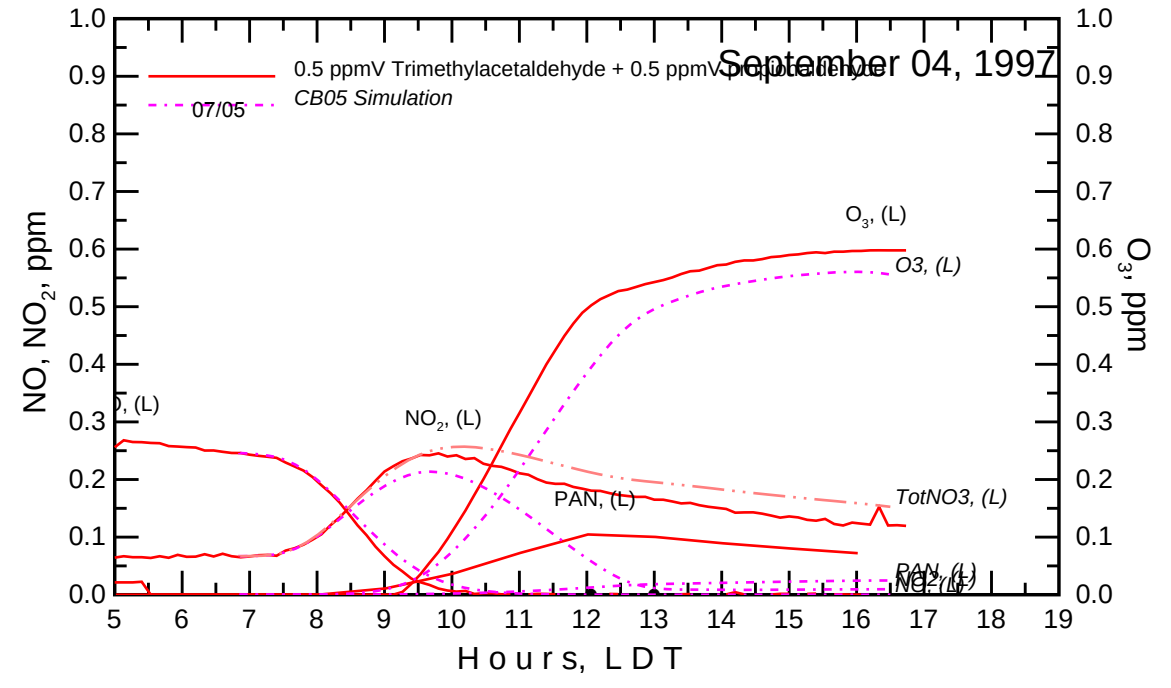

August 12, 1997
CO, (R)
HCHO, (R)
Acetaldehyde, (L)
ALD2, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

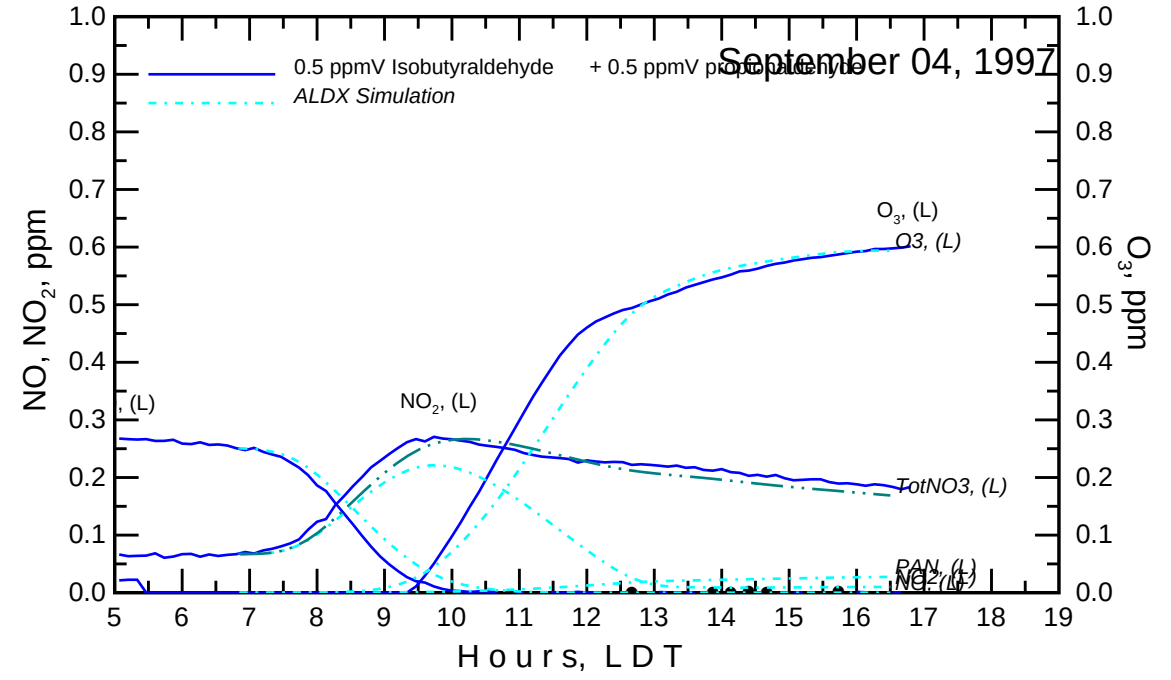


Aldehydes Mix vs Ketones Mix

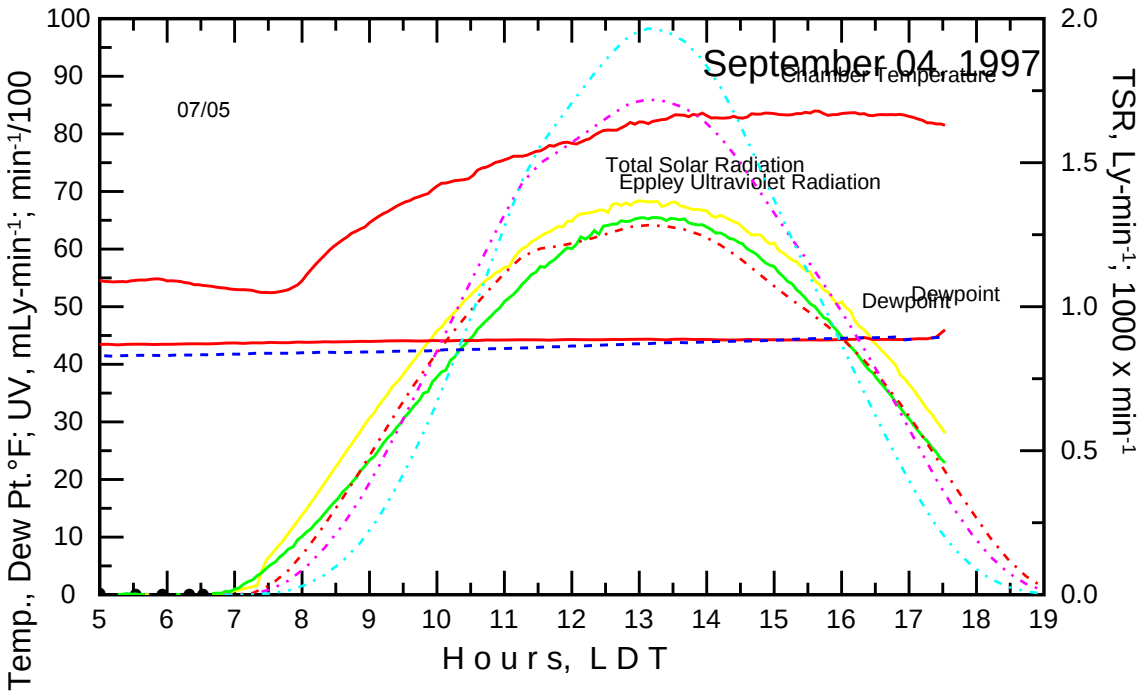

August 12, 1997
Chamber Temperature
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

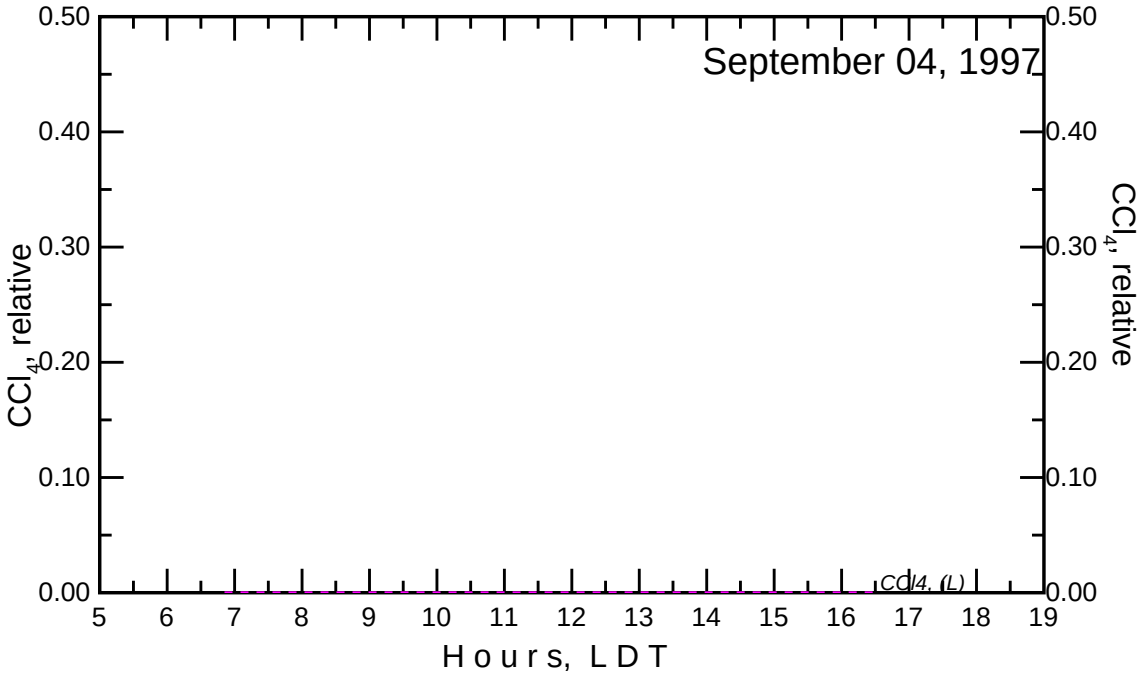

August 12, 1997
CCl4, relative
4, (L)
Hours, LDT

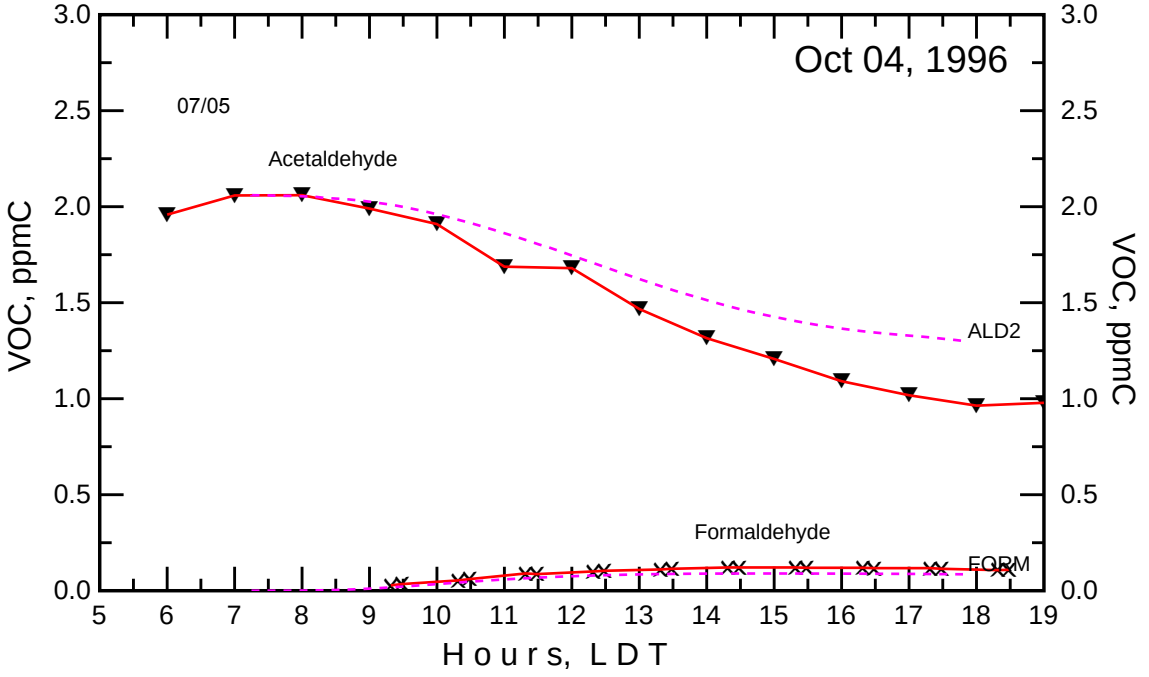


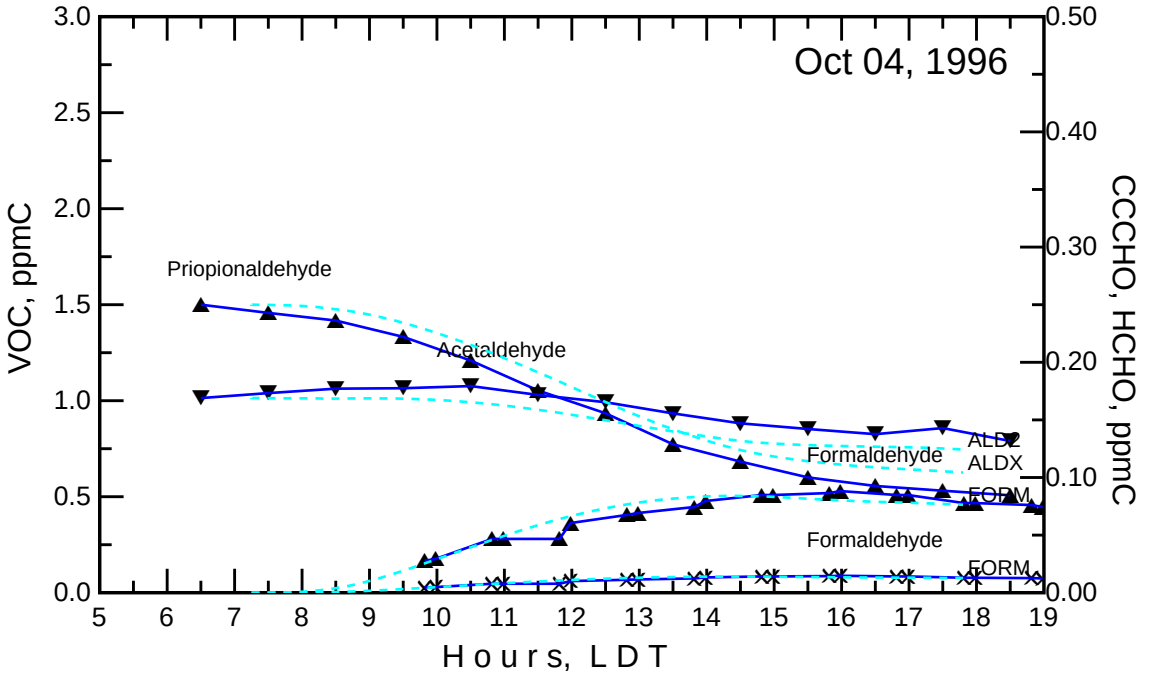


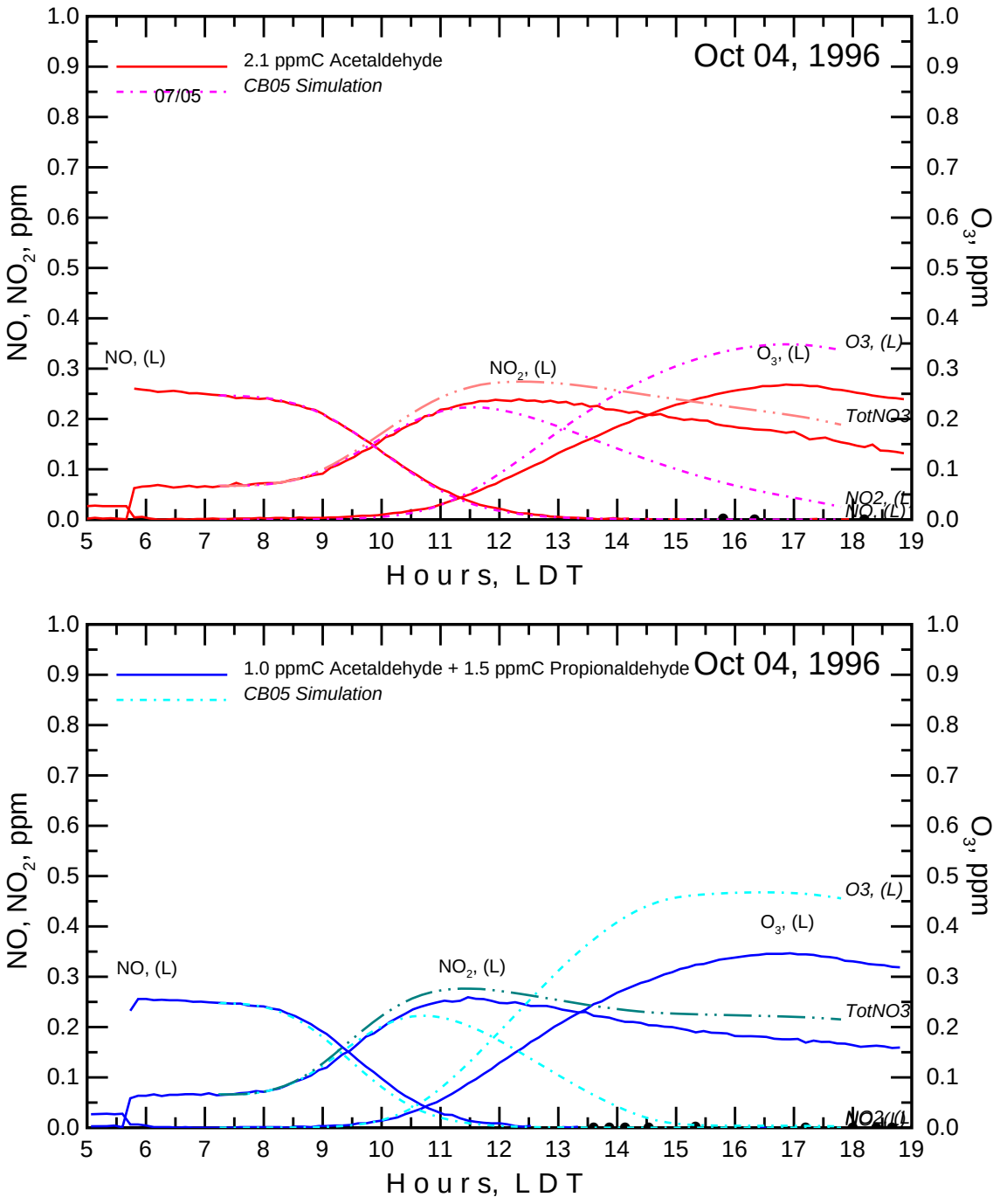
Aldehyde Mix run


September 04, 1997
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

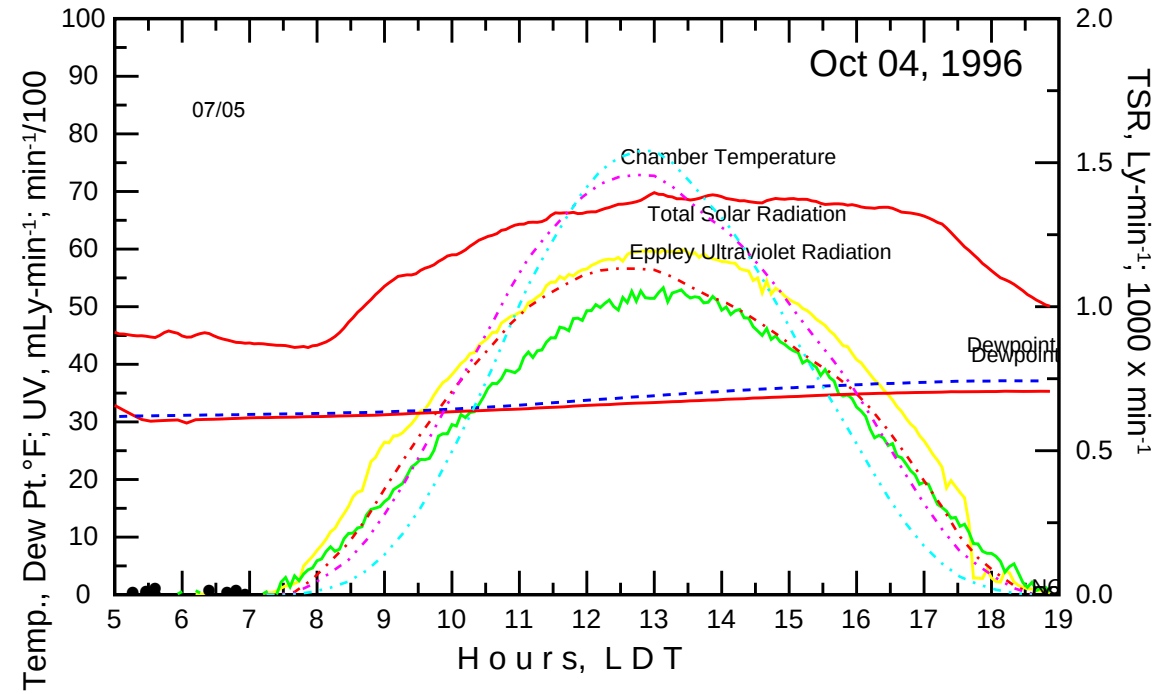

September 04, 1997
CCl4, (L)
CCl4, relative
CCl4, relative
Hours, LDT


Oct 04, 1996
07/05
Acetaldehyde
ALD2
Formaldehyde
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT


Oct 04, 1996
Priopionaldehyde
Acetaldehyde
ALD2
ALDX
Formaldehyde
FORM
Formaldehyde
FORM
VOC, ppmC
CCCHO, HCHO, ppmC
Hours, LDT



1 ppm Acetaldehyde vs 0.5 ppm Acetaldehyde and 0.5 ppm Propionaldehyde


Oct 04, 1996
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
100
90
80
70
60
50
40
30
20
10
0
2.0
1.5
1.0
0.5
0.0
5
6
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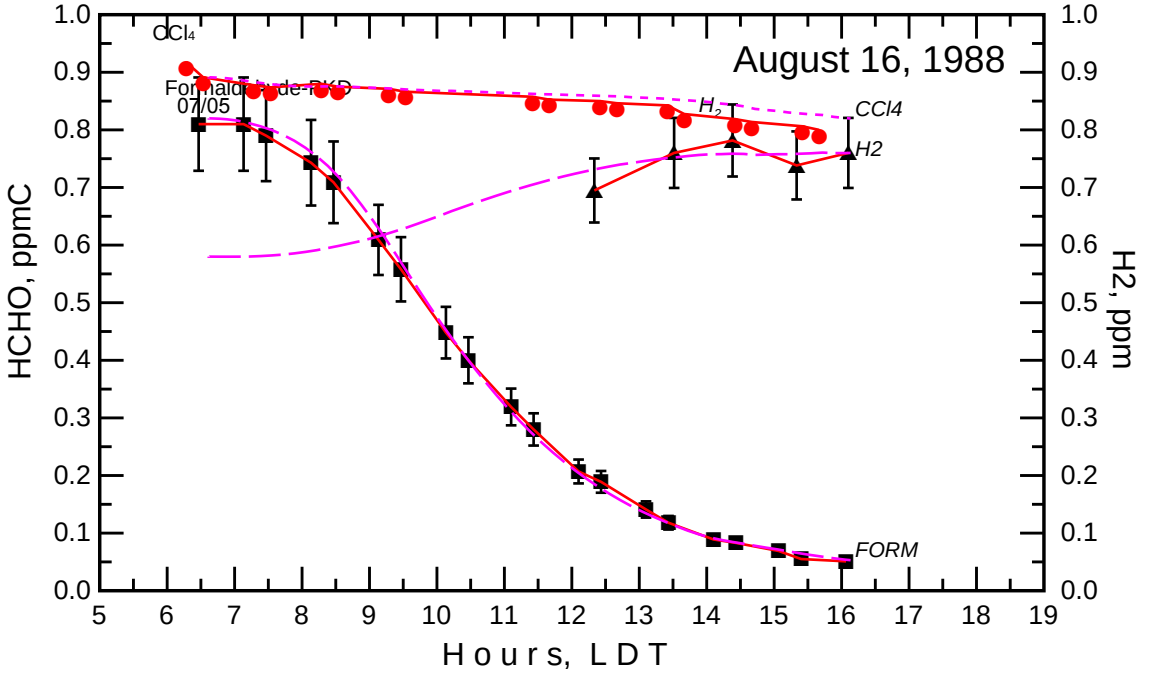
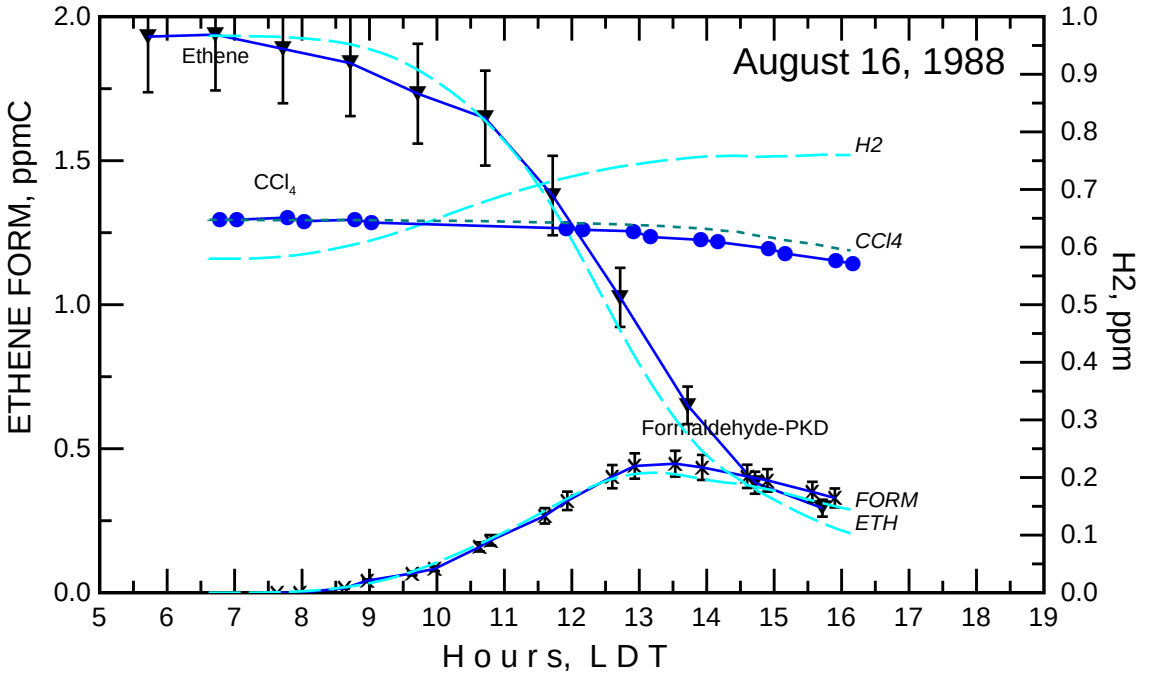
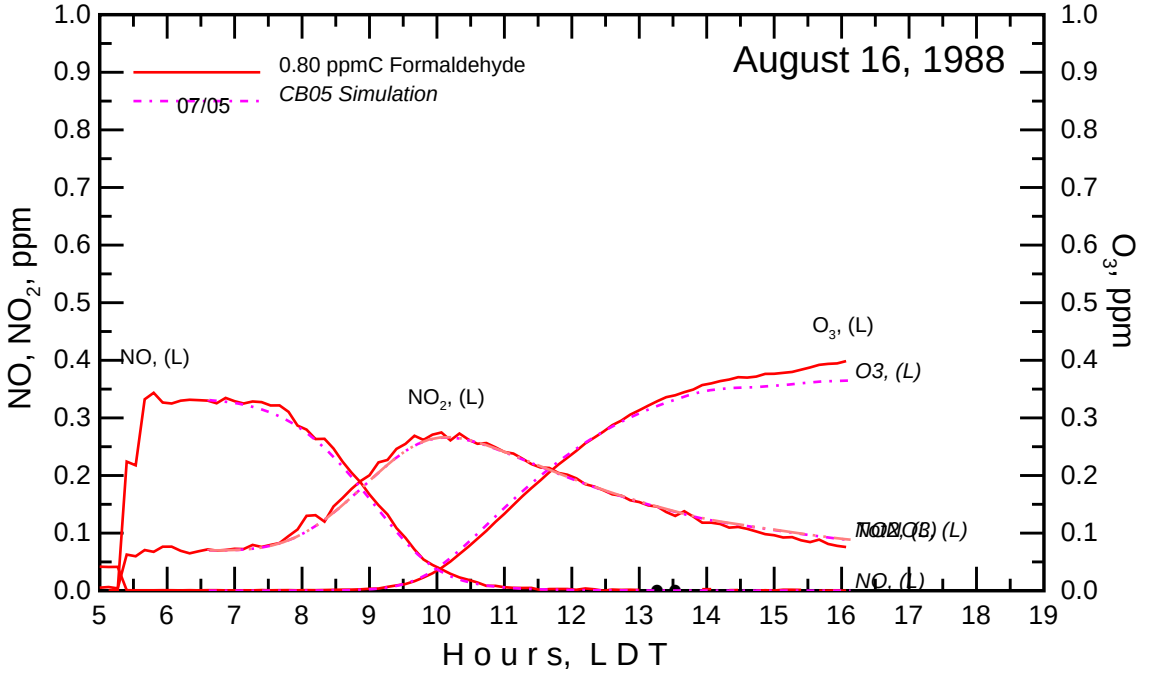
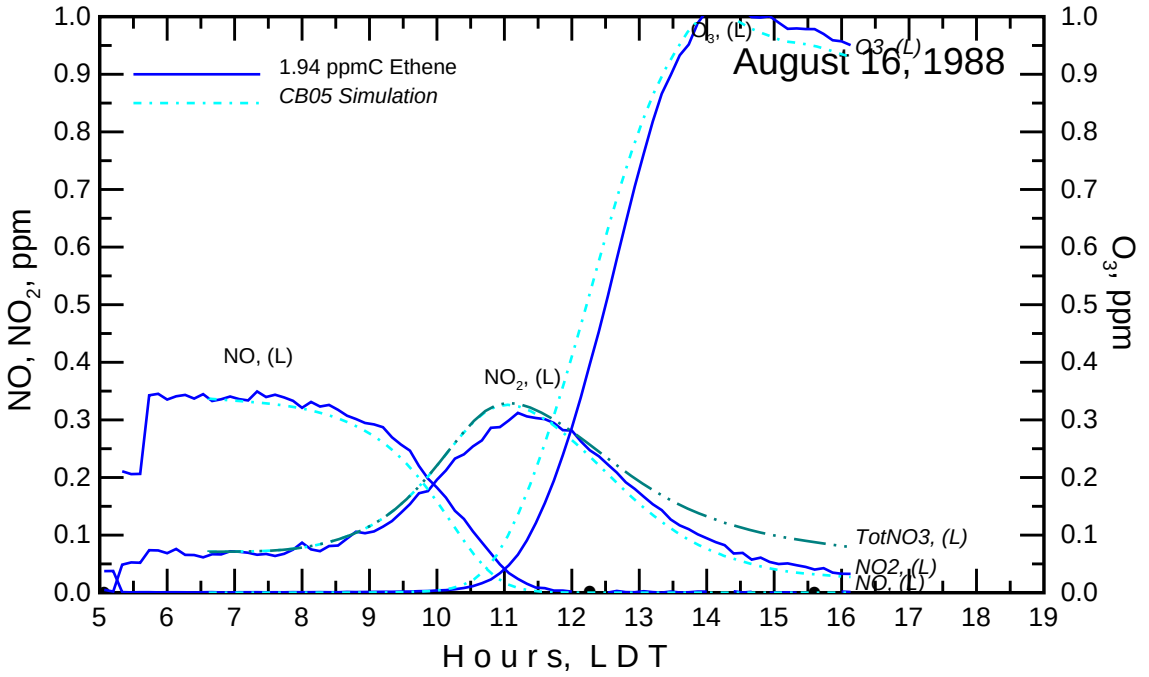
Ethene (ETH)

AU 16 88
Au 24 97

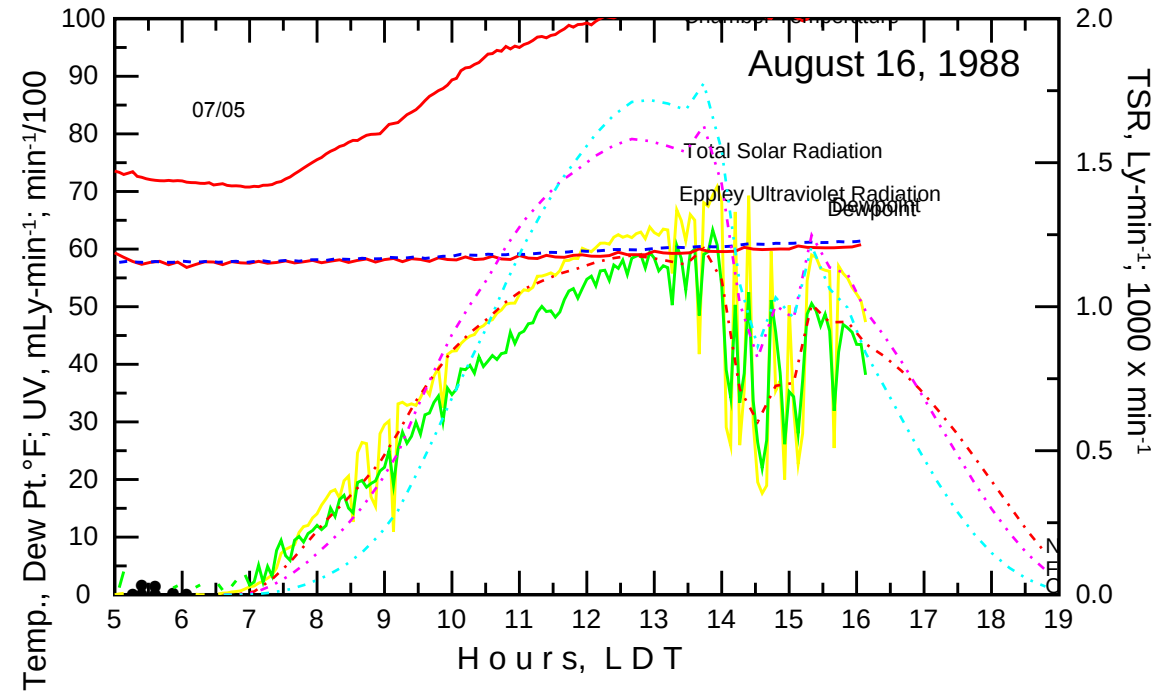

August 16, 1988
CCl4
Formaldehyde-PKD
07/05
H2
CCl4
H2
FORM
HCHO, ppmC
H2, ppm
Hours, LDT


August 16, 1988
Ethene
CCl4
H2
CCl4
Formaldehyde-PKD
FORM
ETH
ETHENE FORM, ppmC
H2, ppm
Hours, LDT





HC Reactivity at 0.39 NO_x


August 16, 1988
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
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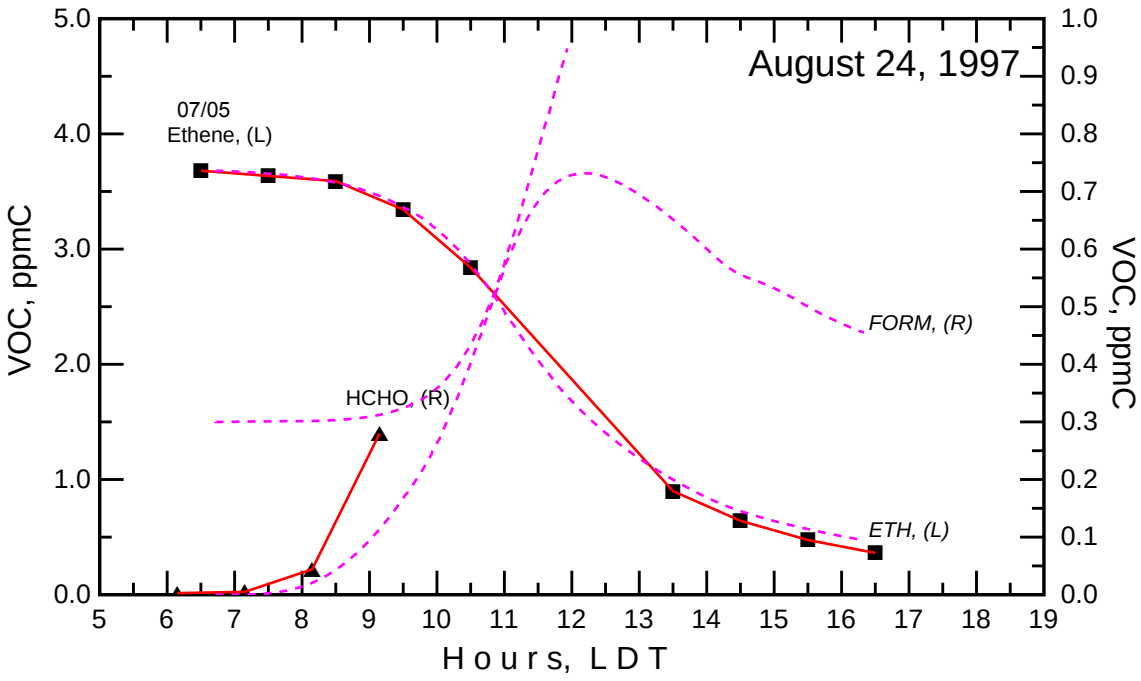
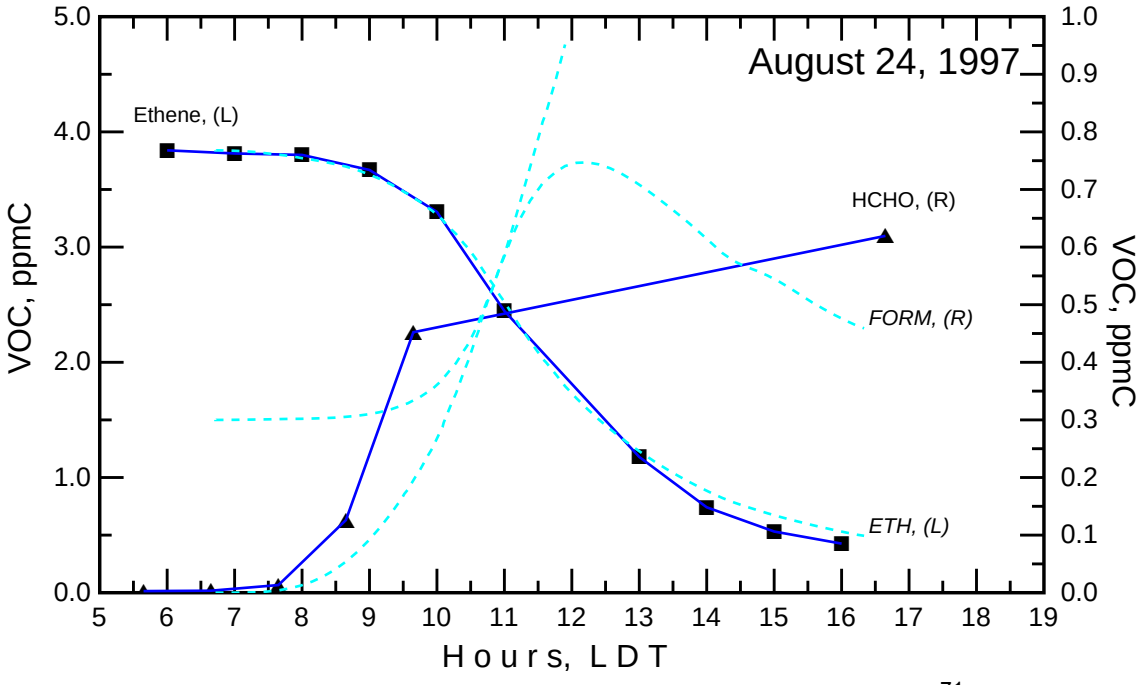
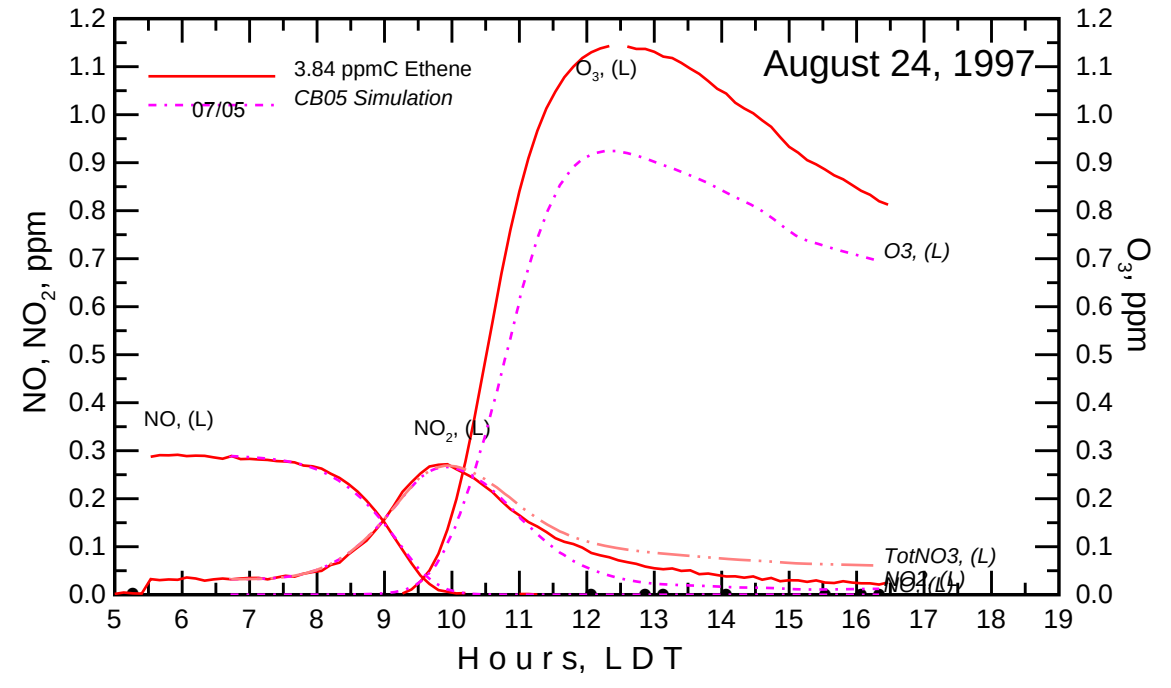
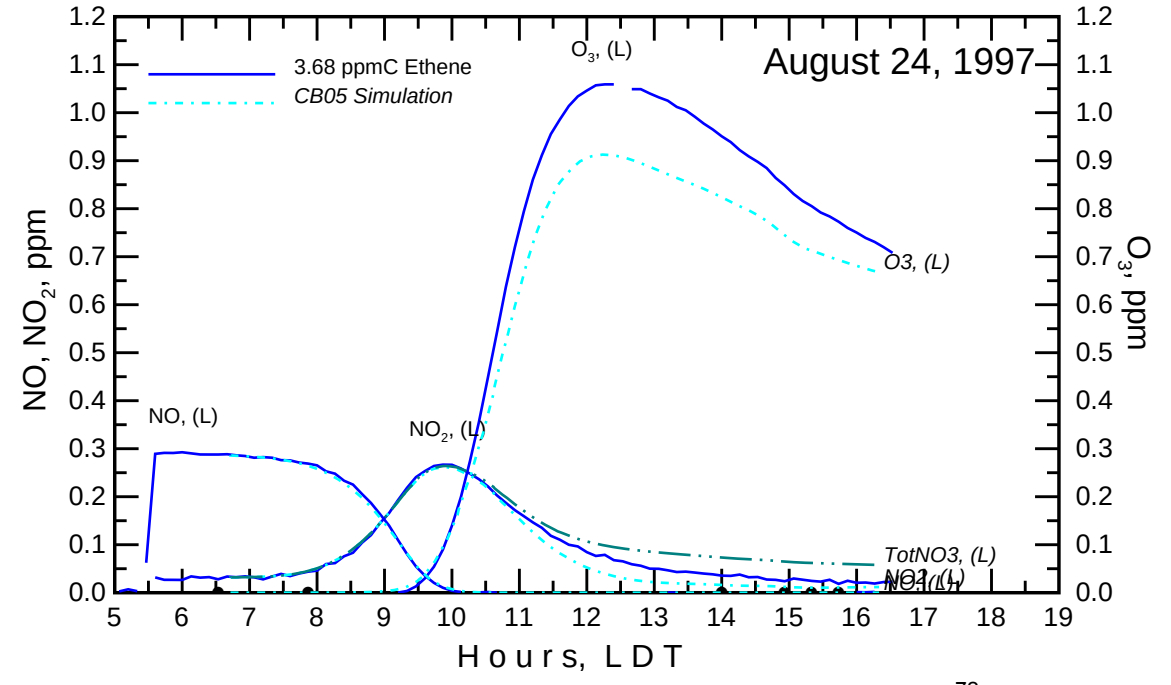
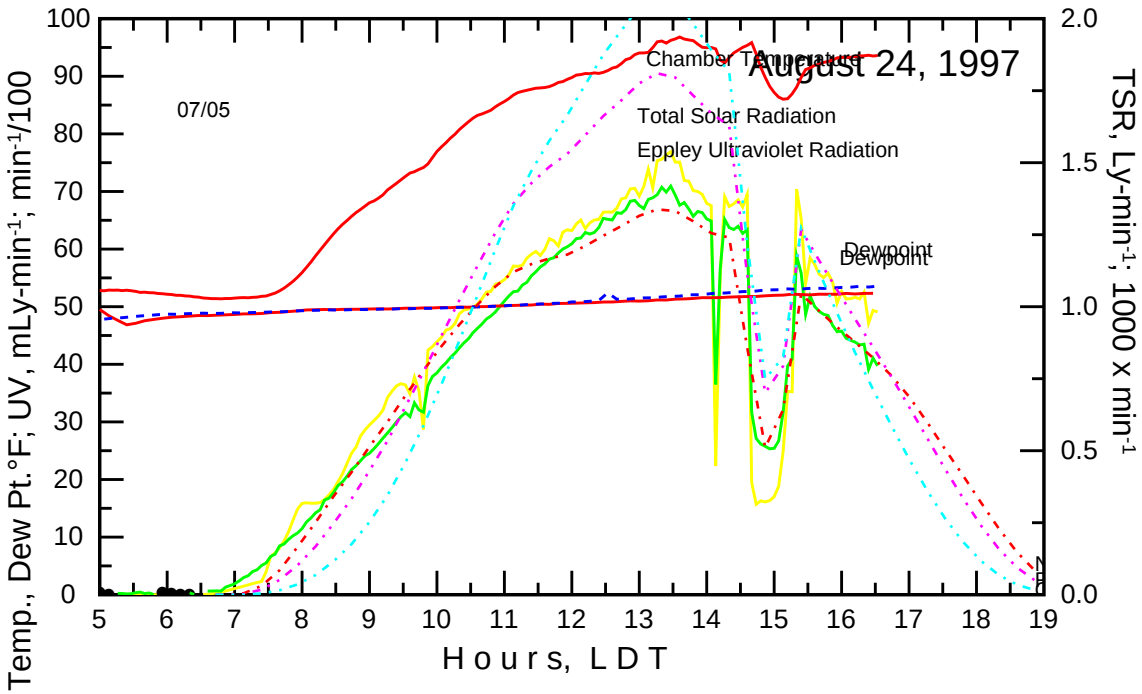

August 24, 1997
07/05
Ethene, (L)
HCHO, (R)
FORM, (R)
ETH, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

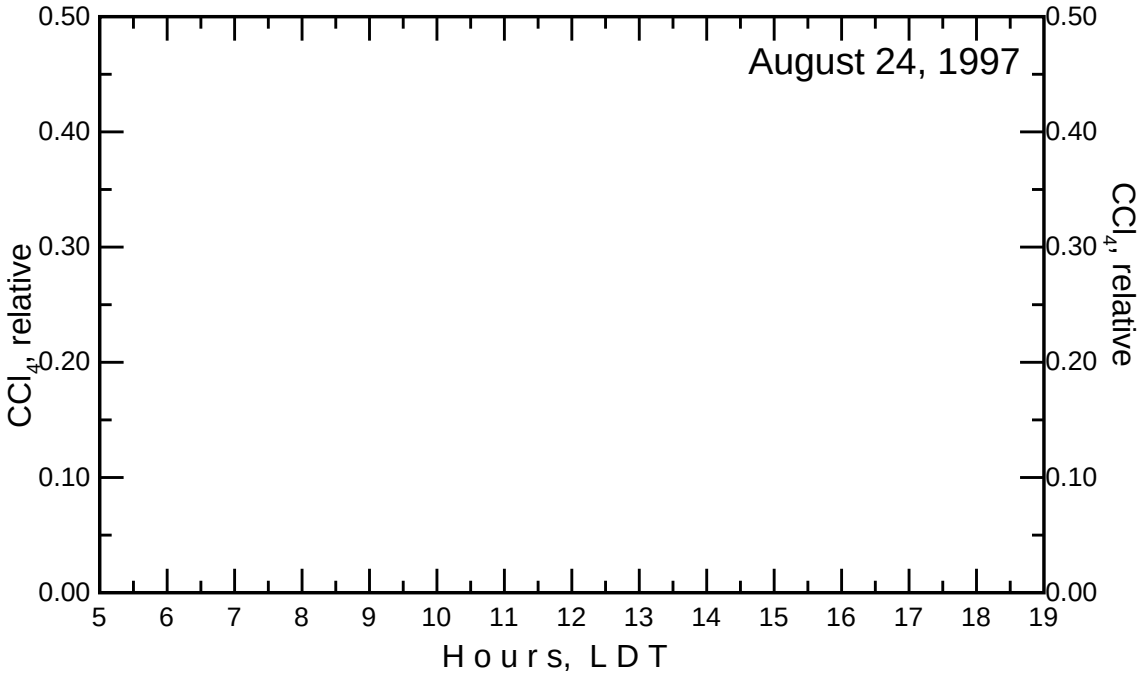

August 24, 1997
Ethene, (L)
HCHO, (R)
FORM, (R)
ETH, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT





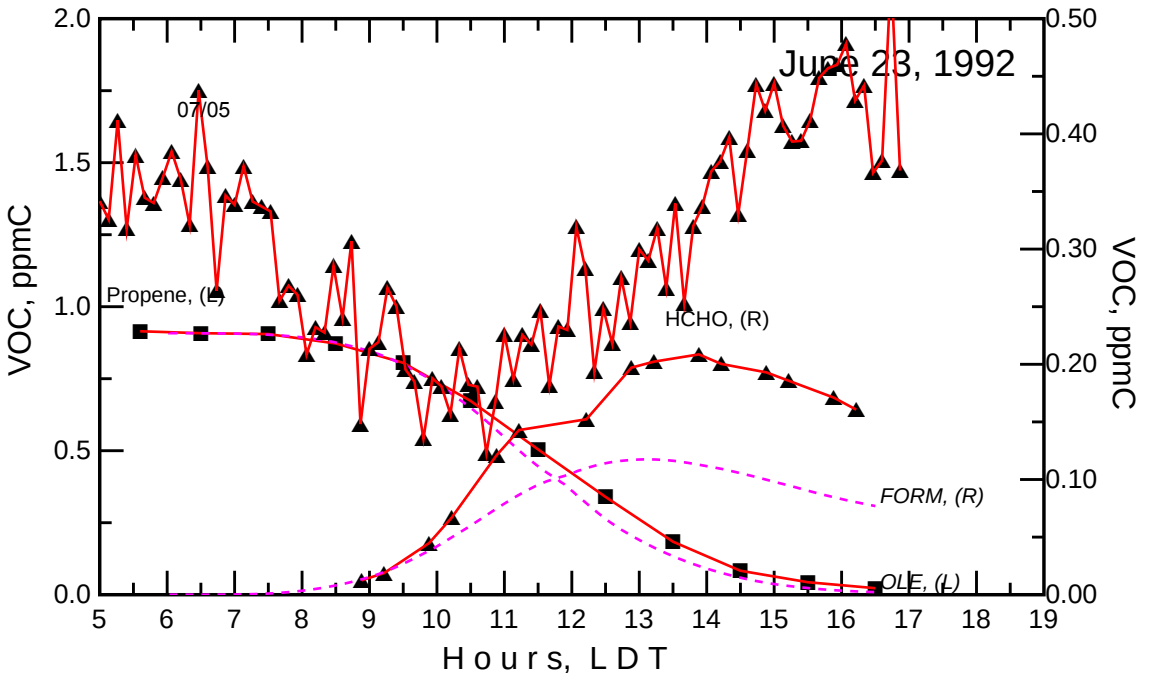
Matched 4 ppmC Ethene

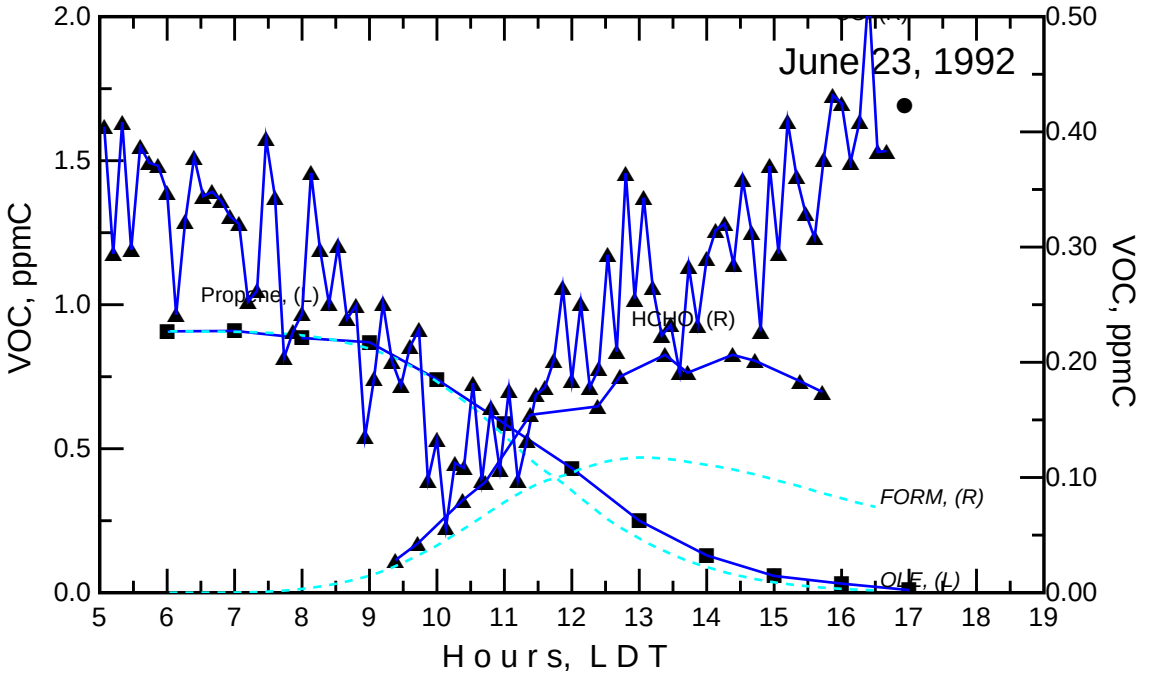

August 24, 1997
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

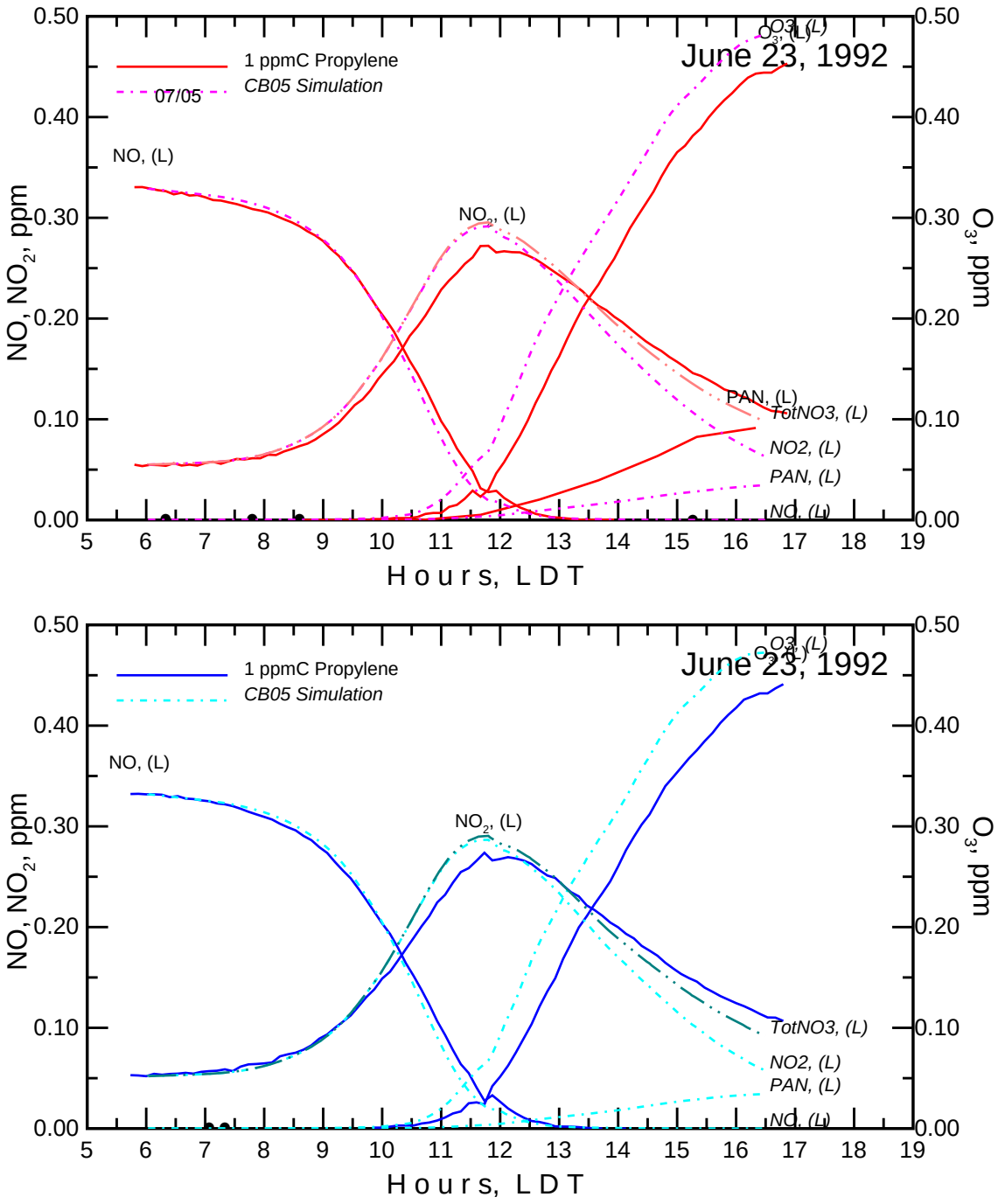

August 24, 1997
CCl4, relative
CCl4, relative
Hours, LDT

Terminal Olefins (OLE)

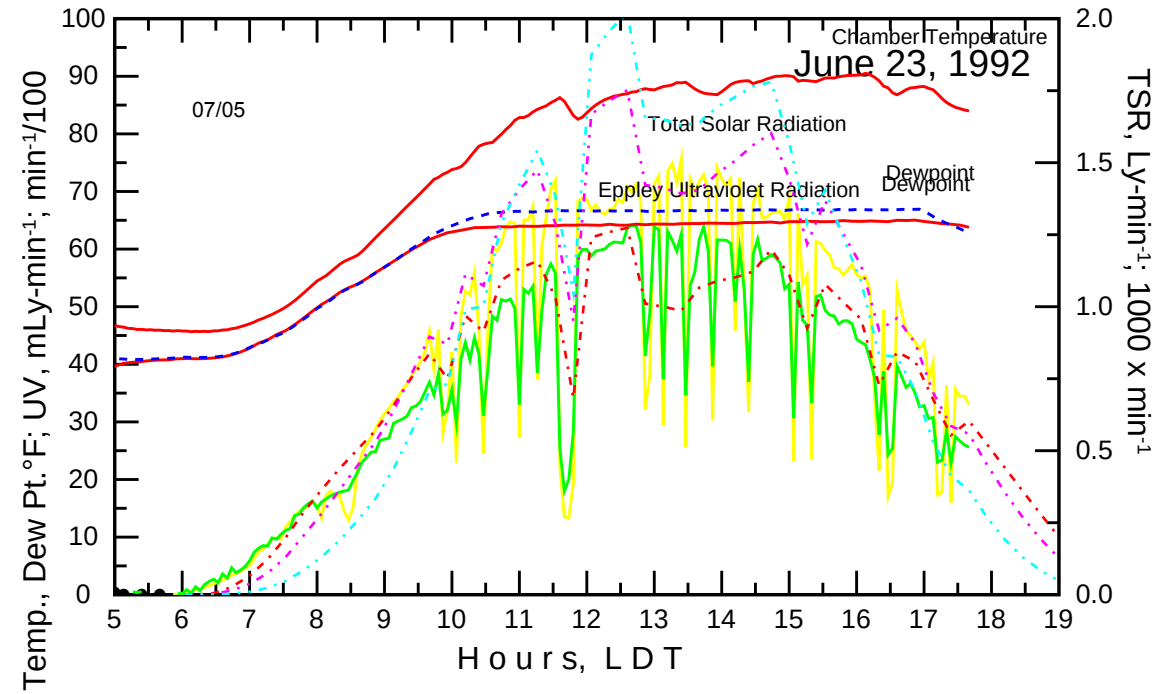
JN 23 92
ST 19 95

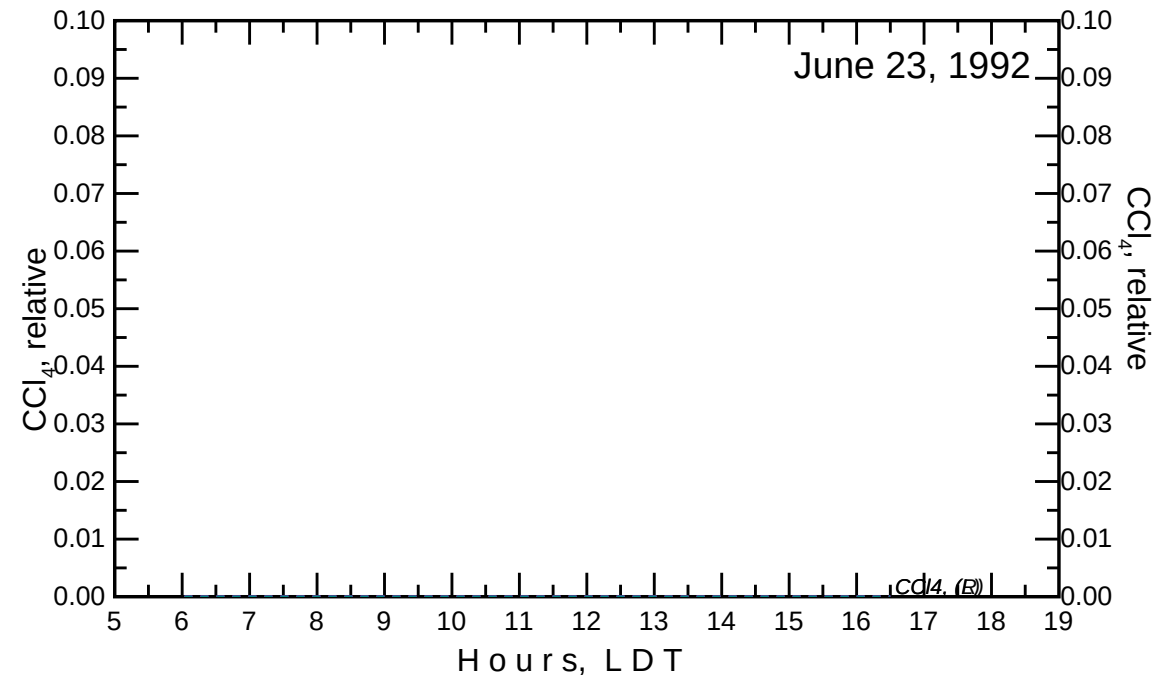

June 23, 1992
07/05
Propene, (L)
HCHO, (R)
FORM, (R)
OLE, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT
2.0
1.5
1.0
0.5
0.0
0.50
0.40
0.30
0.20
0.10
0.00
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

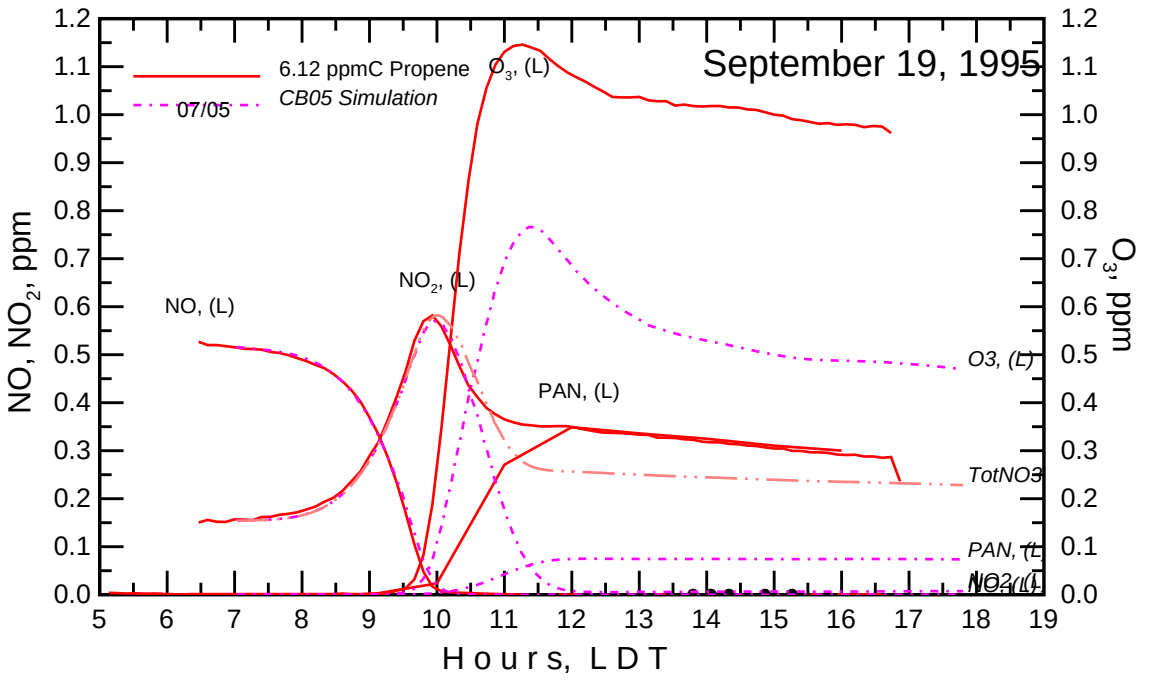

June 23, 1992
Propene, (L)
HCHO, (R)
FORM, (R)
OLE, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT
2.0
1.5
1.0
0.5
0.0
0.50
0.40
0.30
0.20
0.10
0.00
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

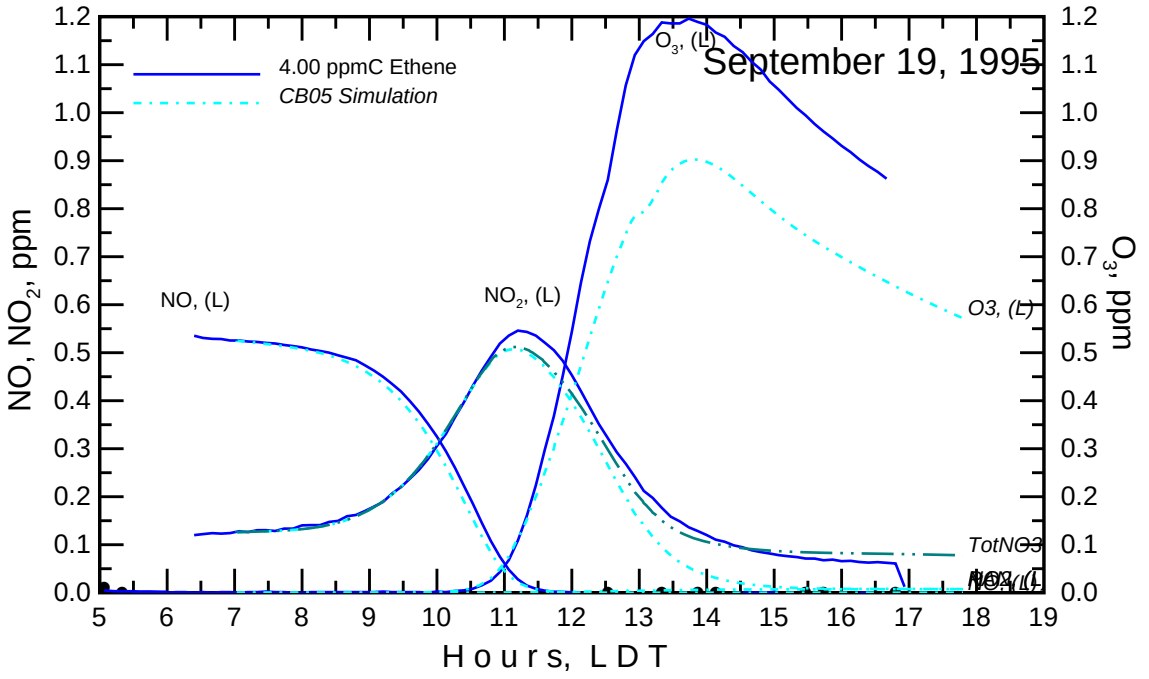


Matched Propylene; Matched NO_x

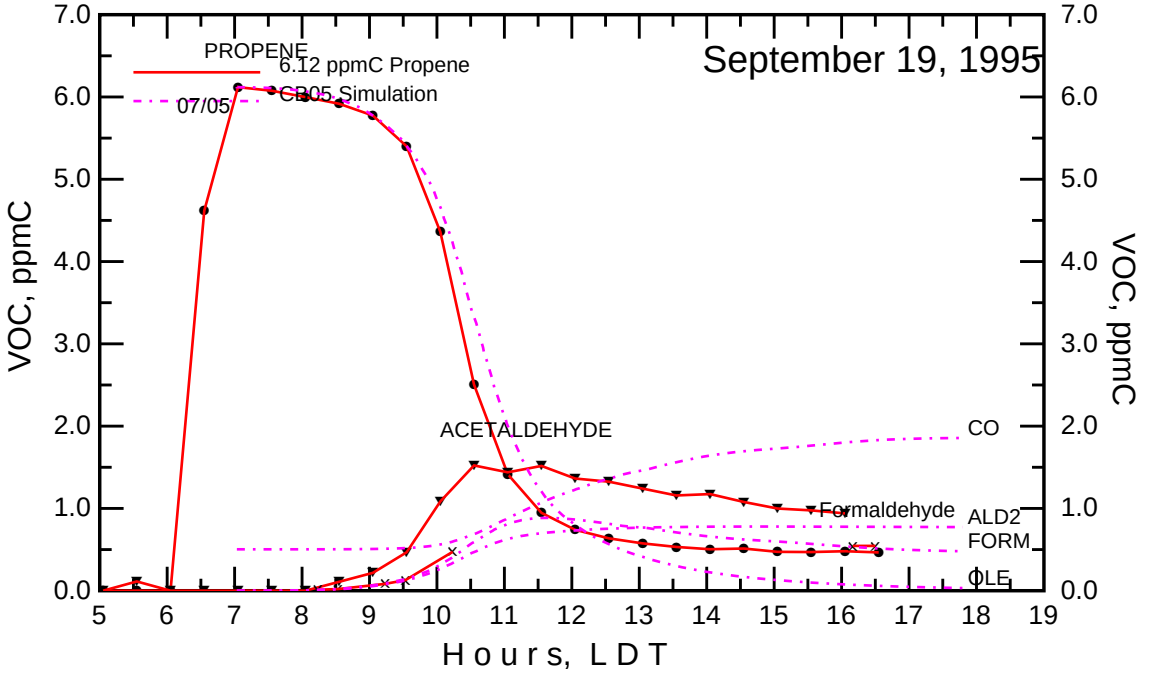

Chamber Temperature
June 23, 1992
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

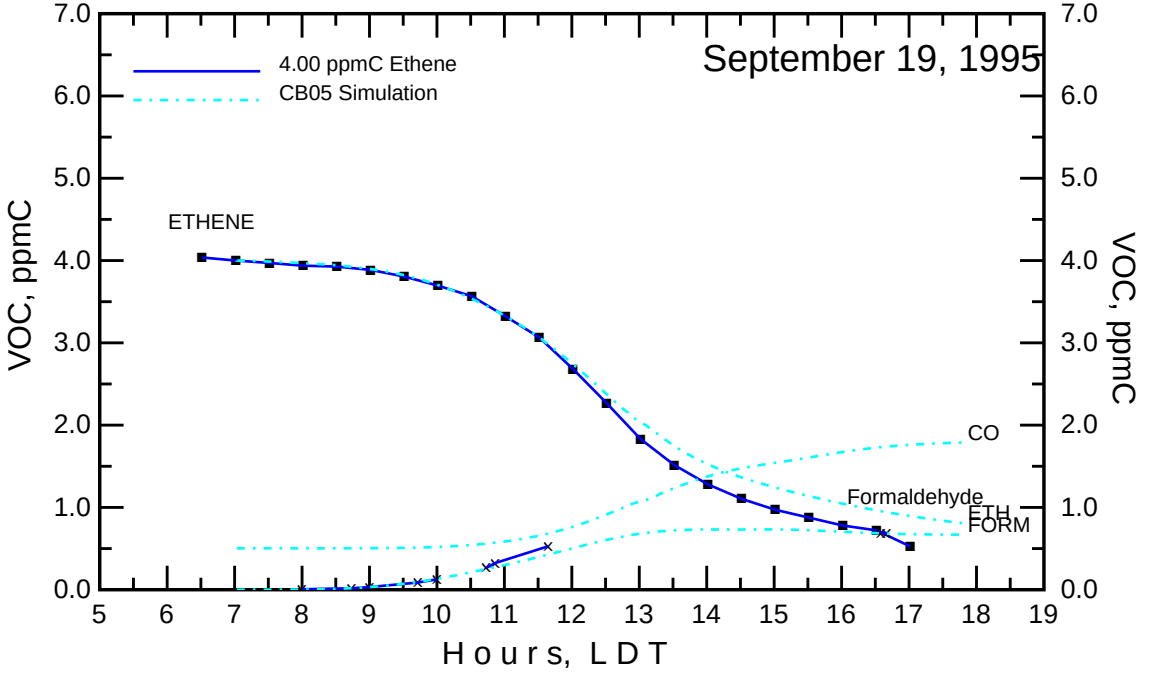

June 23, 1992
CCl4, relative
CCl4, relative
CCl4, (E)
Hours, LDT





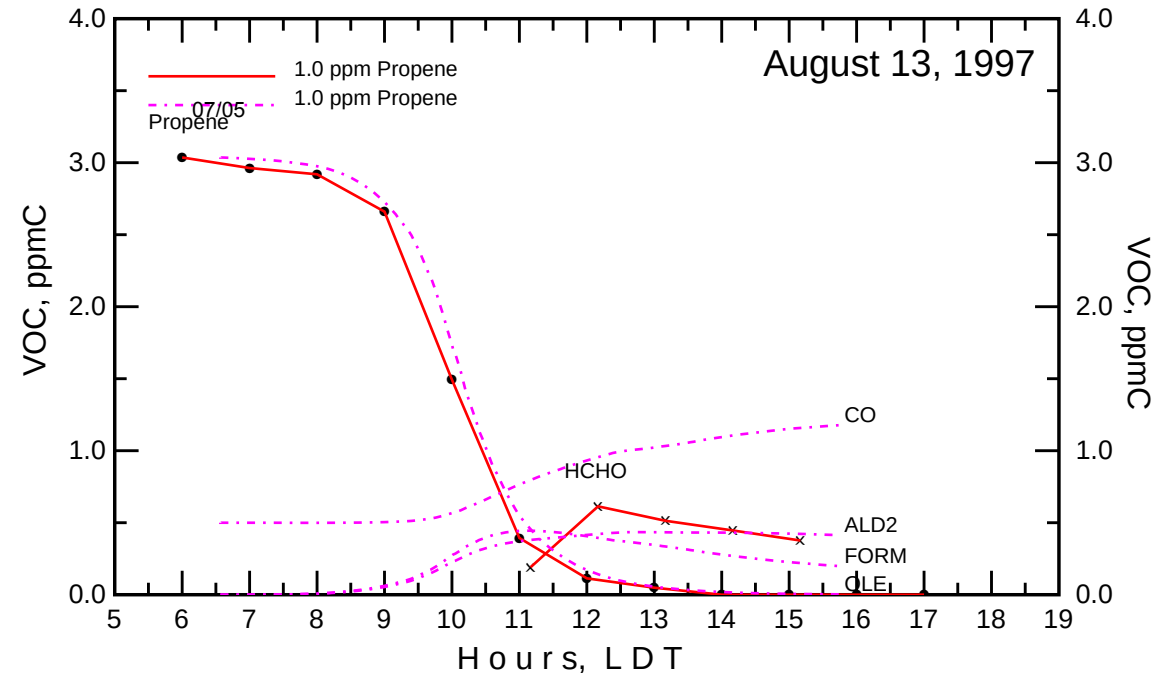
Propene vs Ethene run; Matched NOx

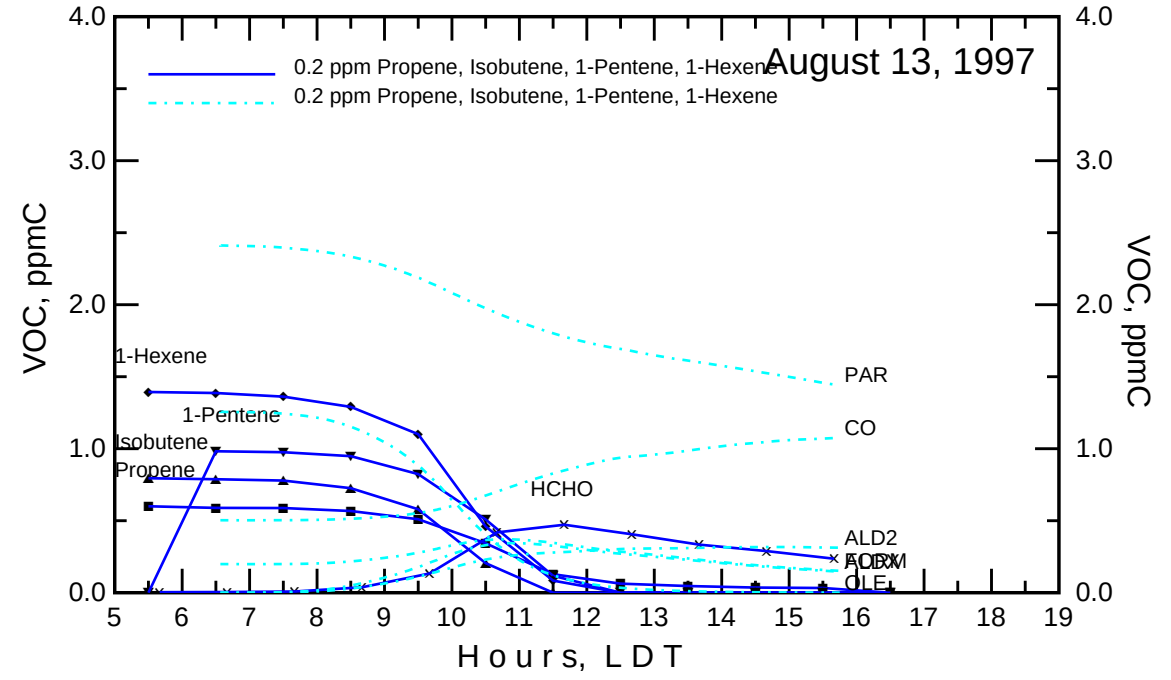

PROPENE
6.12 ppmC Propene
CB05 Simulation
07/05
September 19, 1995
ACETALDEHYDE
CO
Formaldehyde
ALD2
FORM
OLE
VOC, ppmC
VOC, ppmC
Hours, LDT

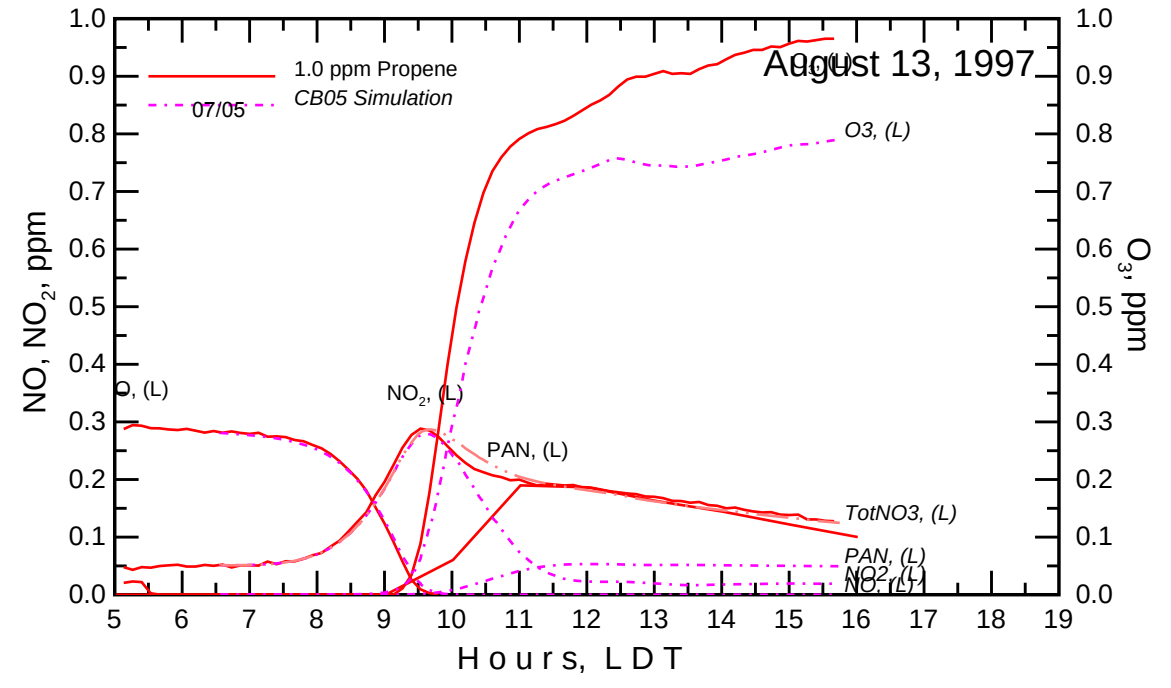

4.00 ppmC Ethene
CB05 Simulation
September 19, 1995
ETHENE
CO
Formaldehyde
ETH
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT

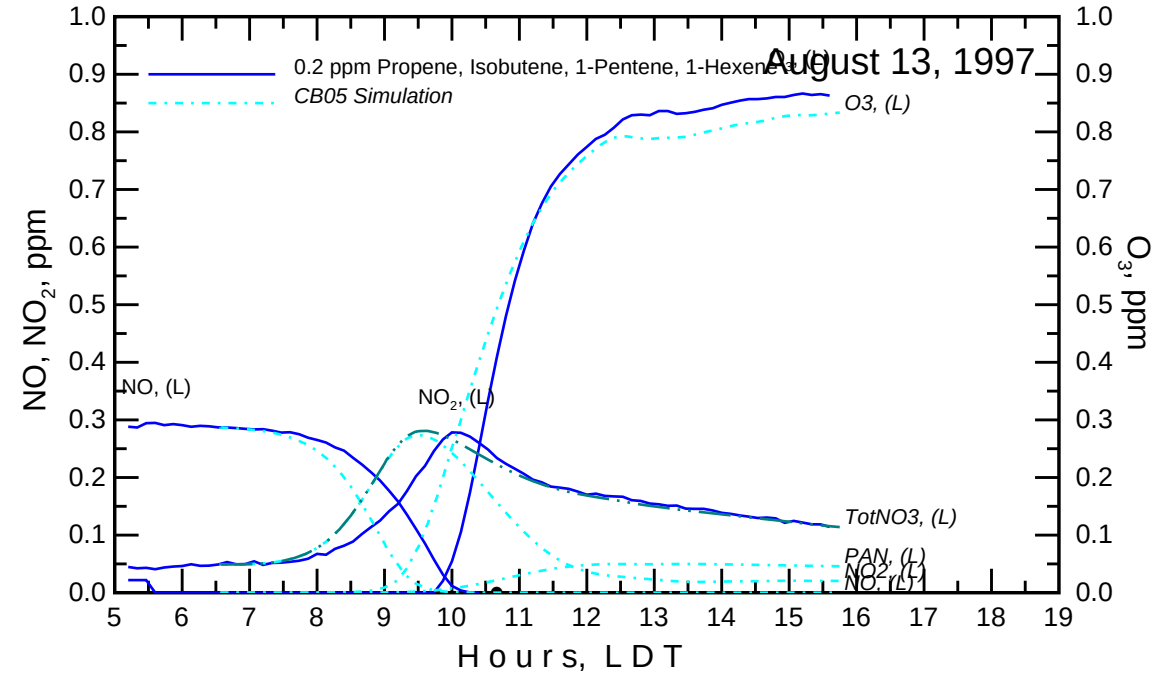
Olefin Mixtures (OLE and IOLE)

AU 13 97
ST 13 02
ST 14 96
OC 16 96

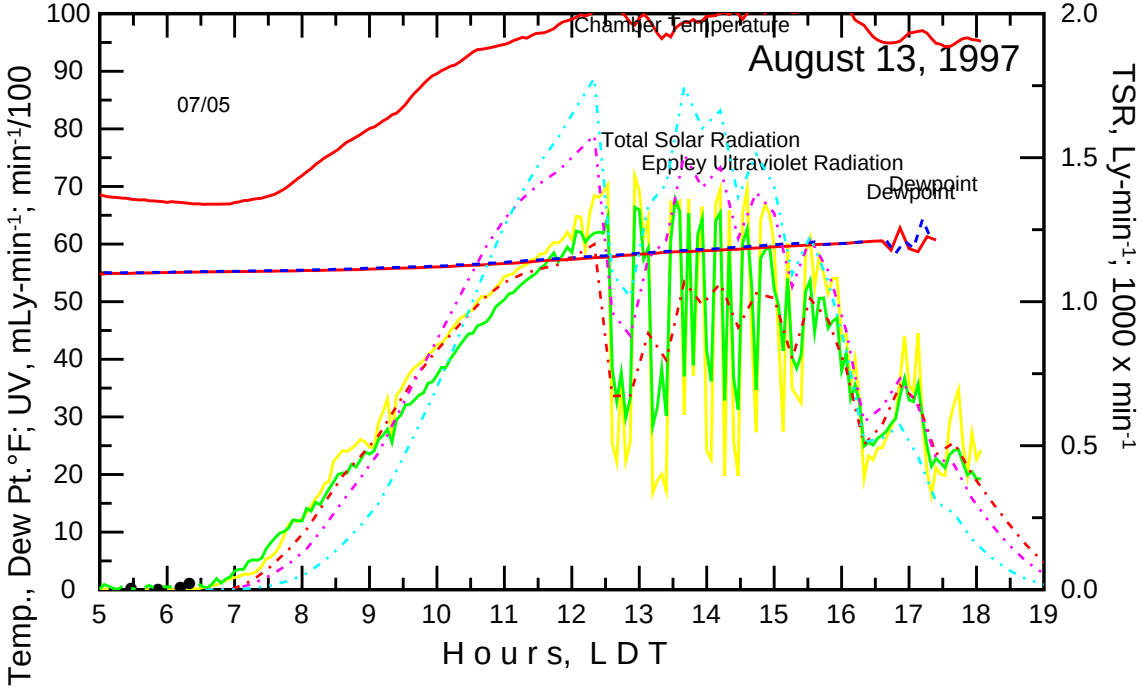

August 13, 1997
1.0 ppm Propene
1.0 ppm Propene
07/05
Propene
CO
HCHO
ALD2
FORM
OLE
VOC, ppmC
VOC, ppmC
Hours, LDT

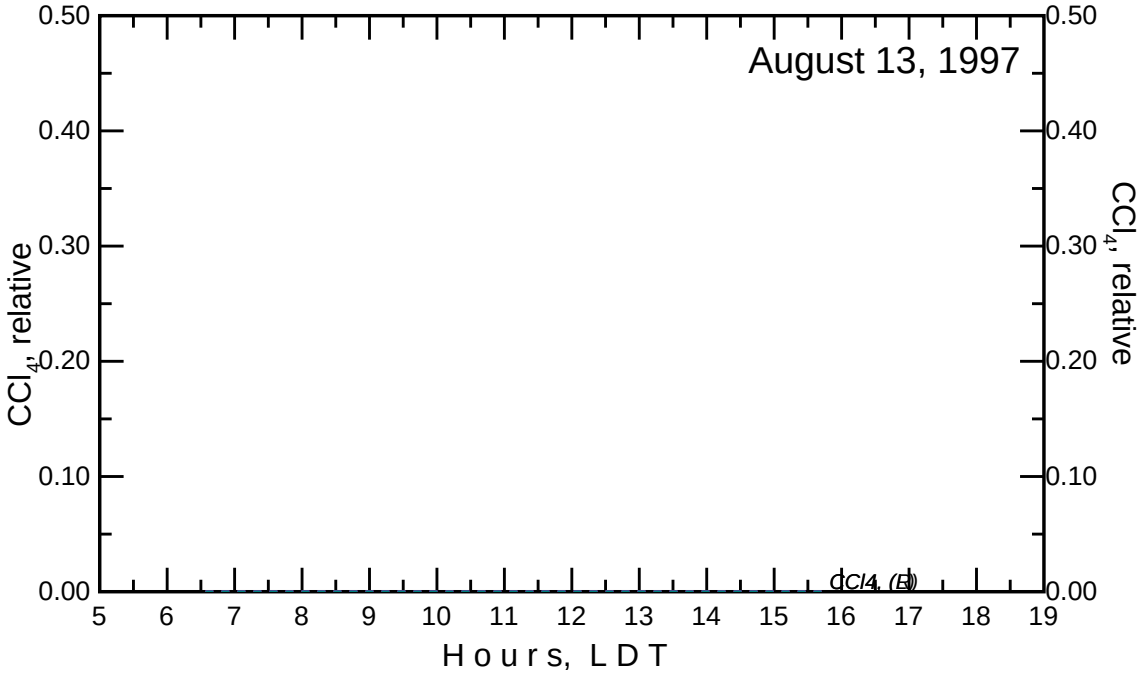

August 13, 1997
0.2 ppm Propene, Isobutene, 1-Pentene, 1-Hexene
0.2 ppm Propene, Isobutene, 1-Pentene, 1-Hexene
1-Hexene
1-Pentene
Isobutene
Propene
PAR
CO
HCHO
ALD2
FORM
OLE
VOC, ppmC
VOC, ppmC
Hours, LDT

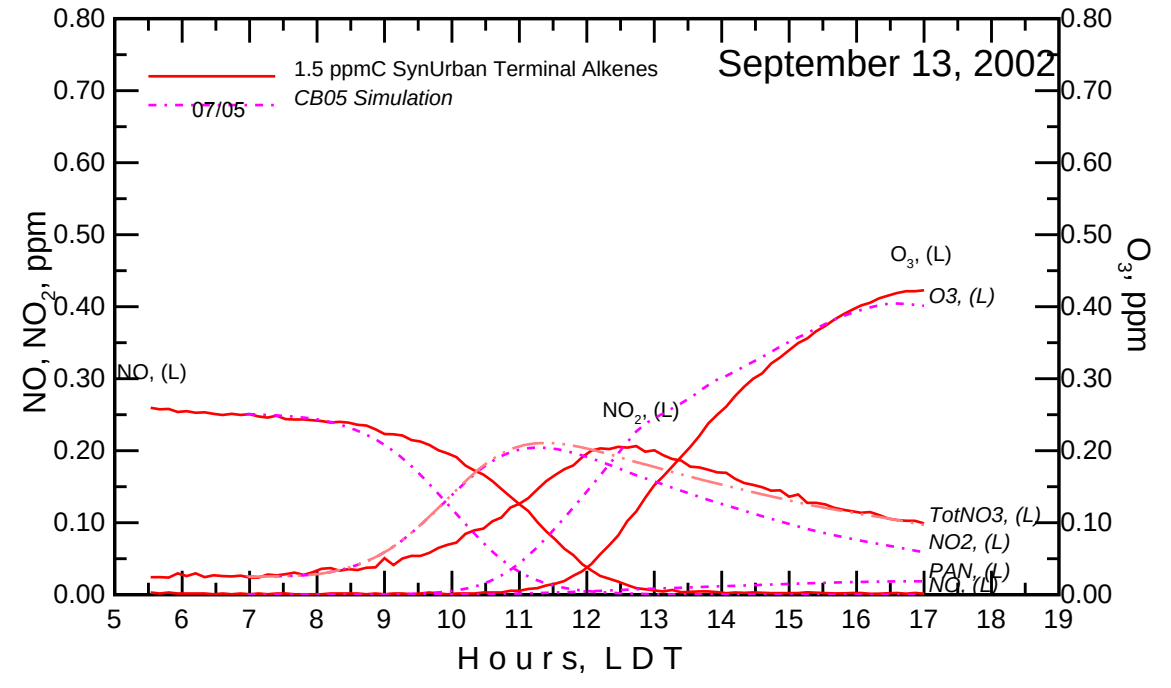


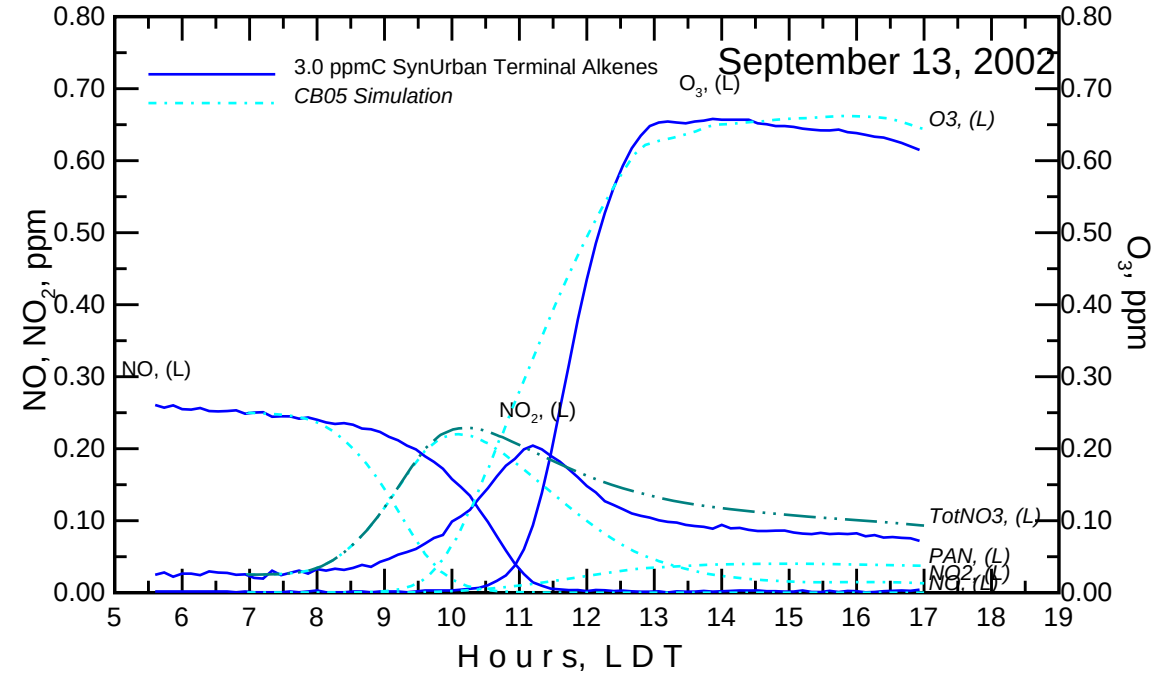


C_3alkene vs. C_3, C_4, C_5, C_6alkenes

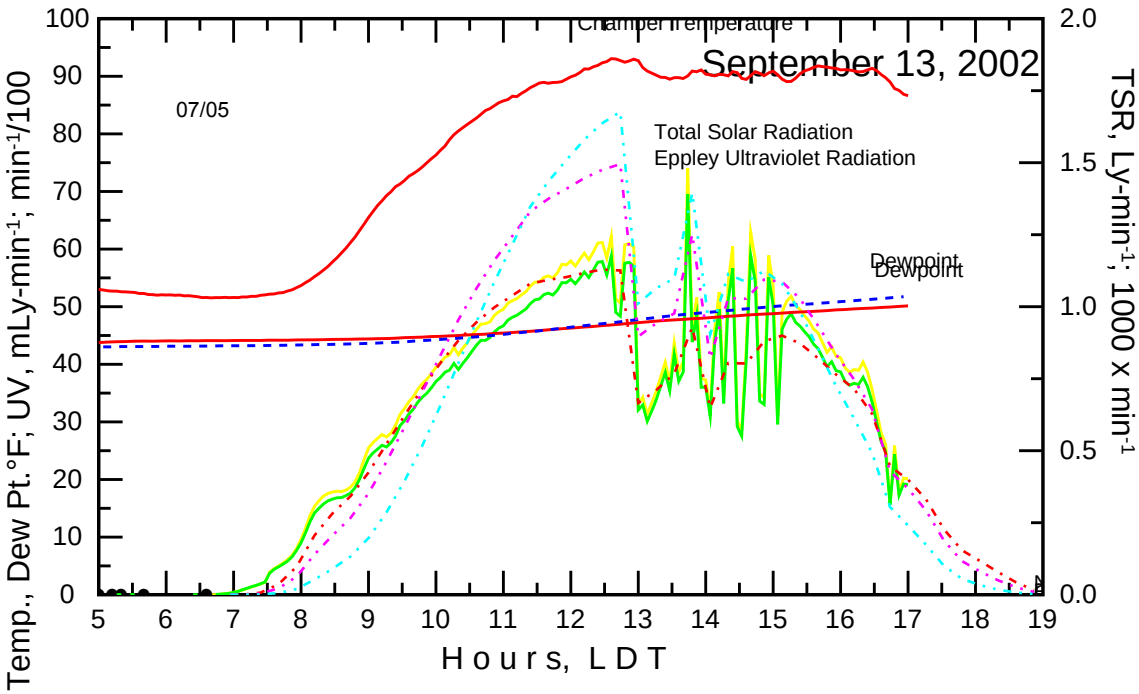

August 13, 1997
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

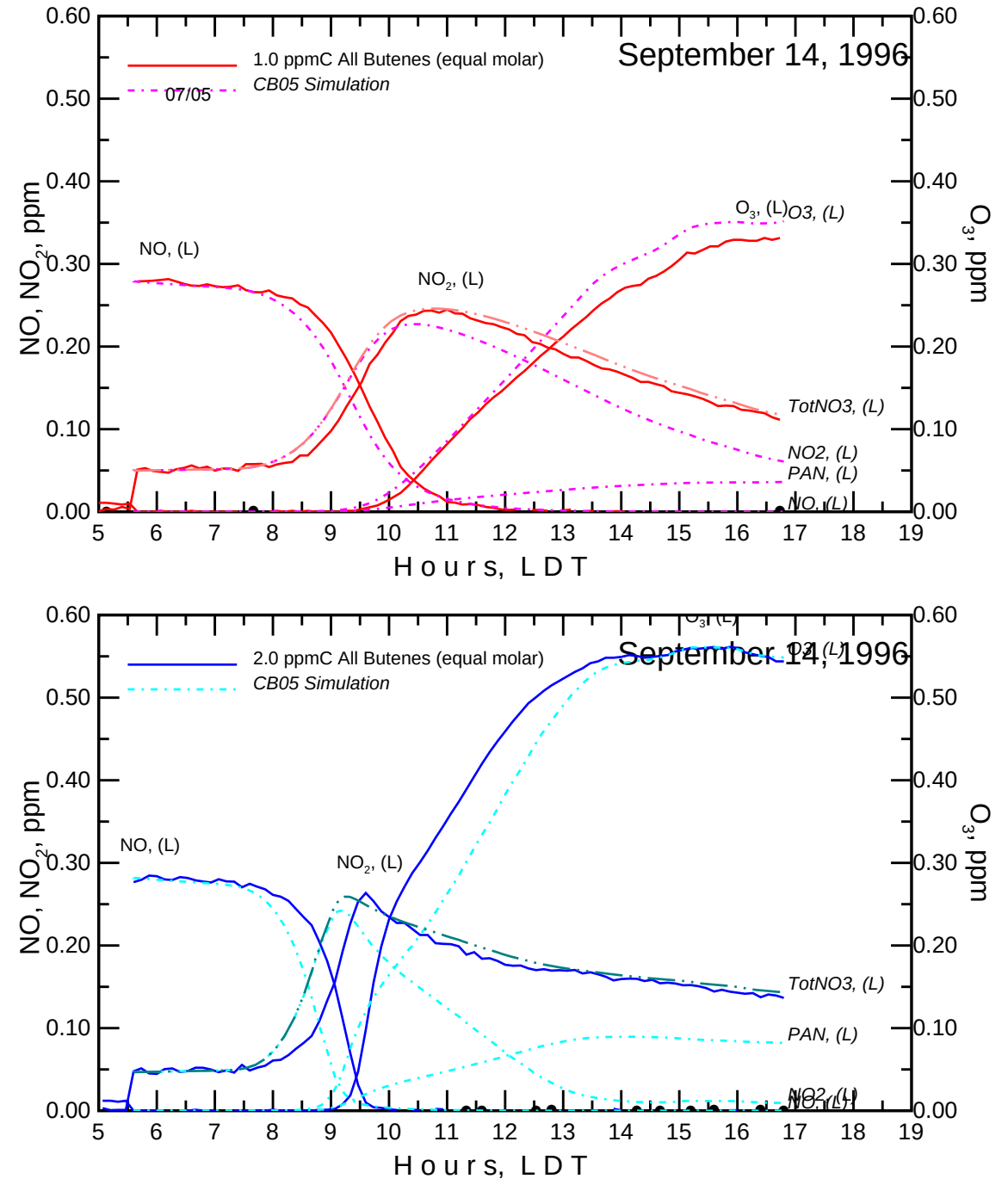

August 13, 1997
CCl4, relative
CCl4, relative
dCl4 (B)
Hours, LDT

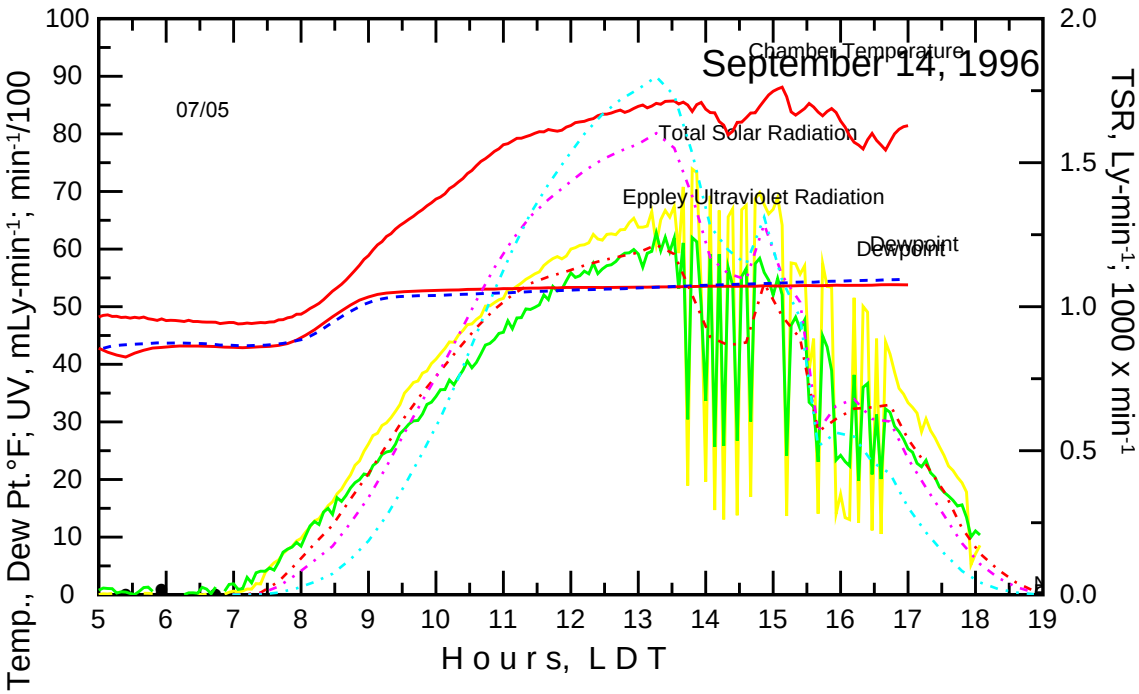


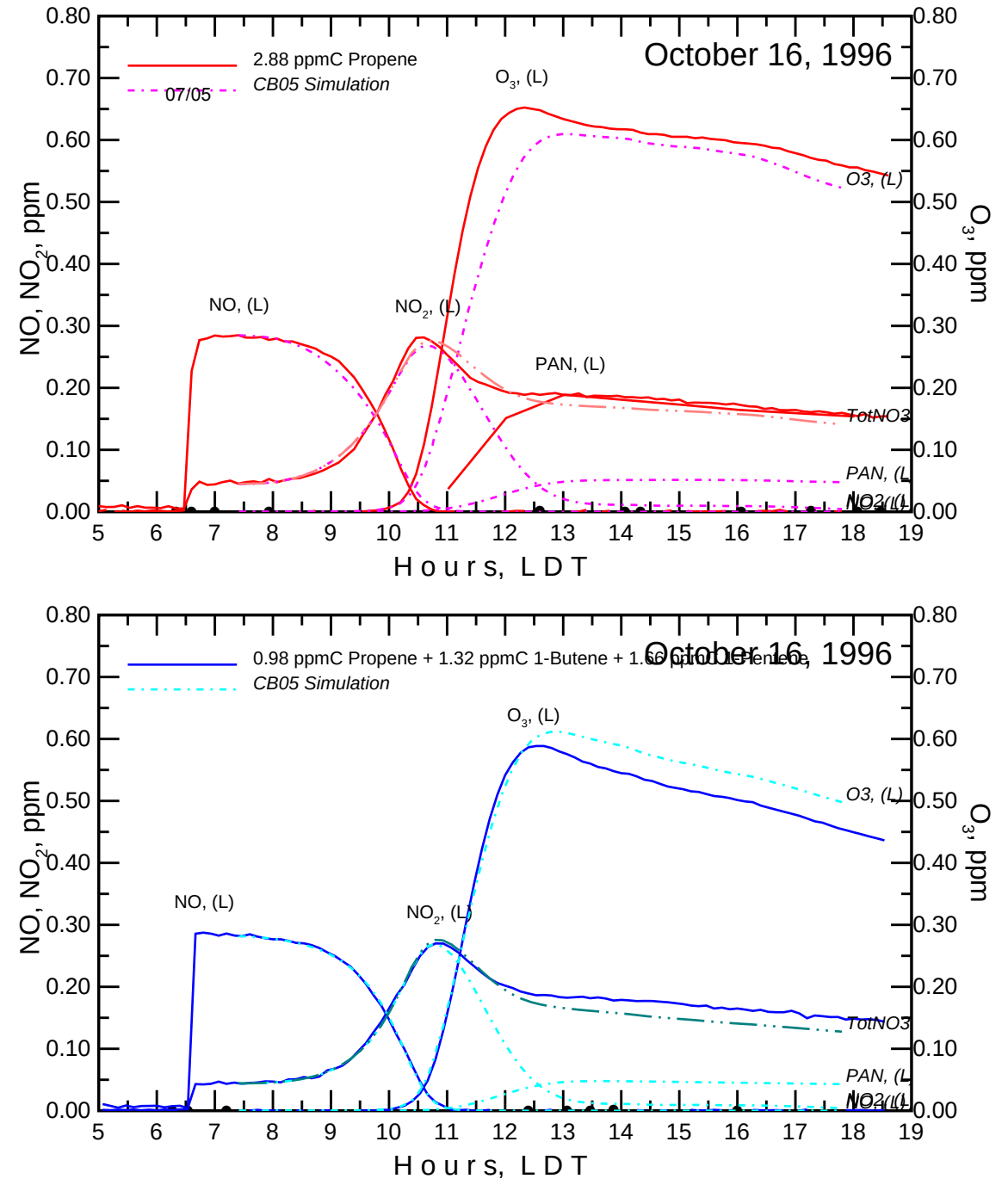


Delta SynUrban Mix Terminal Alkenes

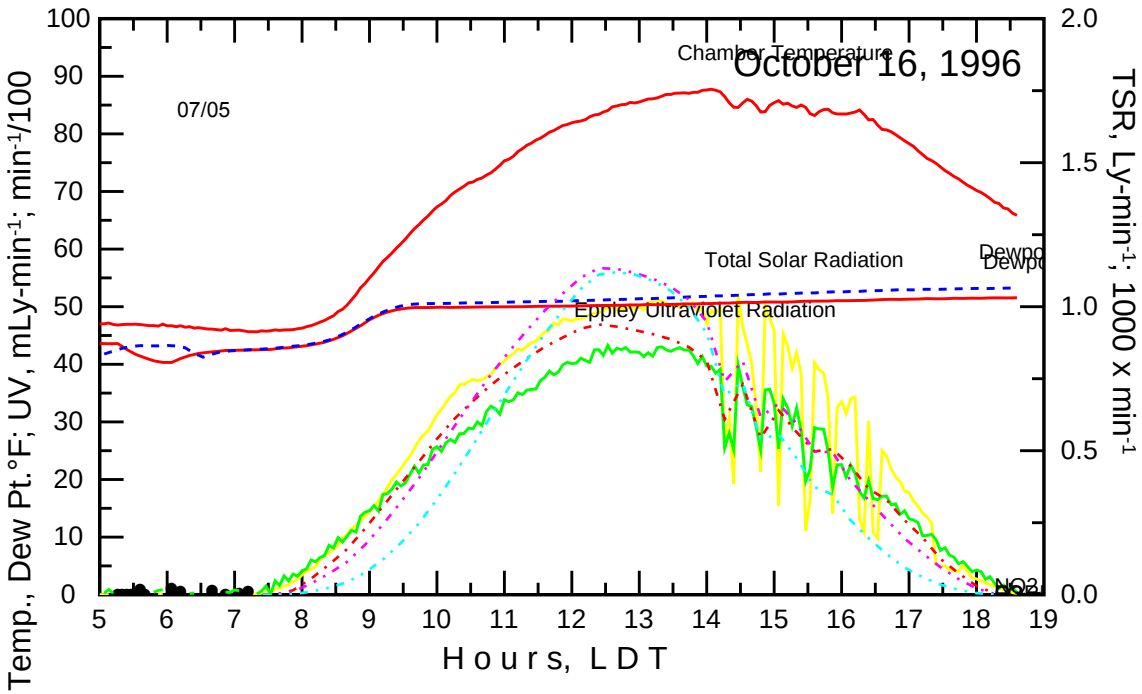

September 13, 2002
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

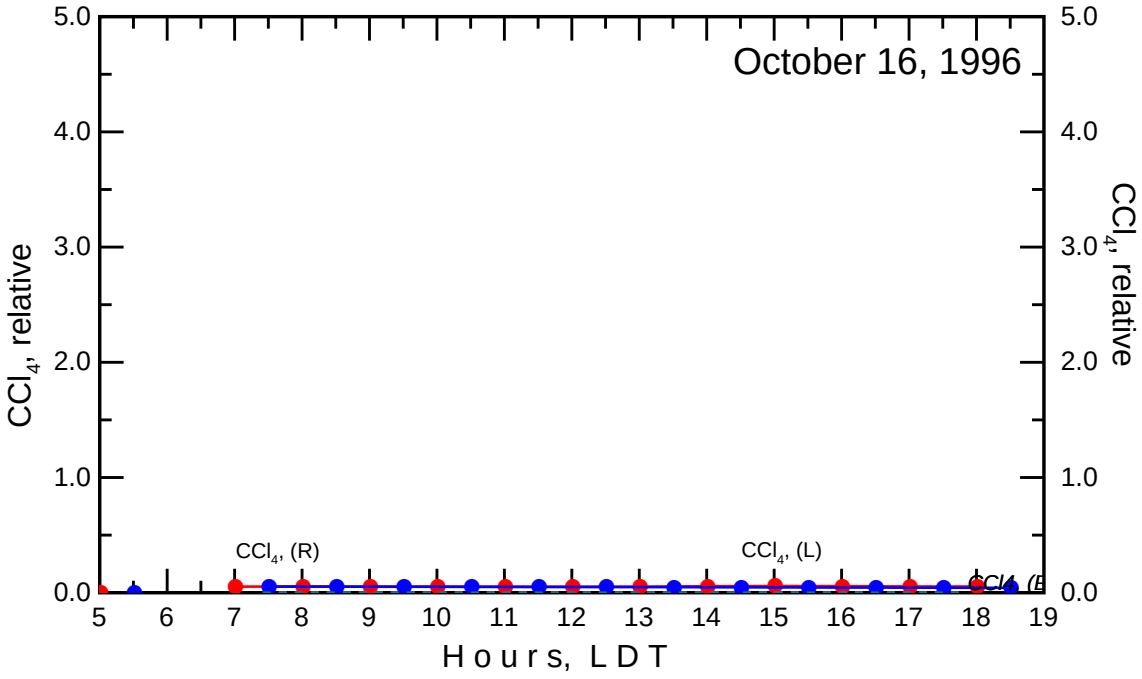

September 14, 1996
1.0 ppmC All Butenes (equal molar)
CB05 Simulation
07/05
NO, (L)
NO2, (L)
O3, (L)
TotNO3, (L)
NO2, (L)
PAN, (L)
NO, (L)
NO, NO2, ppm
O3, ppm
Hours, LDT
September 14, 1996
2.0 ppmC All Butenes (equal molar)
CB05 Simulation
NO, (L)
NO2, (L)
TotNO3, (L)
PAN, (L)
NO2, (L)
NO, (L)
NO, NO2, ppm
O3, ppm
Hours, LDT


September 14, 1996
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19



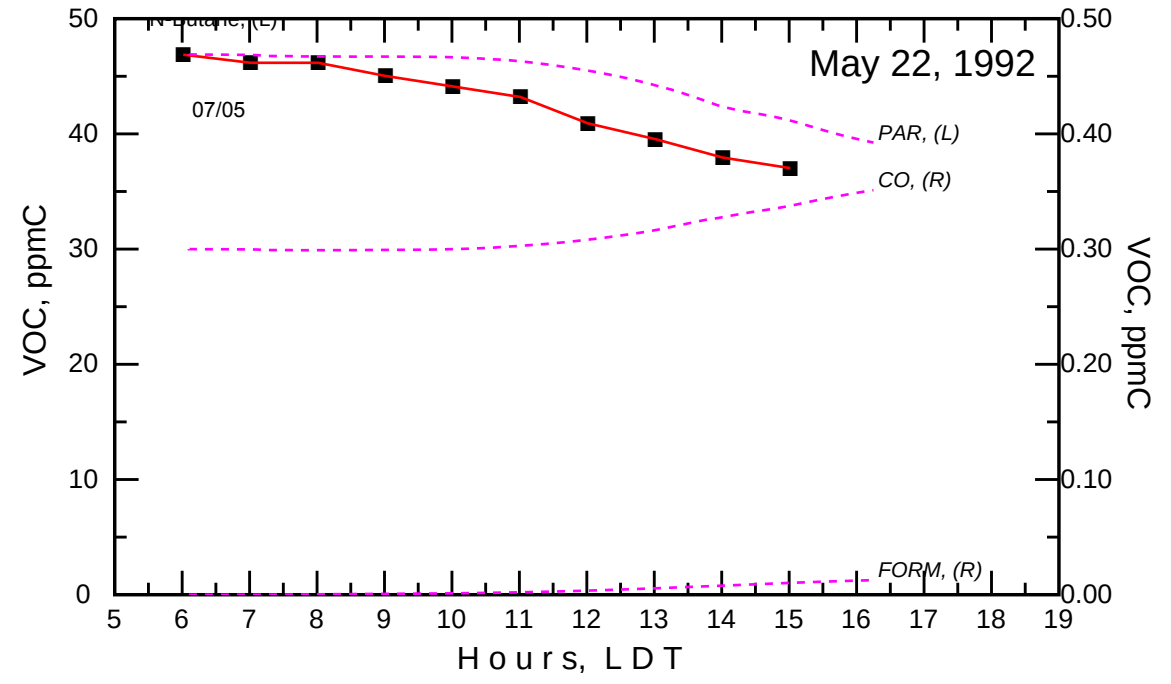
Propene vs Propene, 1-Butene, 1-Pentene

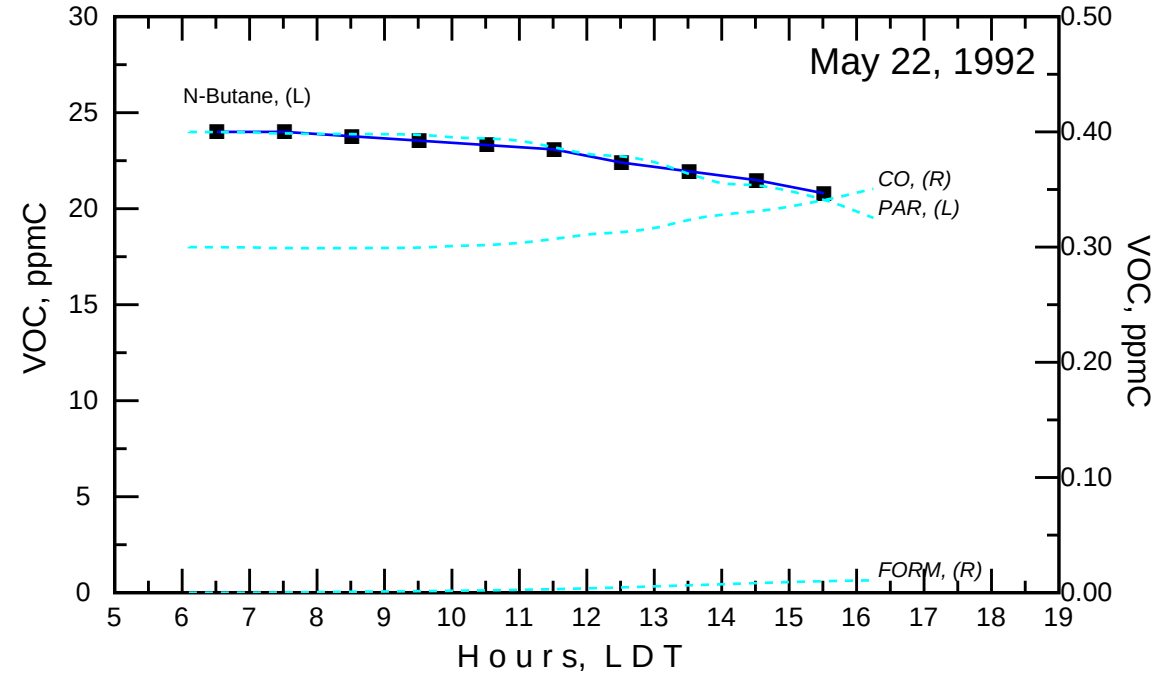

October 16, 1996
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpo
Dewpt
NO2
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

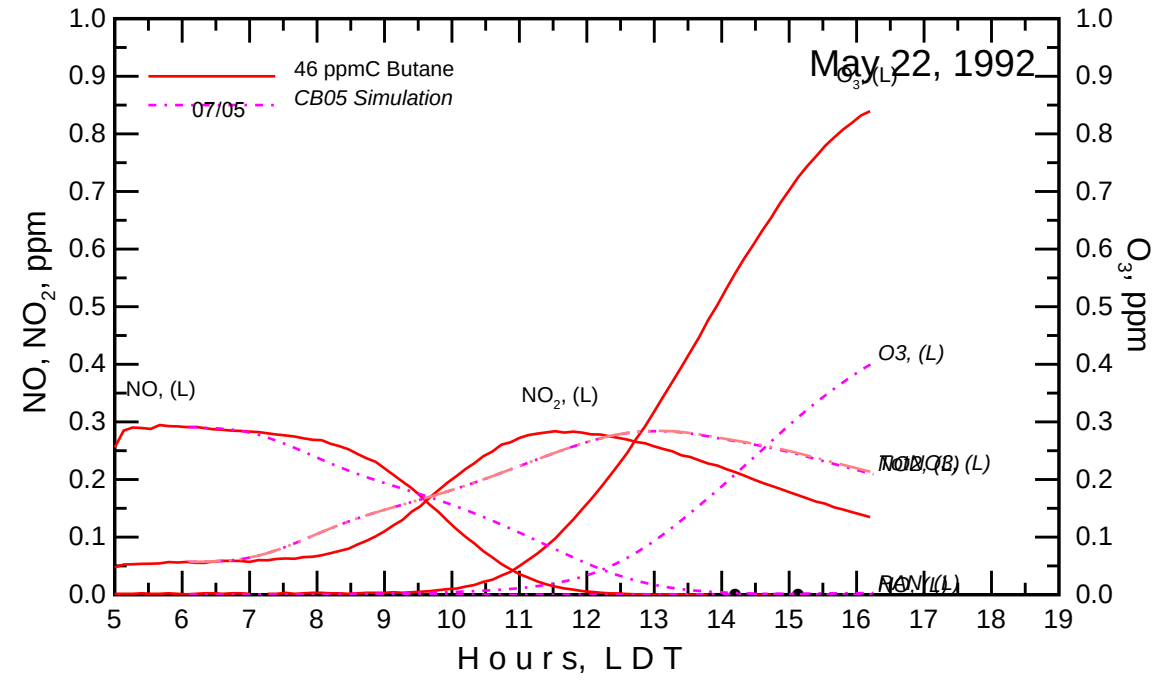

October 16, 1996
CCl4, relative
CCl4, (R)
CCl4, (L)
Hours, LDT

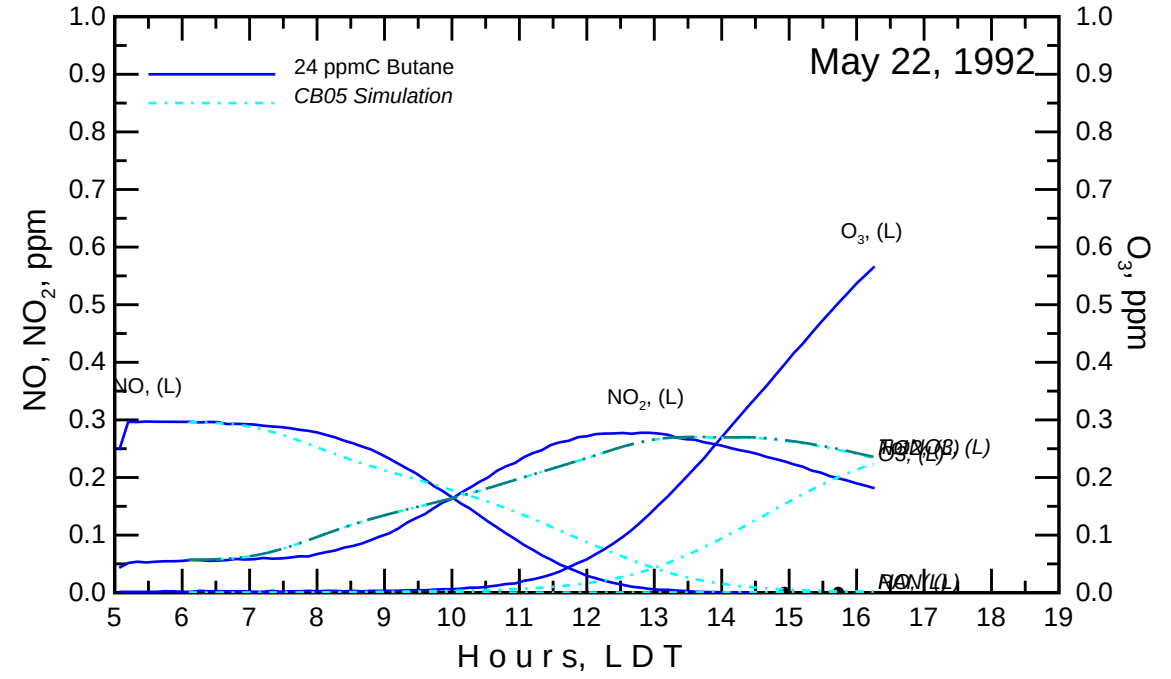
Alkanes (PAR)

MY 22 92
MY 23 92
AU 16 96
AU 19 83
OC 11 01

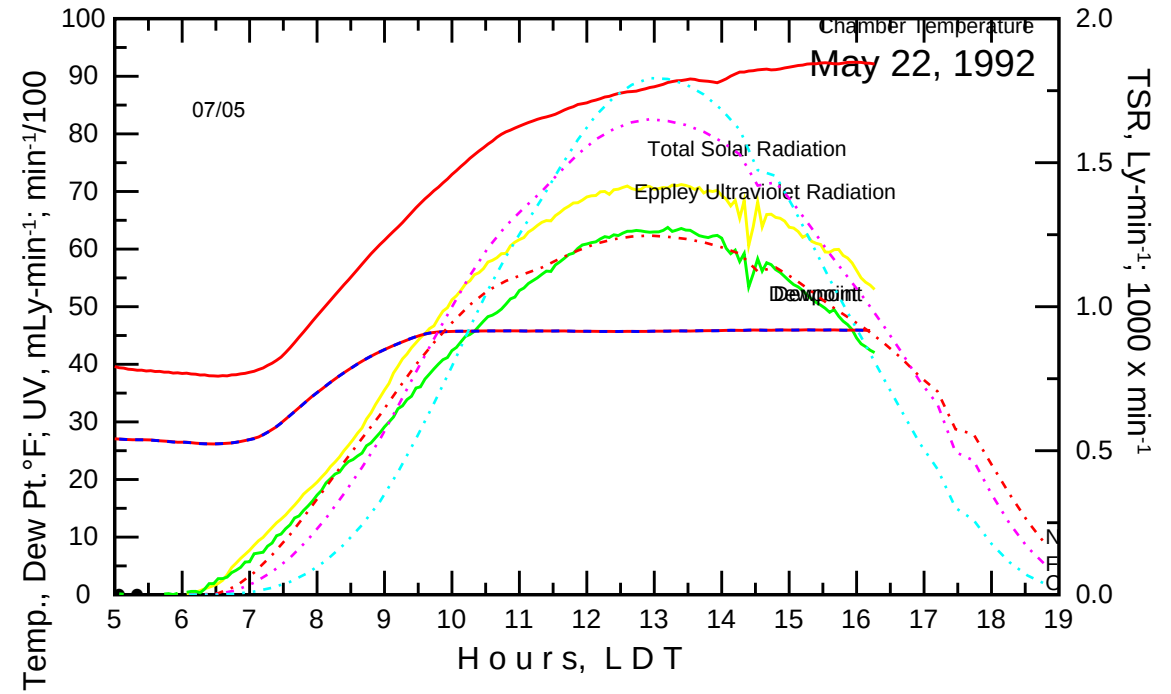

May 22, 1992
07/05
PAR, (L)
CO, (R)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

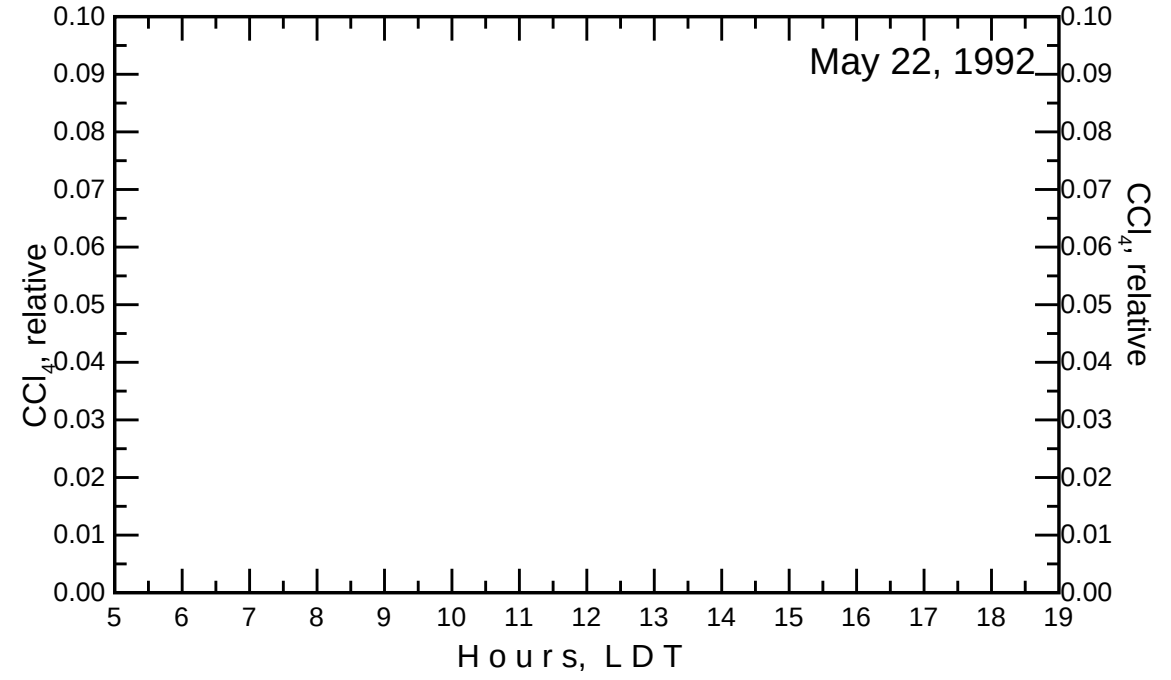

May 22, 1992
N-Butane, (L)
CO, (R)
PAR, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

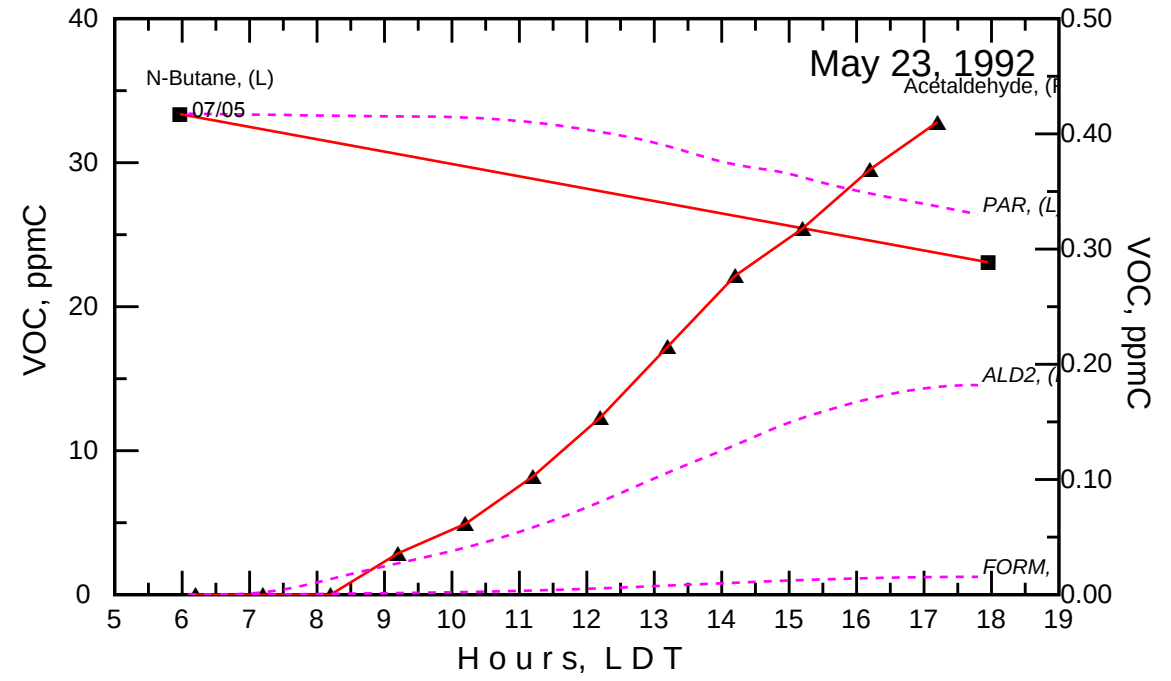


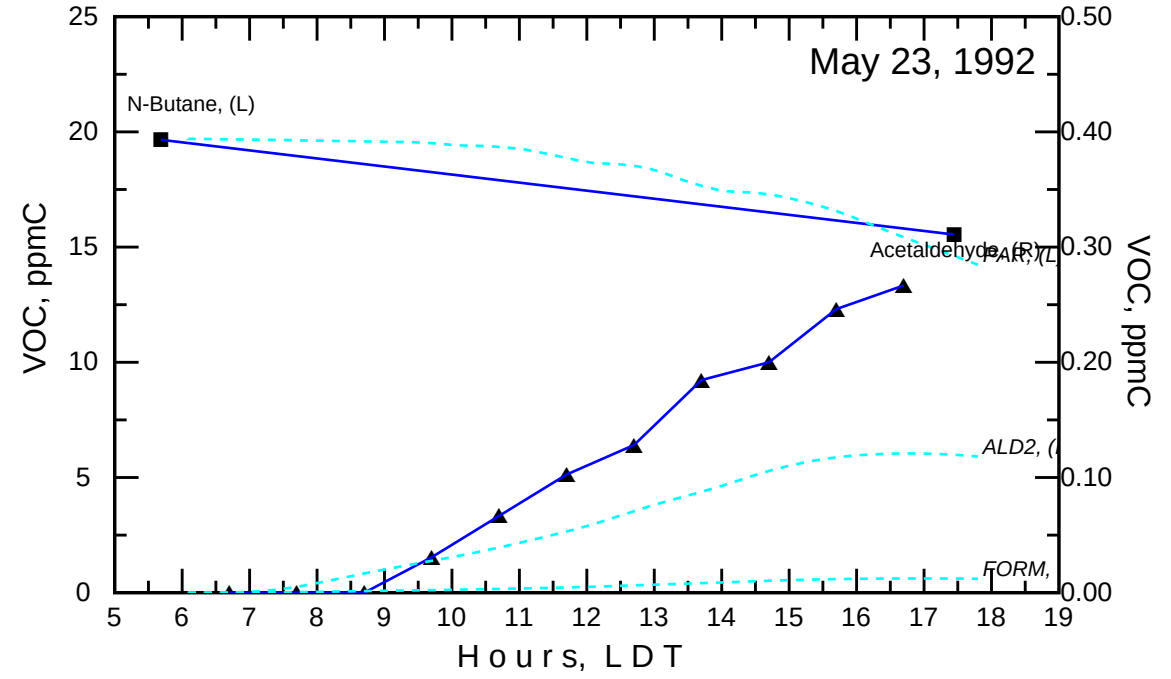


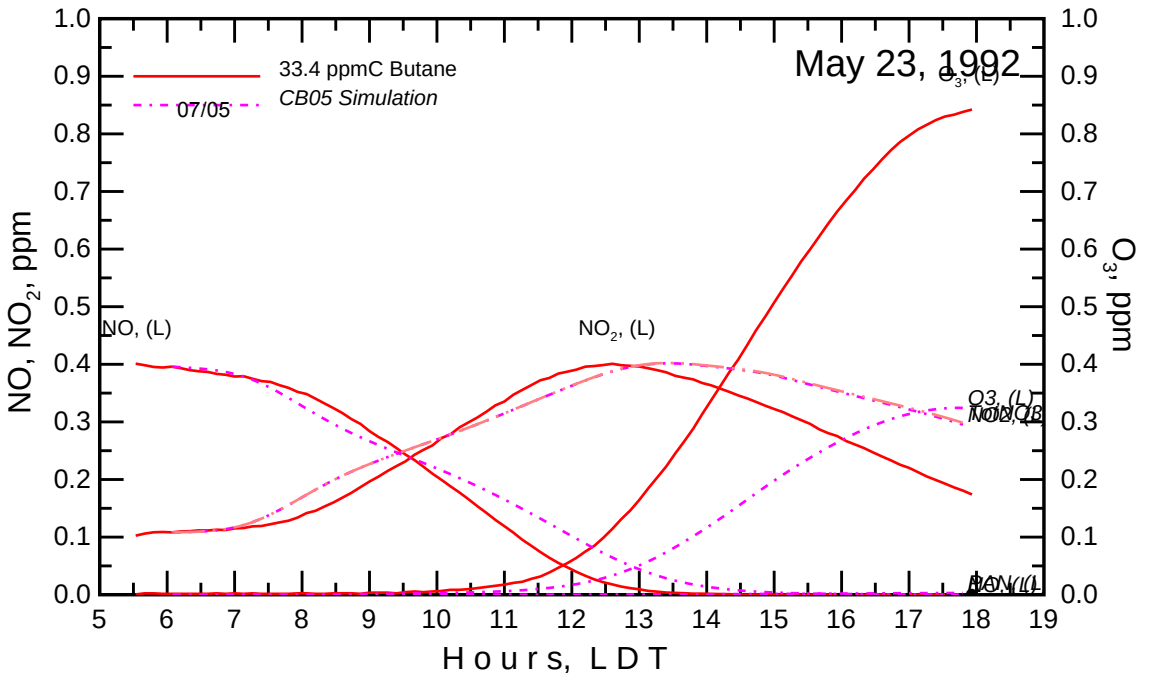
Delta Butane Run

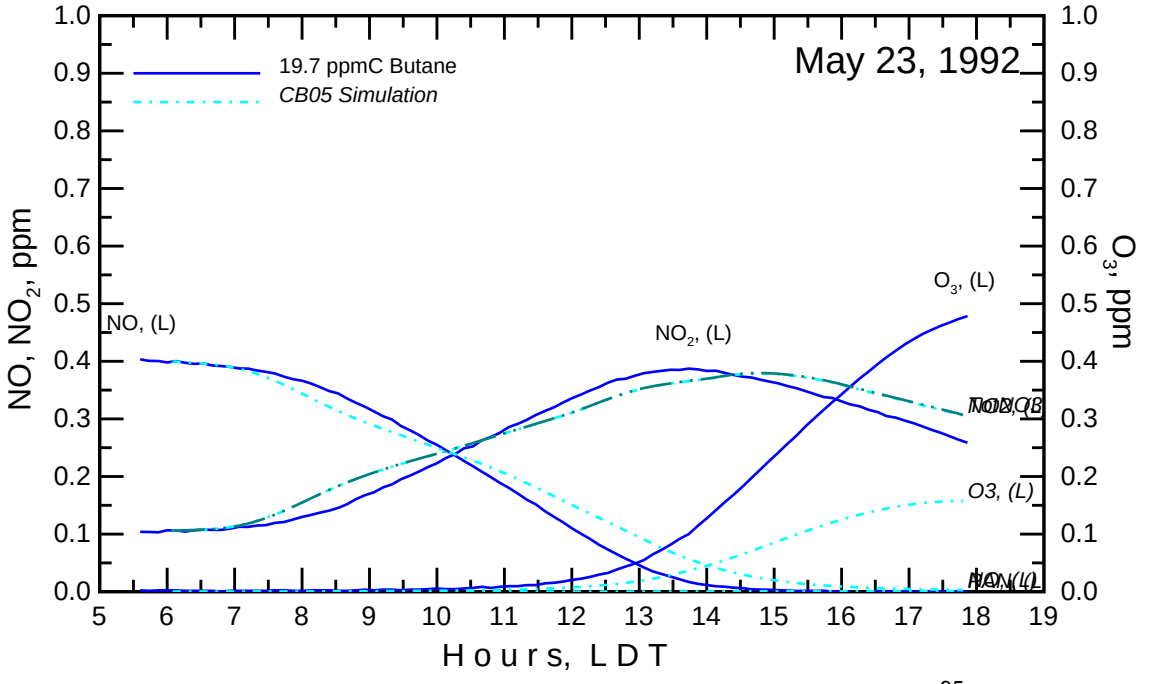

Chamber Temperature
May 22, 1992
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


May 22, 1992
CCl4, relative
CCl4, relative
Hours, LDT

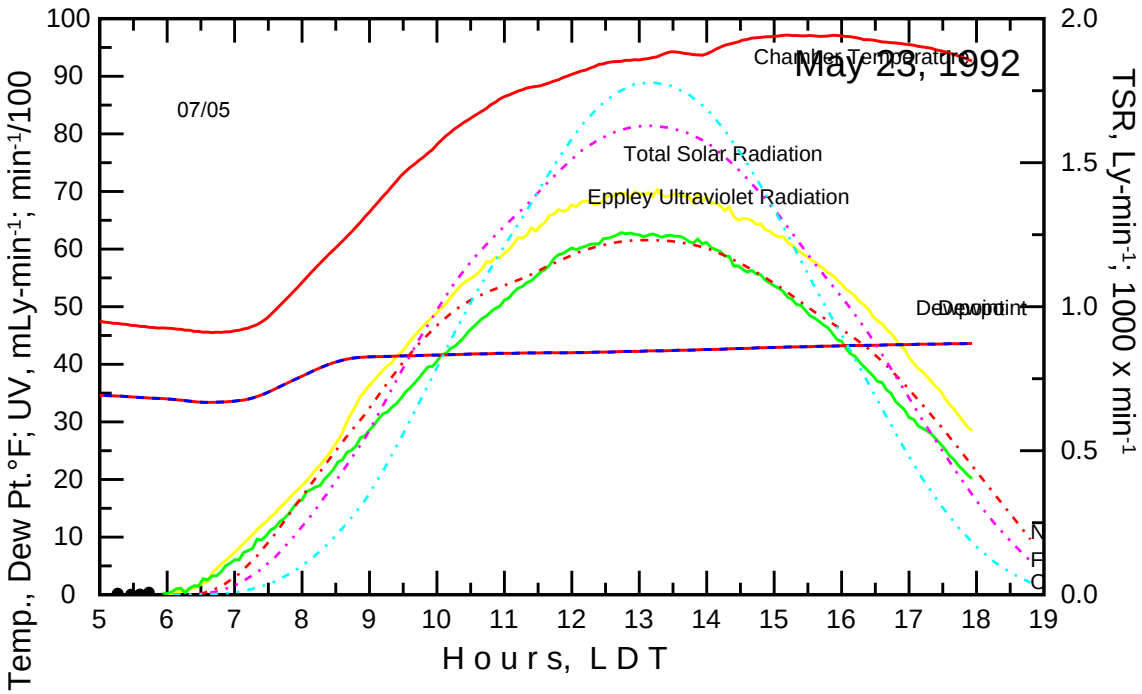

May 23, 1992
N-Butane, (L)
07/05
Acetaldehyde, (R
PAR, (L
ALD2, (
FORM,
VOC, ppmC
VOC, ppmC
Hours, LDT
0
10
20
30
40
0.00
0.10
0.20
0.30
0.40
0.50
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

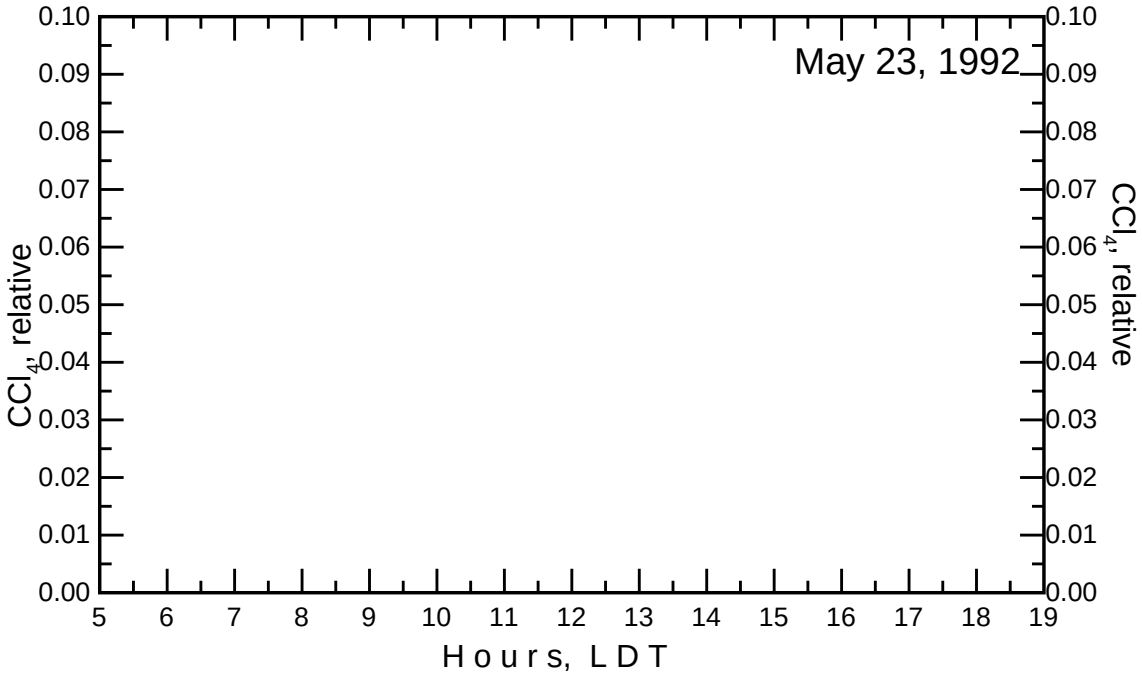

May 23, 1992
N-Butane, (L)
Acetaldehyde, (R)
PAR, (L
ALD2, (
FORM,
VOC, ppmC
VOC, ppmC
Hours, LDT
0
5
10
15
20
25
0.00
0.10
0.20
0.30
0.40
0.50
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

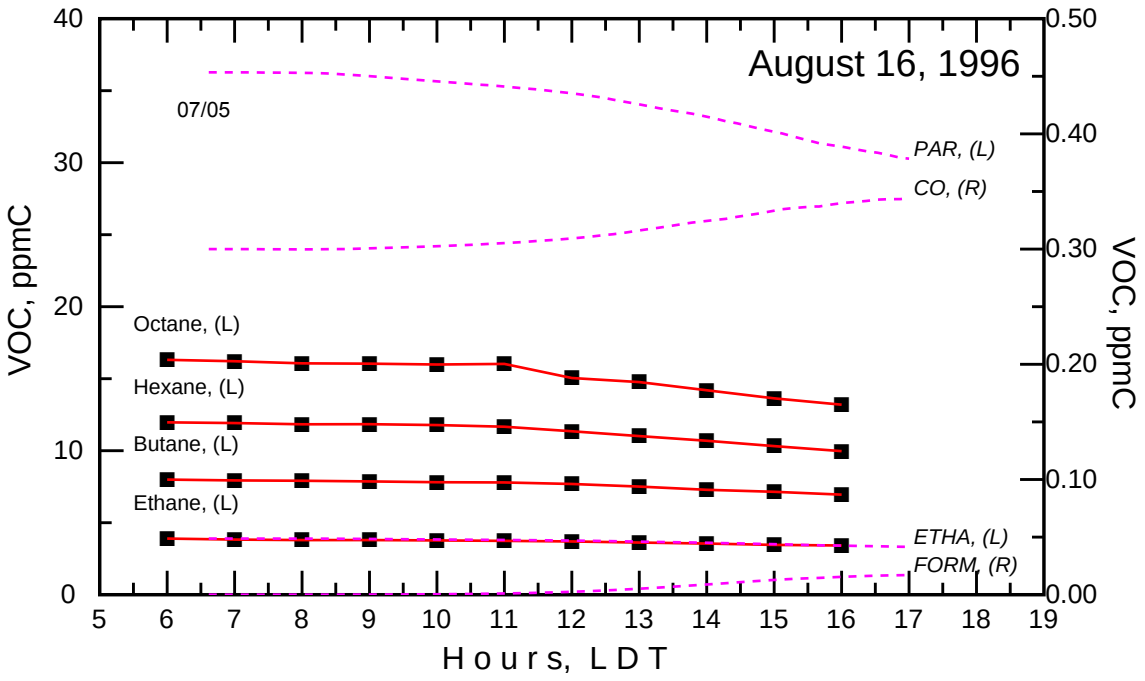


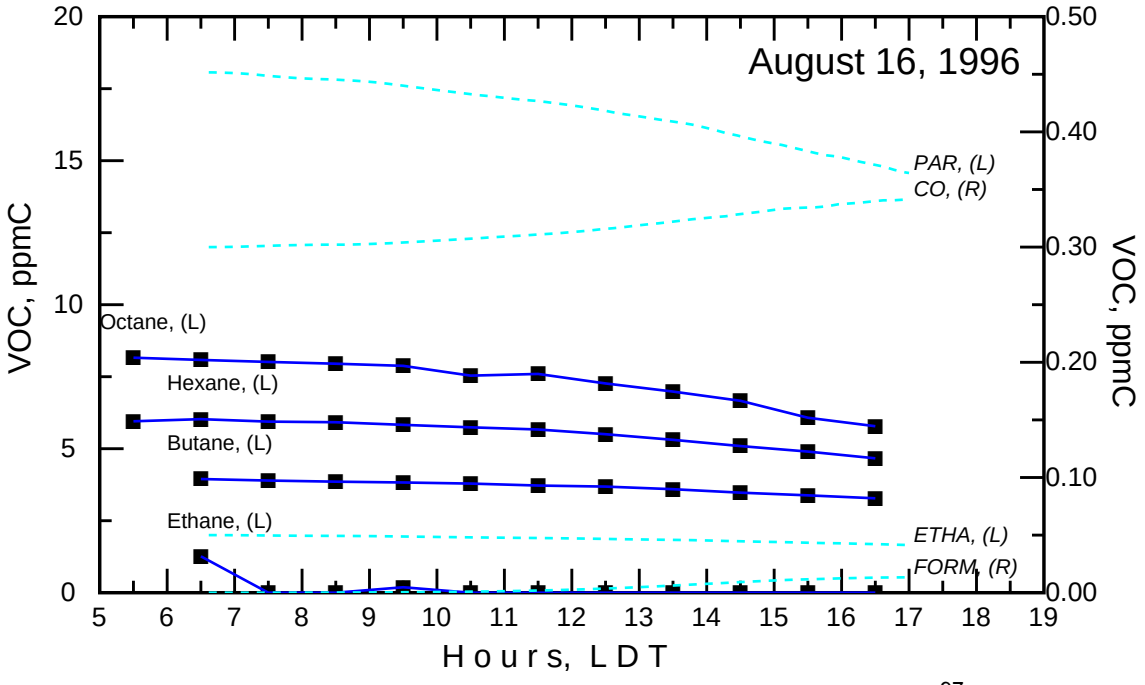


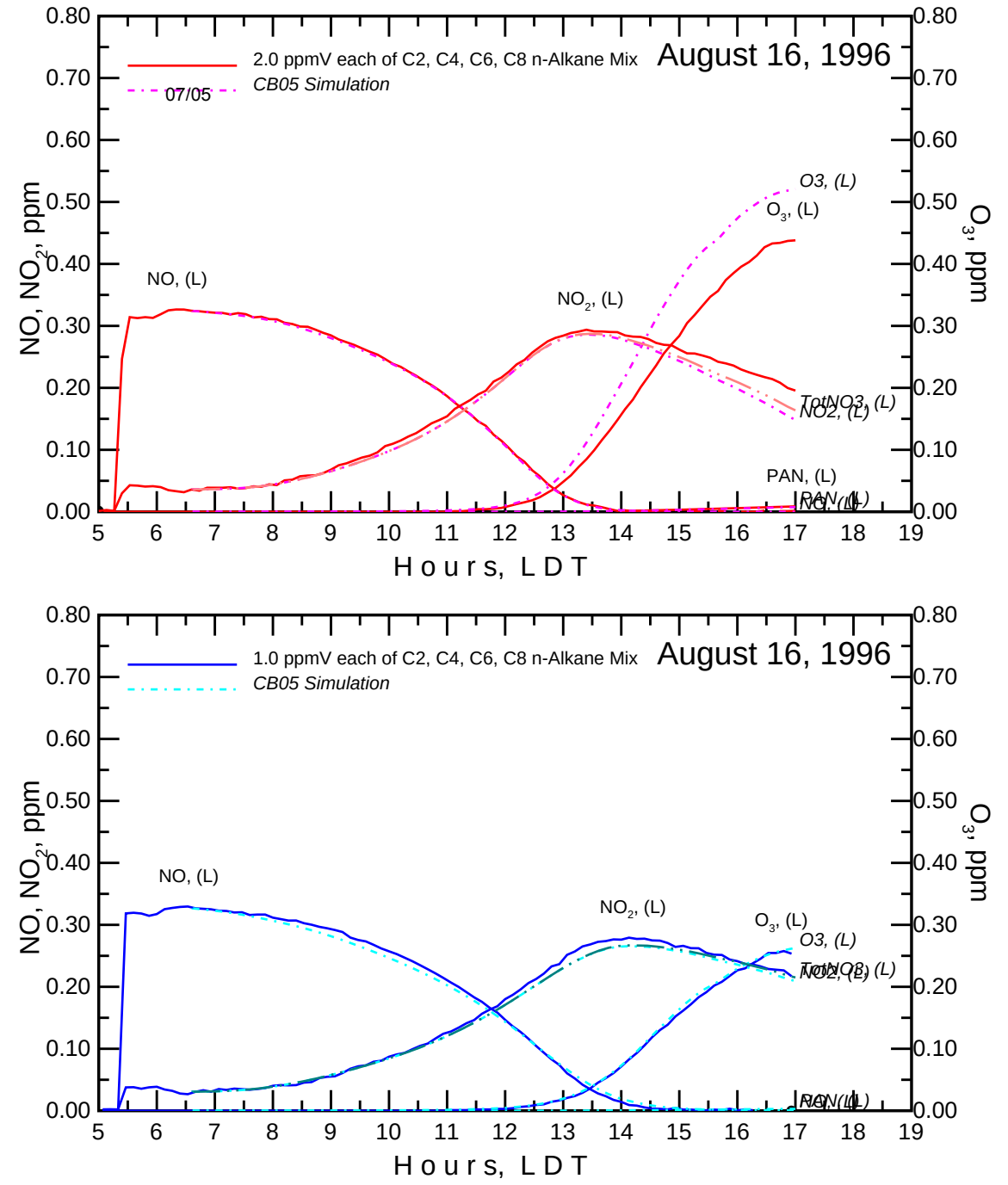
Delta Butane Run


May 23, 1992
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

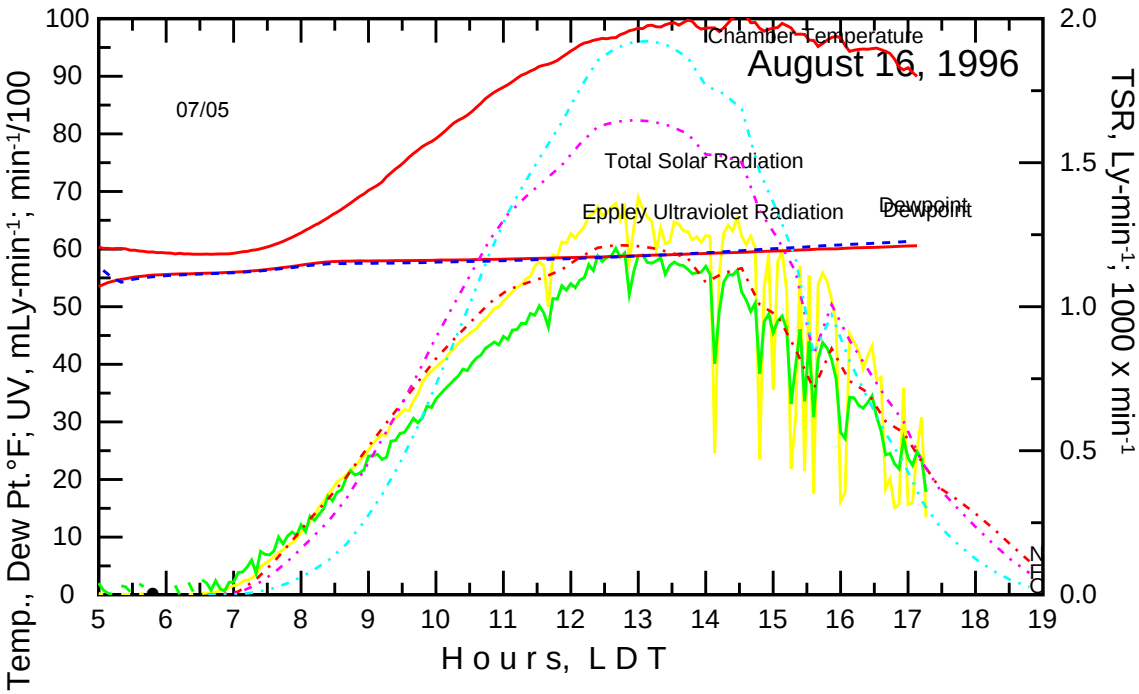

May 23, 1992
CCl4, relative
Hours, LDT

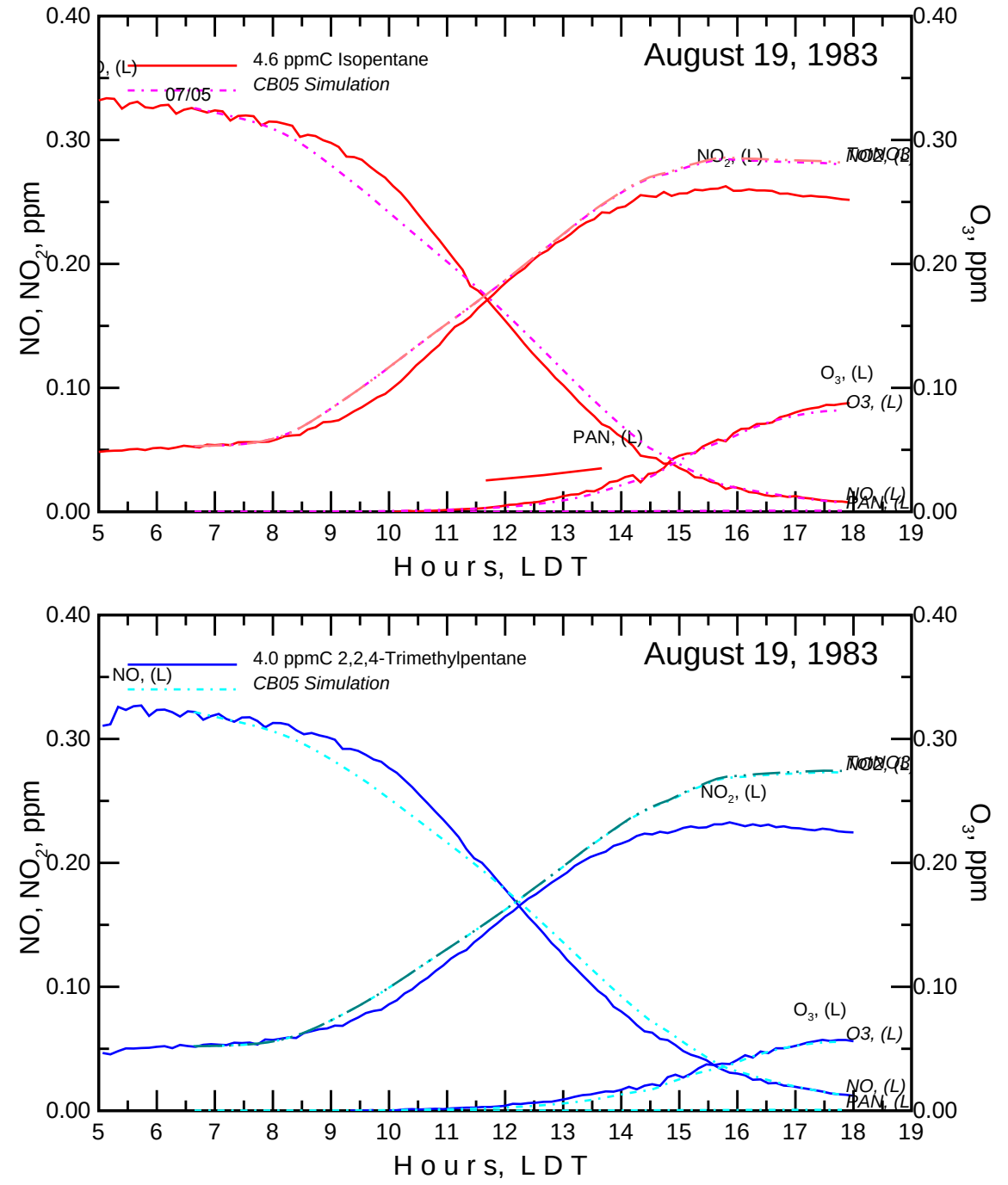

August 16, 1996
07/05
PAR, (L)
CO, (R)
Octane, (L)
Hexane, (L)
Butane, (L)
Ethane, (L)
ETHA, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT


August 16, 1996
PAR, (L)
CO, (R)
Octane, (L)
Hexane, (L)
Butane, (L)
Ethane, (L)
ETHA, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

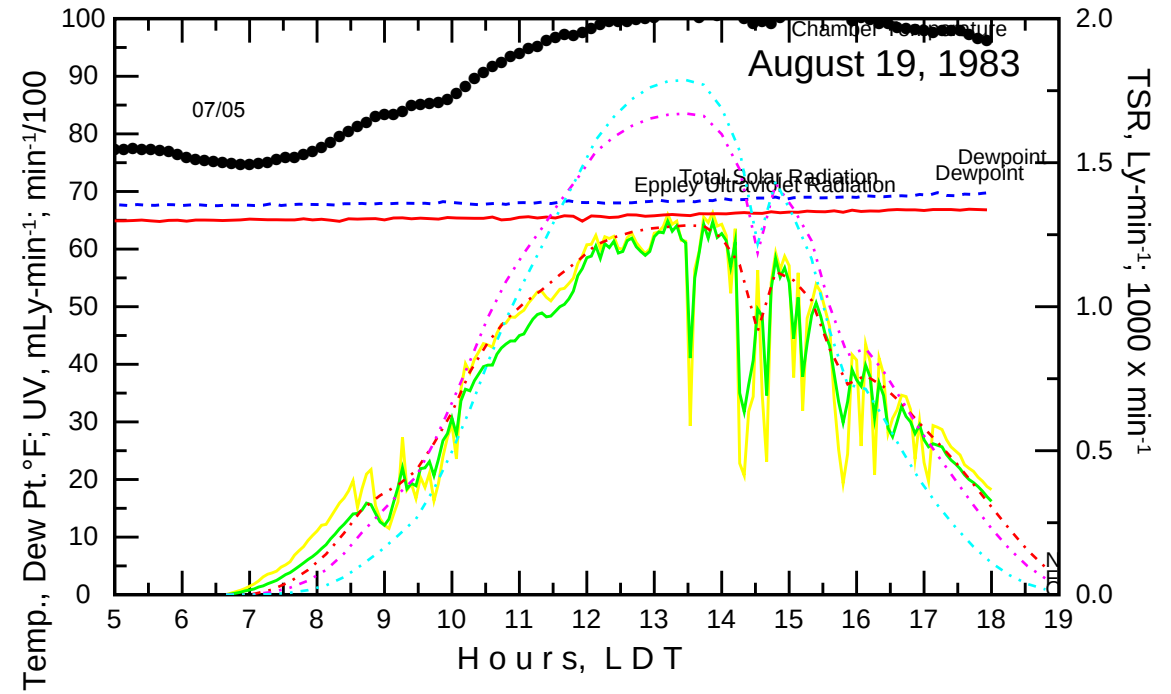


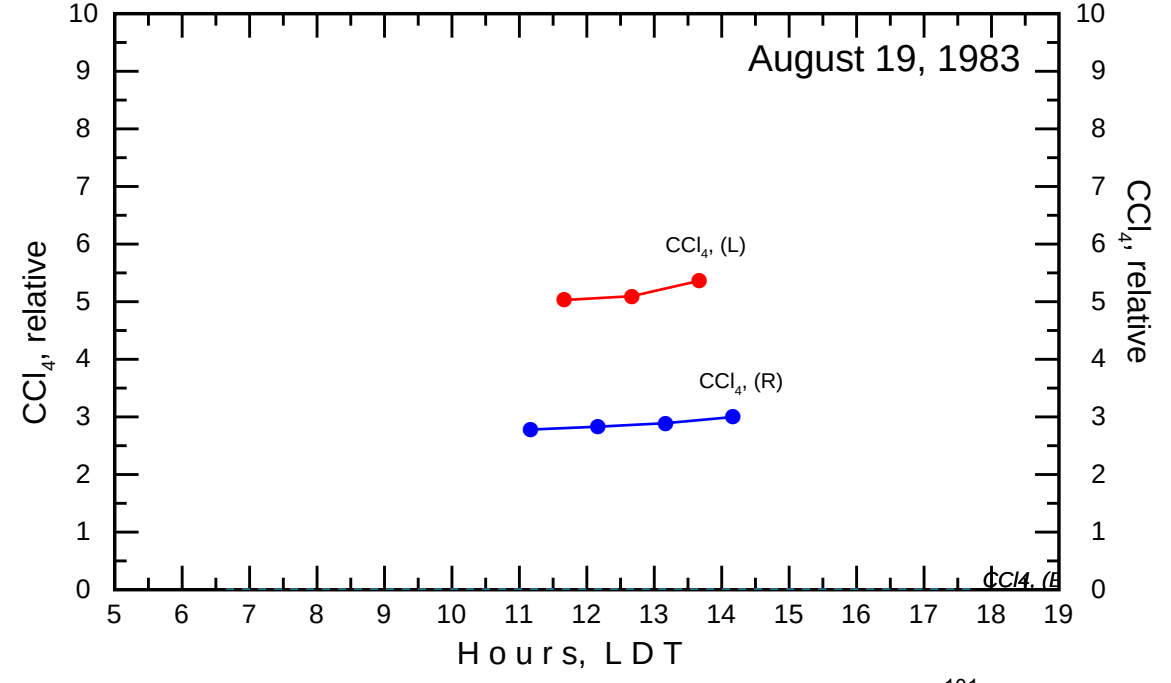
40 ppmC Alkane Mix vs 20 ppmC Alkane Mix

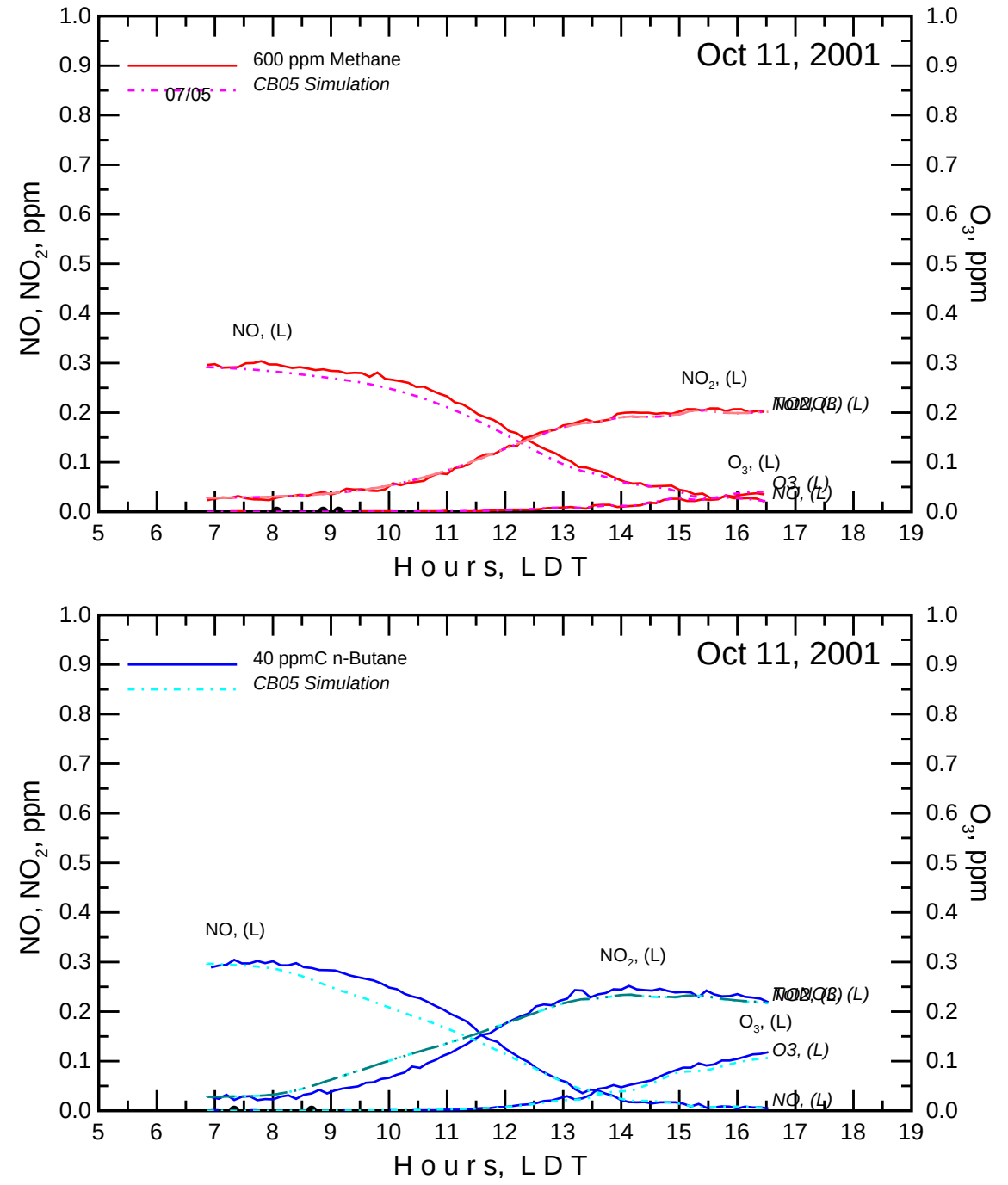

August 16, 1996
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
100
90
80
70
60
50
40
30
20
10
0
2.0
1.5
1.0
0.5
0.0
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19



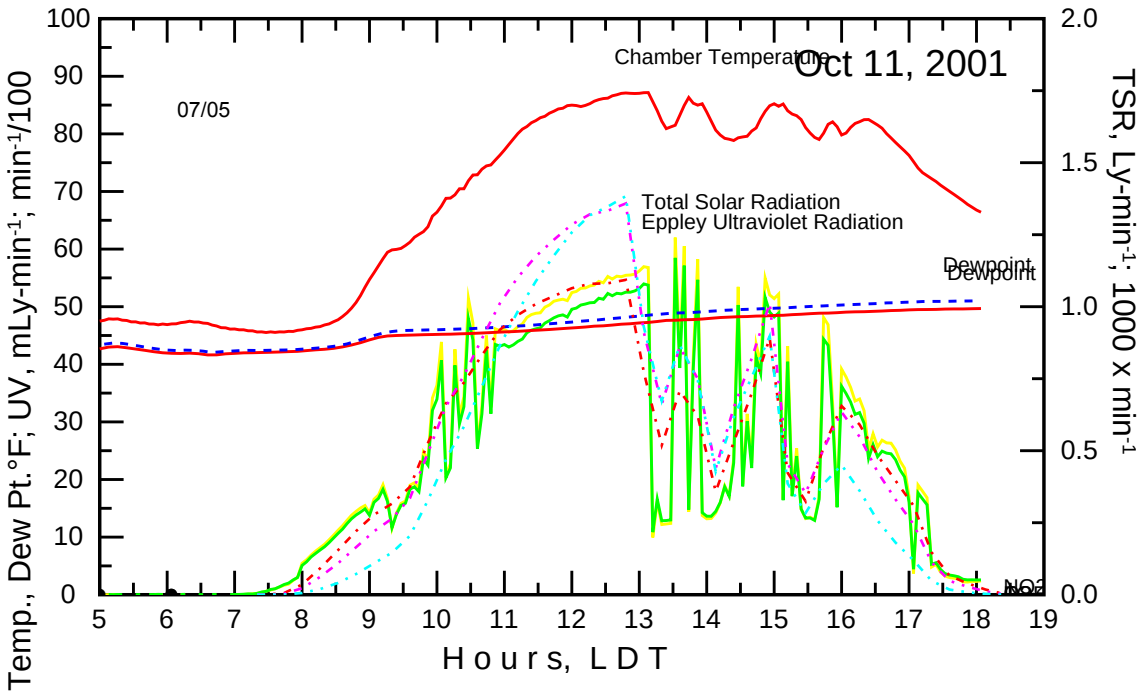
HC Reactivity at 0.37 NO_x

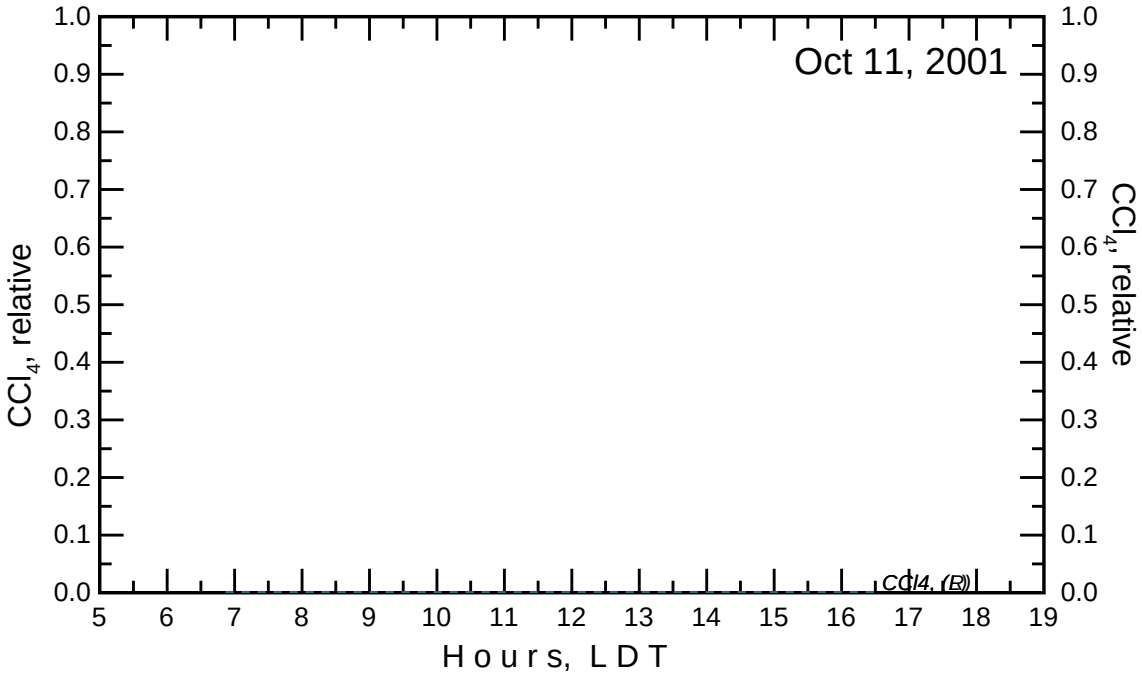

August 19, 1983
07/05
Dewpoint
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


August 19, 1983
CCl4, (L)
CCl4, (R)
CCl4, relative
Hours, LDT



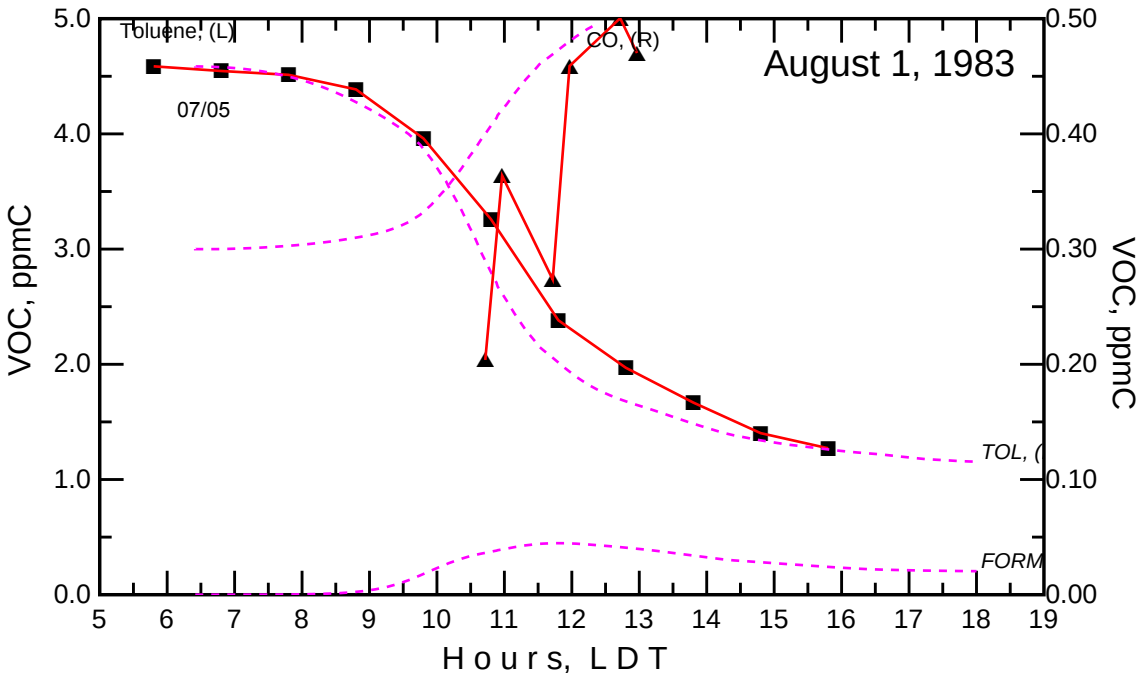
Characterization Experiment: CH4 vs Butane

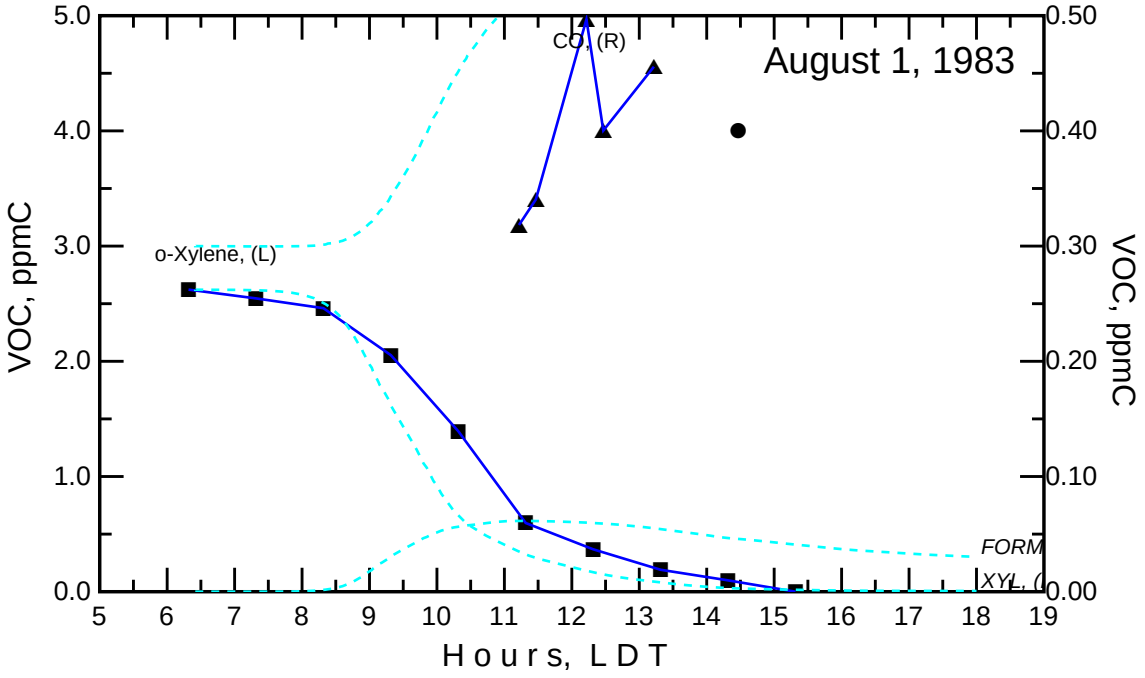

Oct 11, 2001
Chamber Temperature
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
NO2
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


Oct 11, 2001
CCl4, relative
CCl4, relative
CCl4 (B)
Hours, LDT

Aromatics (TOL and XYL)

AU 01 83
AU 03 95
AU 17 88
AU 22 97
AU 30 95
ST 13 93
ST 14 81
ST 24 96


Toluene, (L)
CO, (R)
August 1, 1983
07/05
TOL, (
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT
5.0
4.0
3.0
2.0
1.0
0.0
0.50
0.40
0.30
0.20
0.10
0.00
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19


CO, (R)
August 1, 1983
o-Xylene, (L)
FORM
XYL, (
VOC, ppmC
VOC, ppmC
Hours, LDT
5.0
4.0
3.0
2.0
1.0
0.0
0.50
0.40
0.30
0.20
0.10
0.00
5
6
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16
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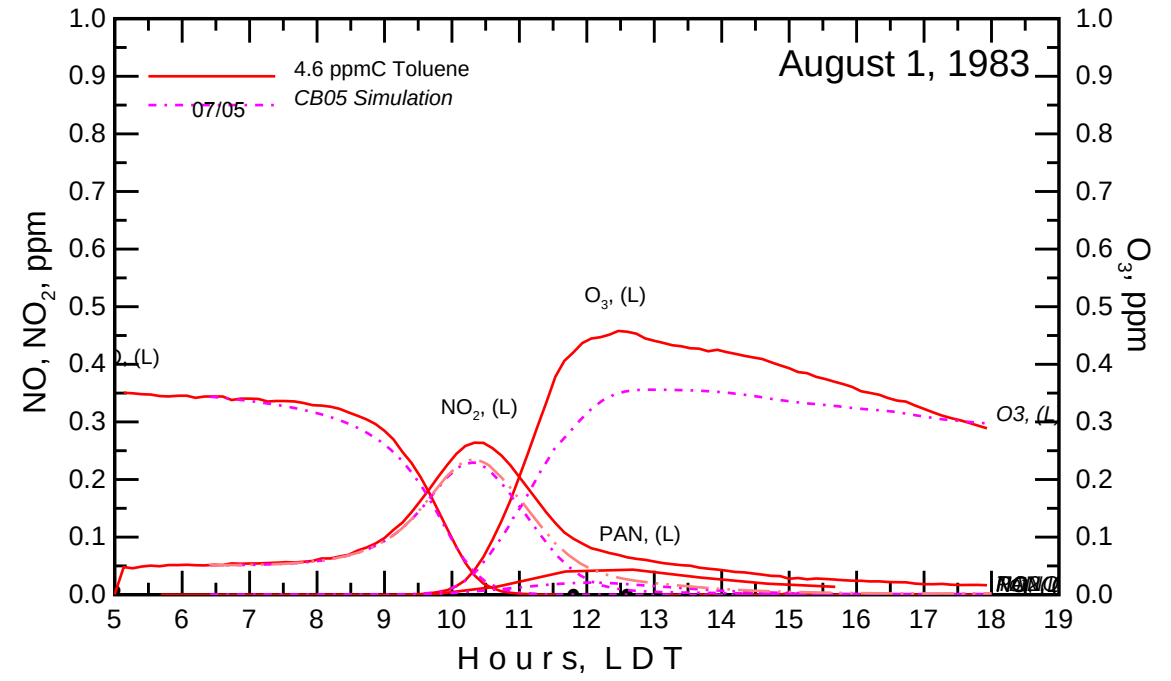
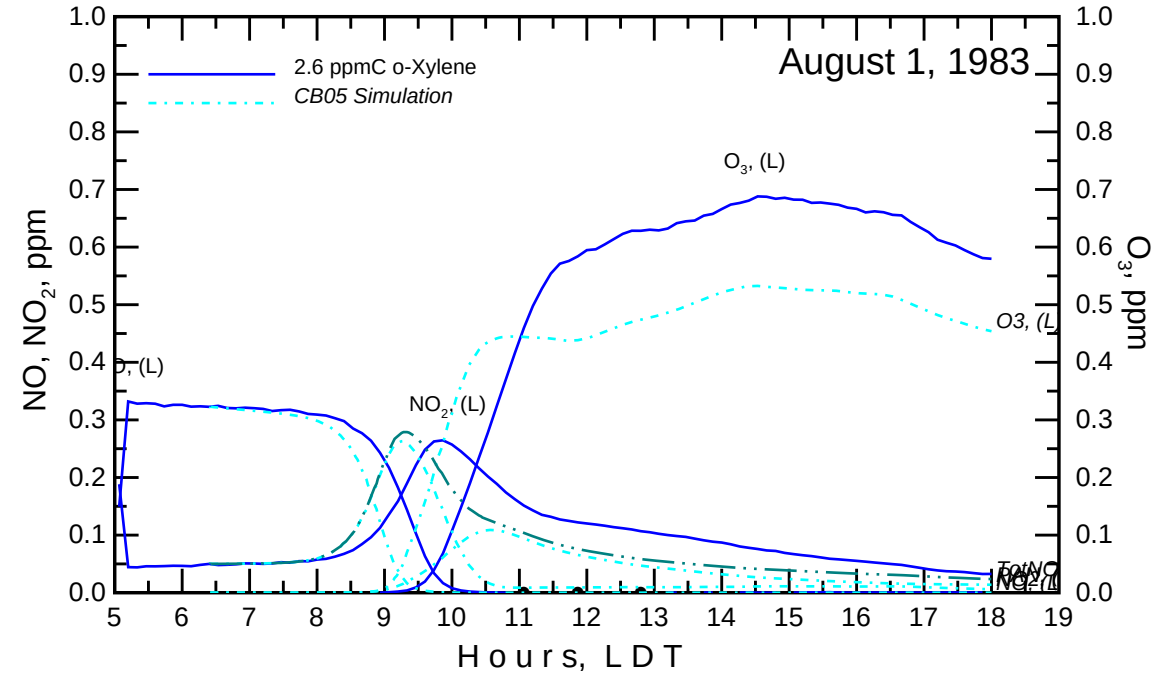
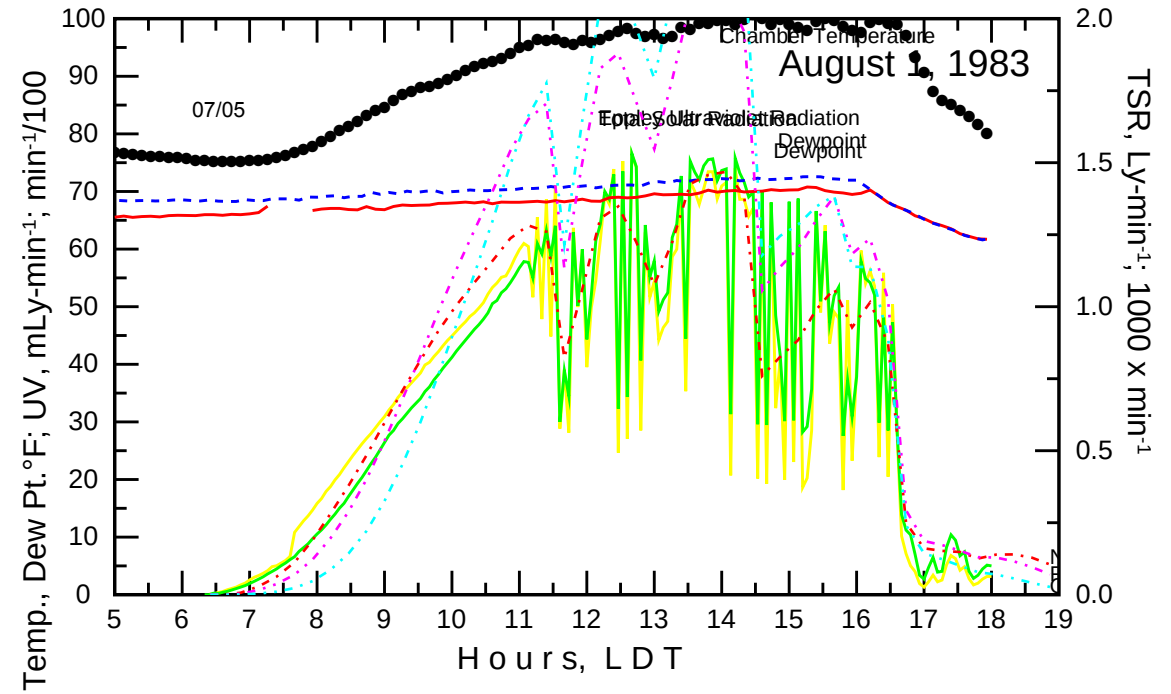
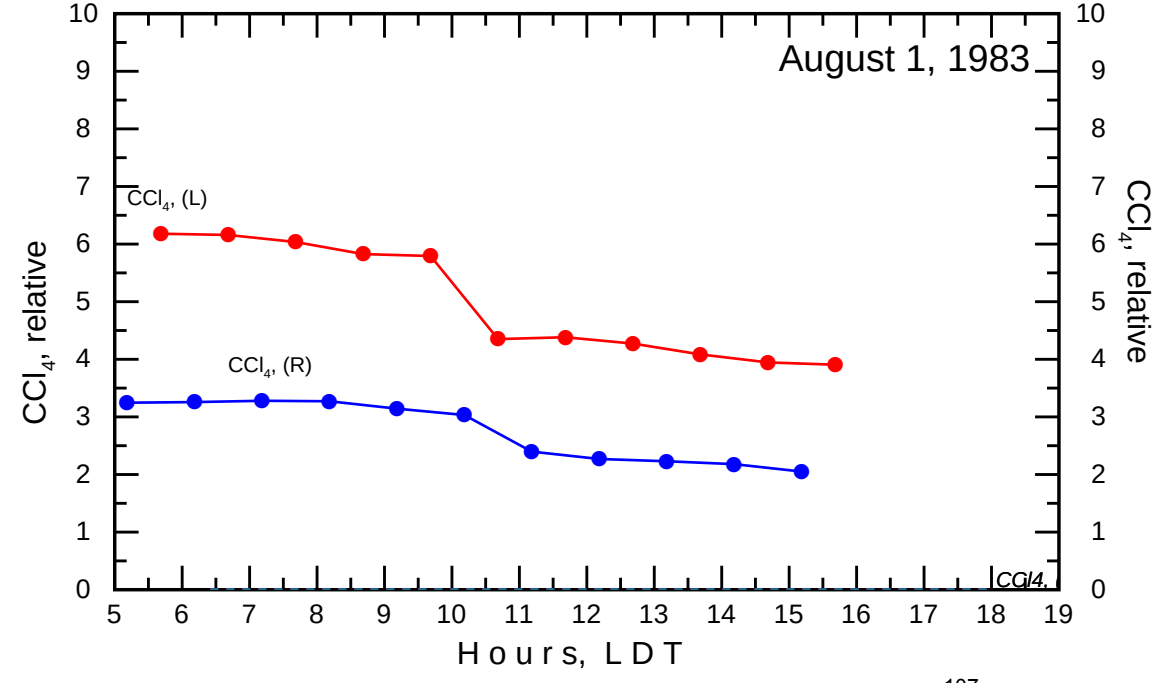
18
19

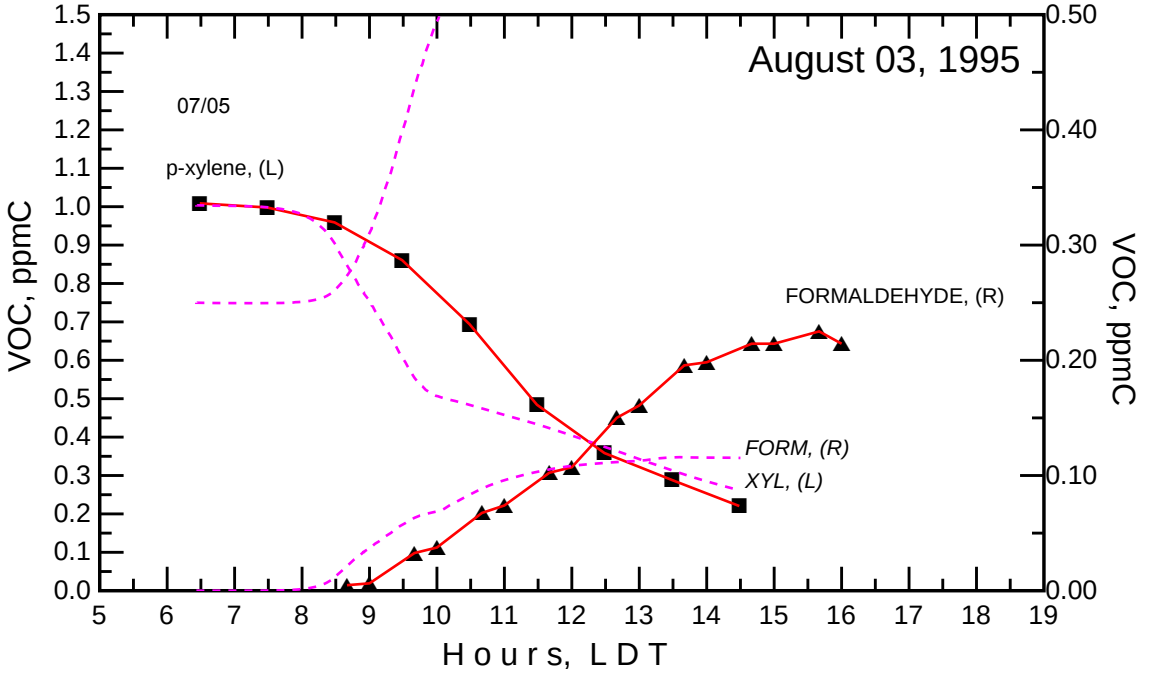


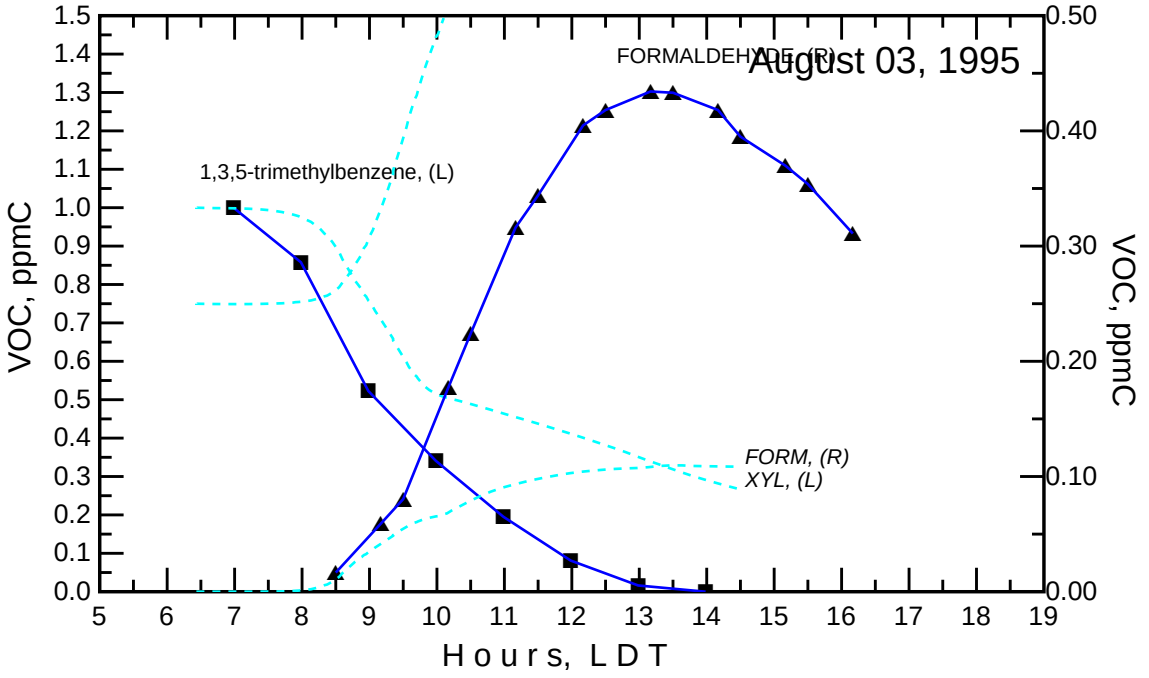


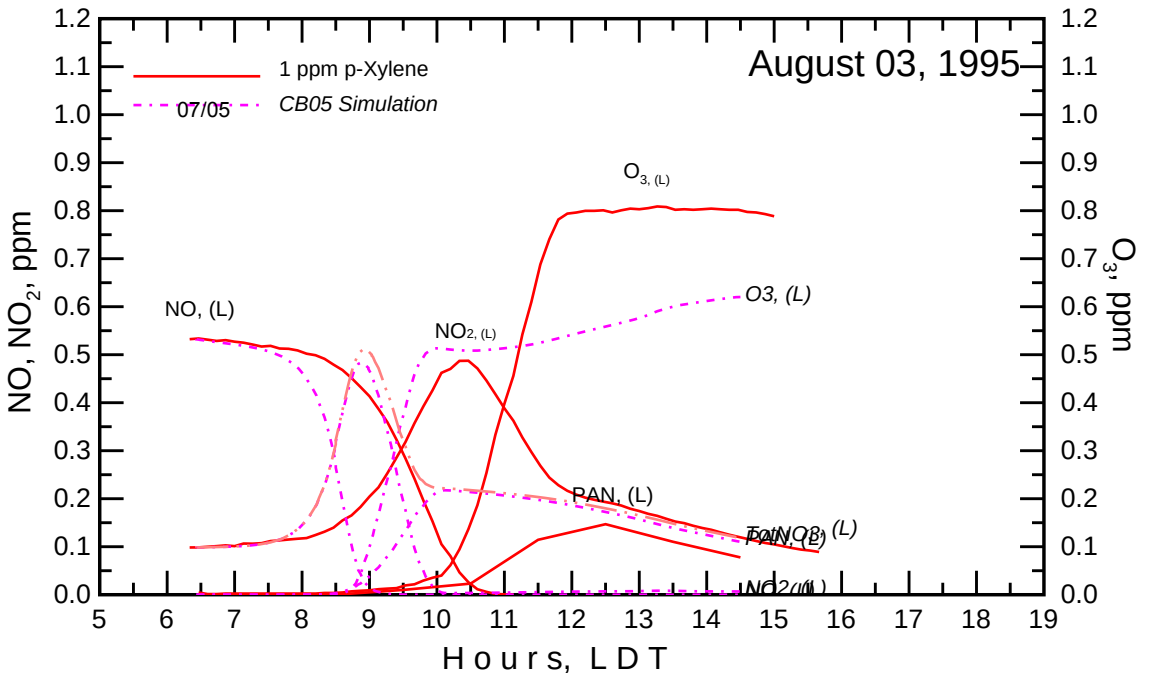
HC Reactivity at 0.38 pm NO_x

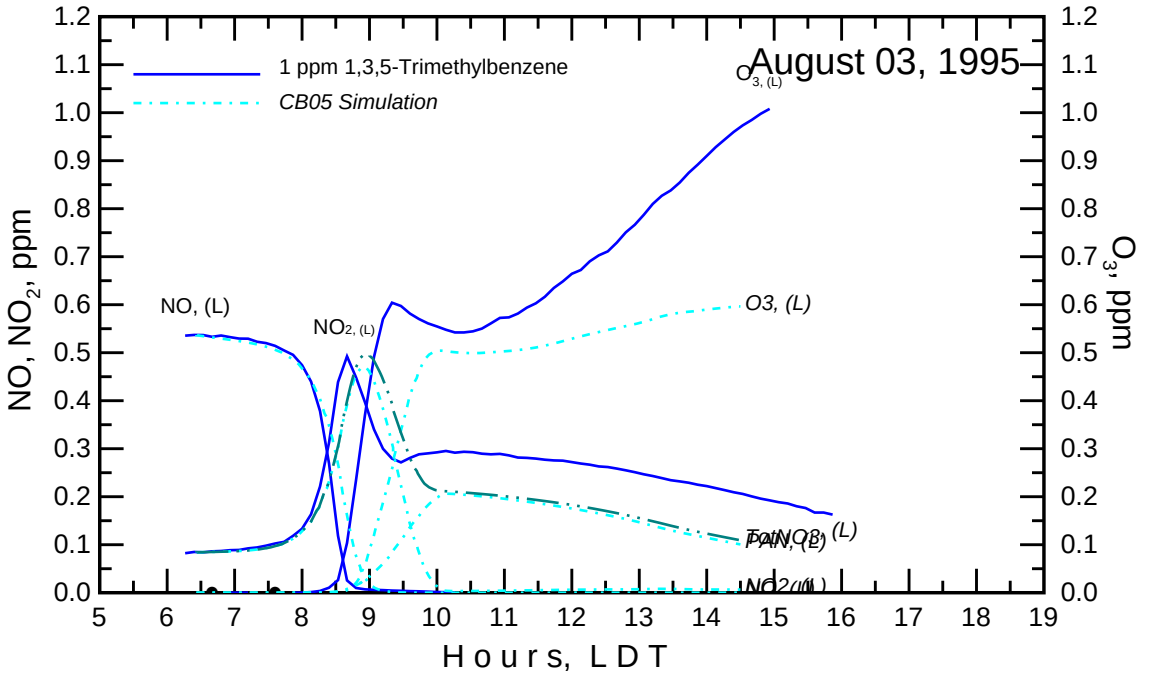

August 1, 1983
07/05
Chamber Temperature
Total Solar Radiation
Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


August 1, 1983
CCl4, (L)
CCl4, (R)
CCl4, relative
CCl4, relative
Hours, LDT

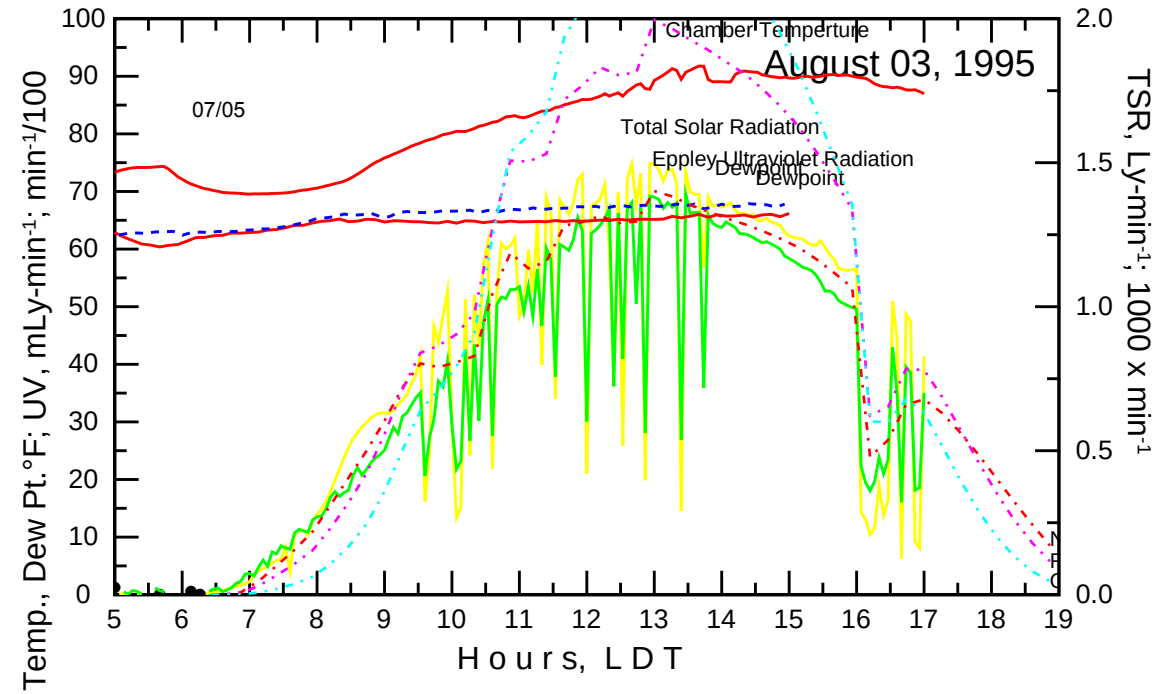

August 03, 1995
07/05
p-xylene, (L)
FORMALDEHYDE, (R)
FORM, (R)
XYL, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

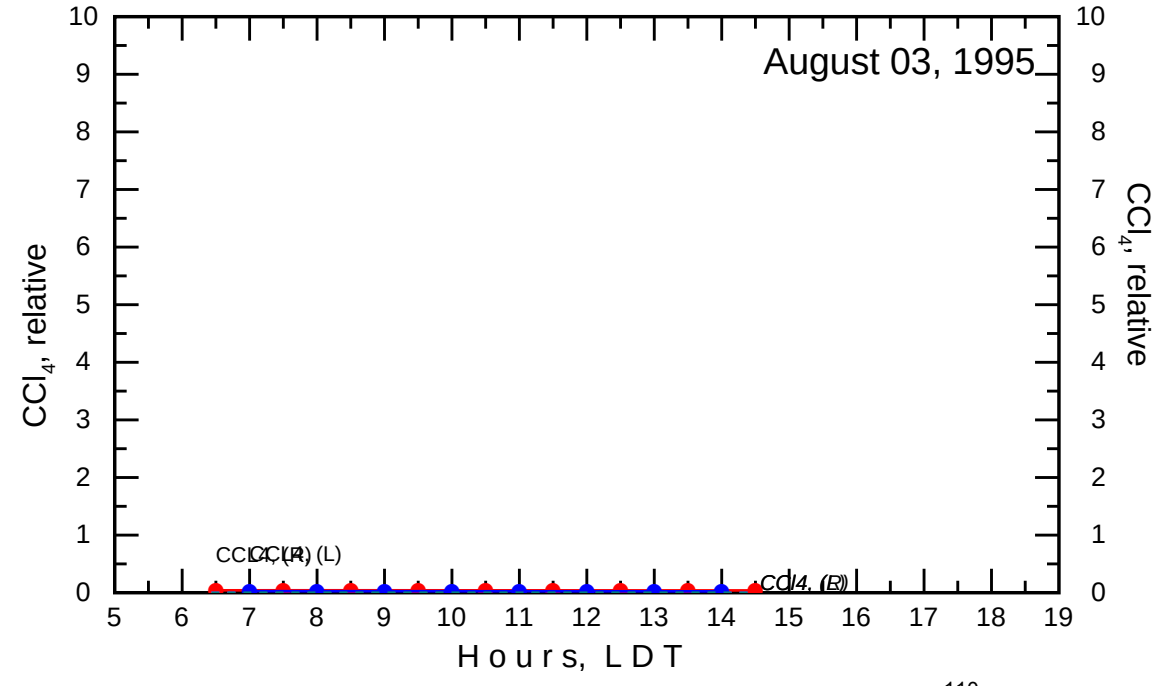

August 03, 1995
FORMALDEHYDE, (R)
1,3,5-trimethylbenzene, (L)
FORM, (R)
XYL, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

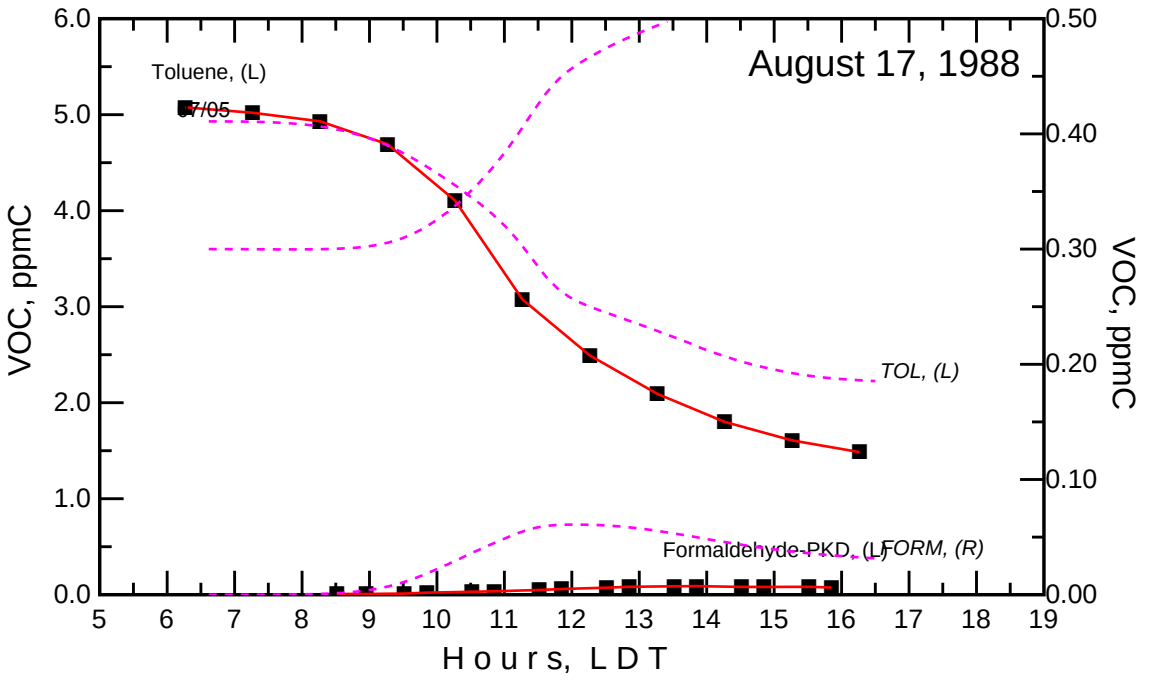


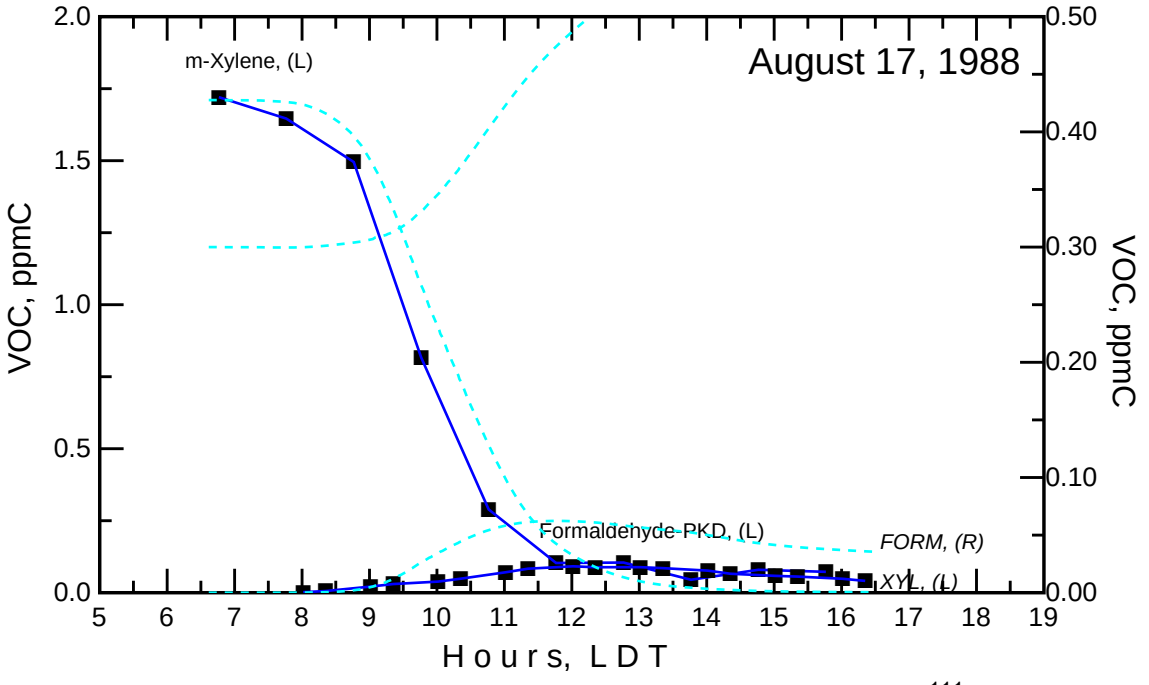


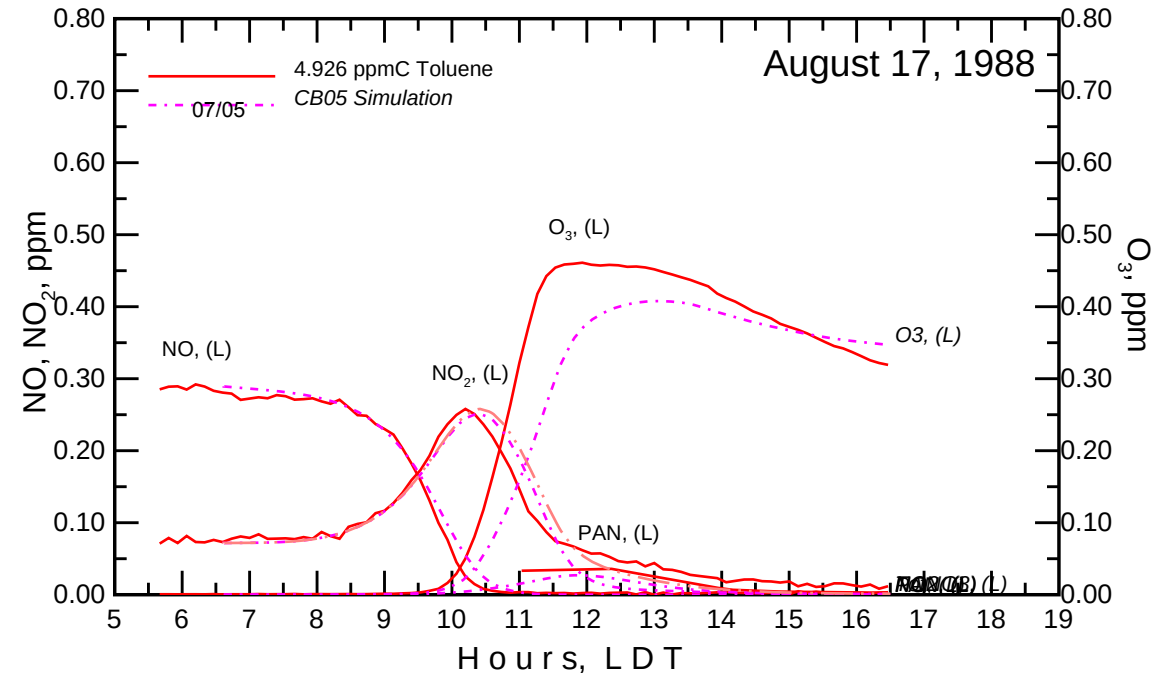
Aromatics Experiments;

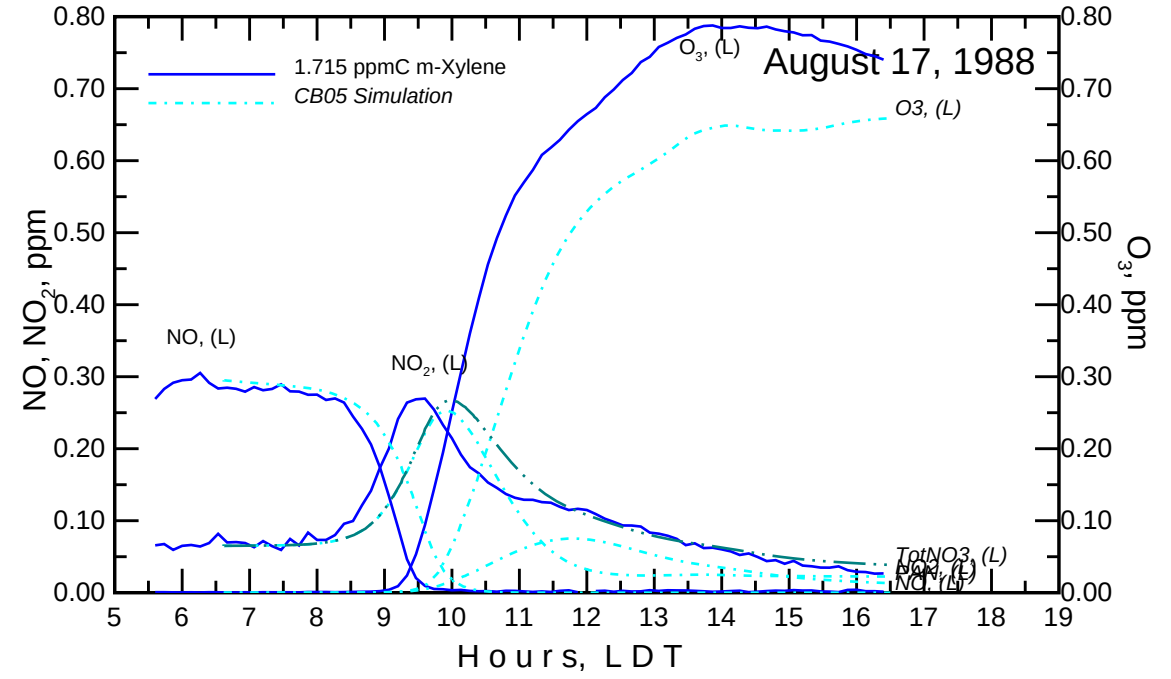

August 03, 1995
07/05
Chamber Temperture
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


August 03, 1995
CCl4, relative
CCl4, relative
CCl4, (R) (L)
CCl4, (R)
Hours, LDT

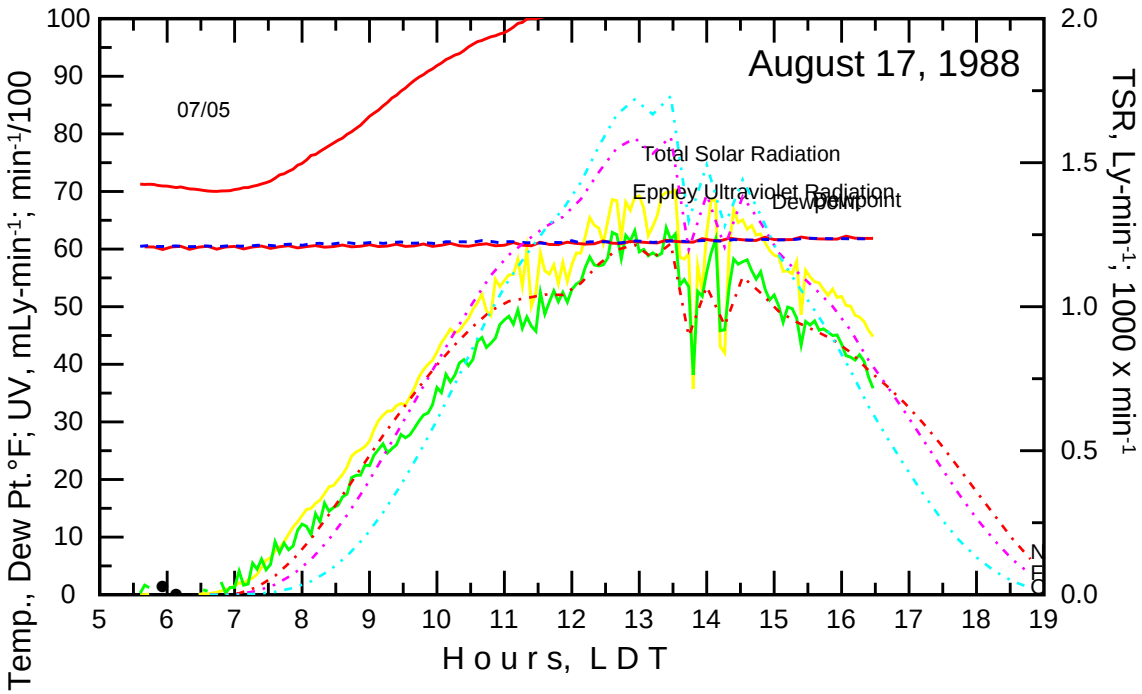

August 17, 1988
Toluene, (L)
8/7/05
TOL, (L)
Formaldehyde-PKD, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

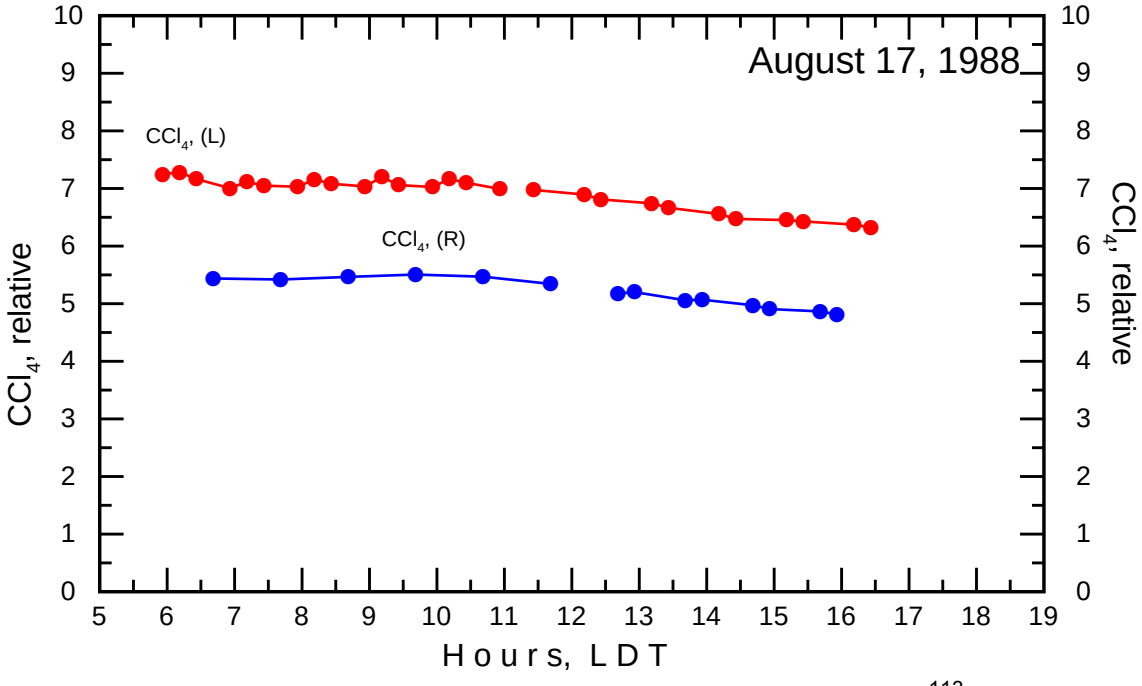

August 17, 1988
m-Xylene, (L)
Formaldehyde-PKD, (L)
FORM, (R)
XYL, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

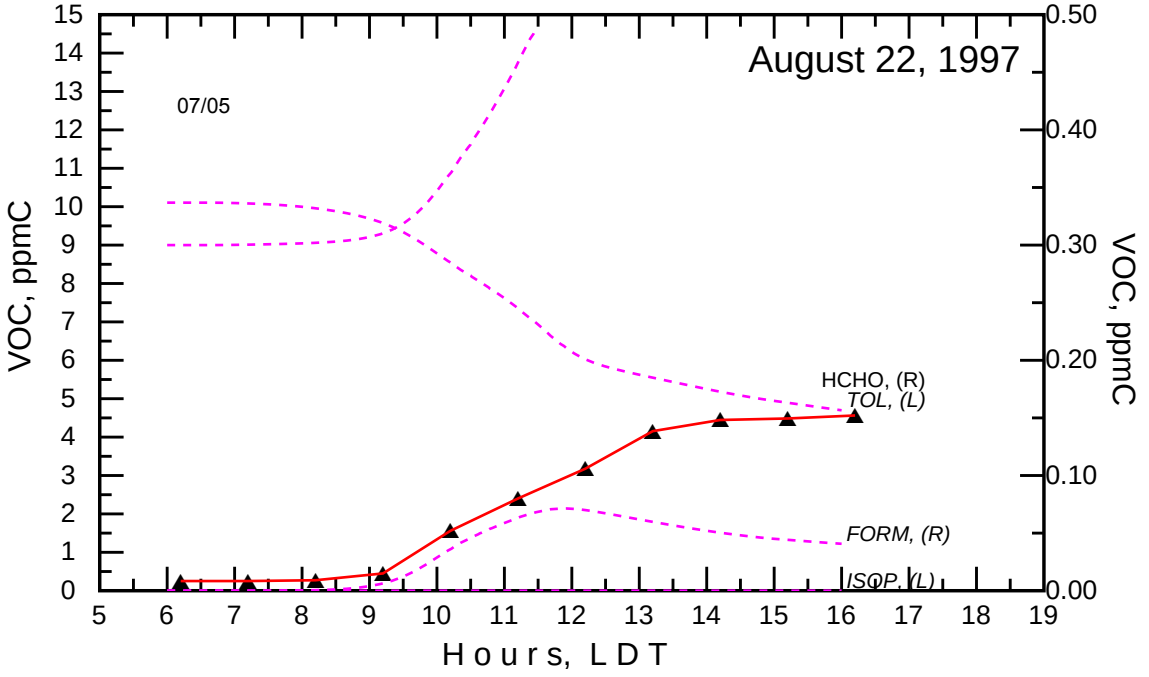


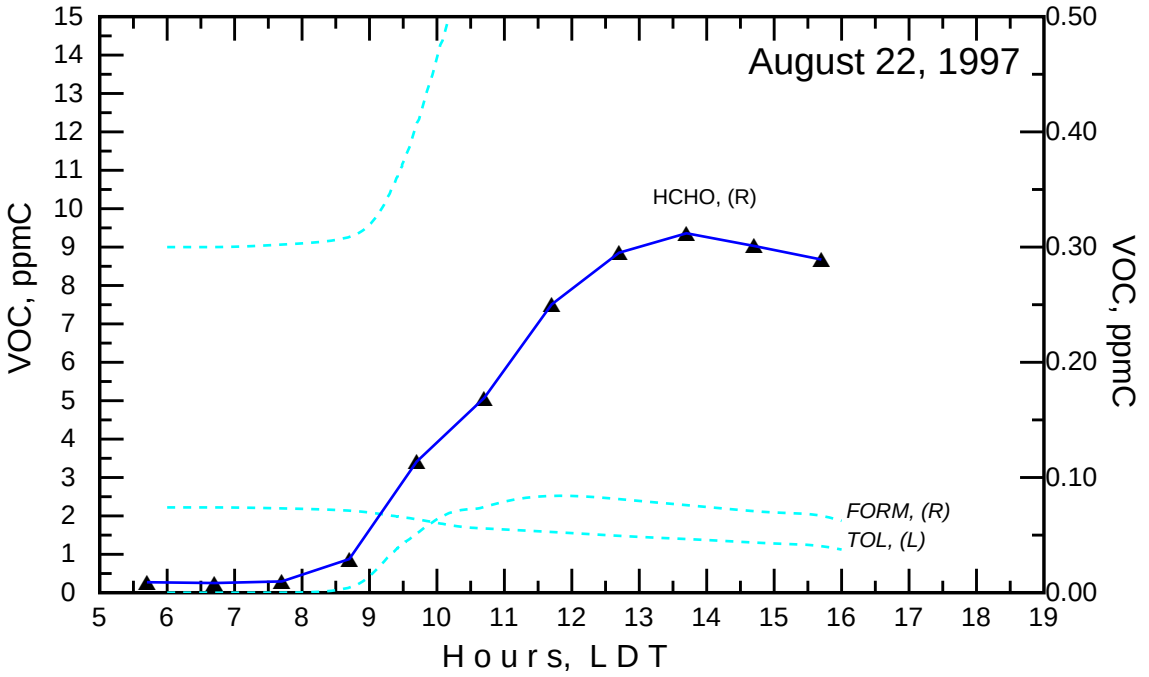


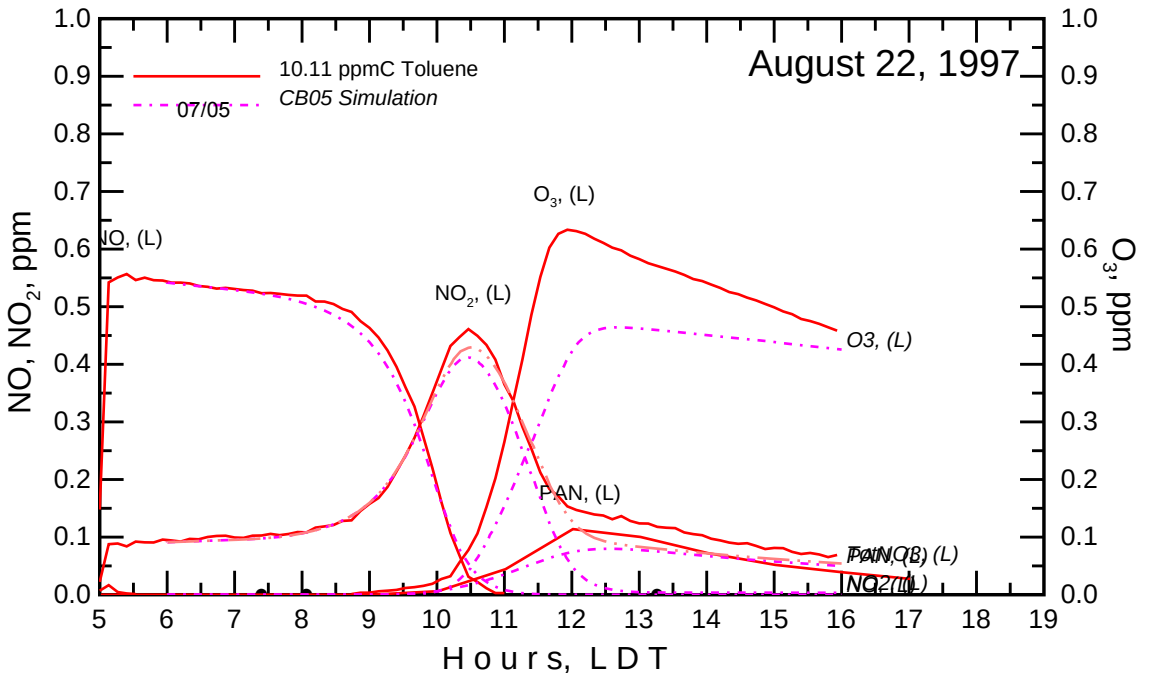
HC Reactivity at 0.36 ppm NO_x

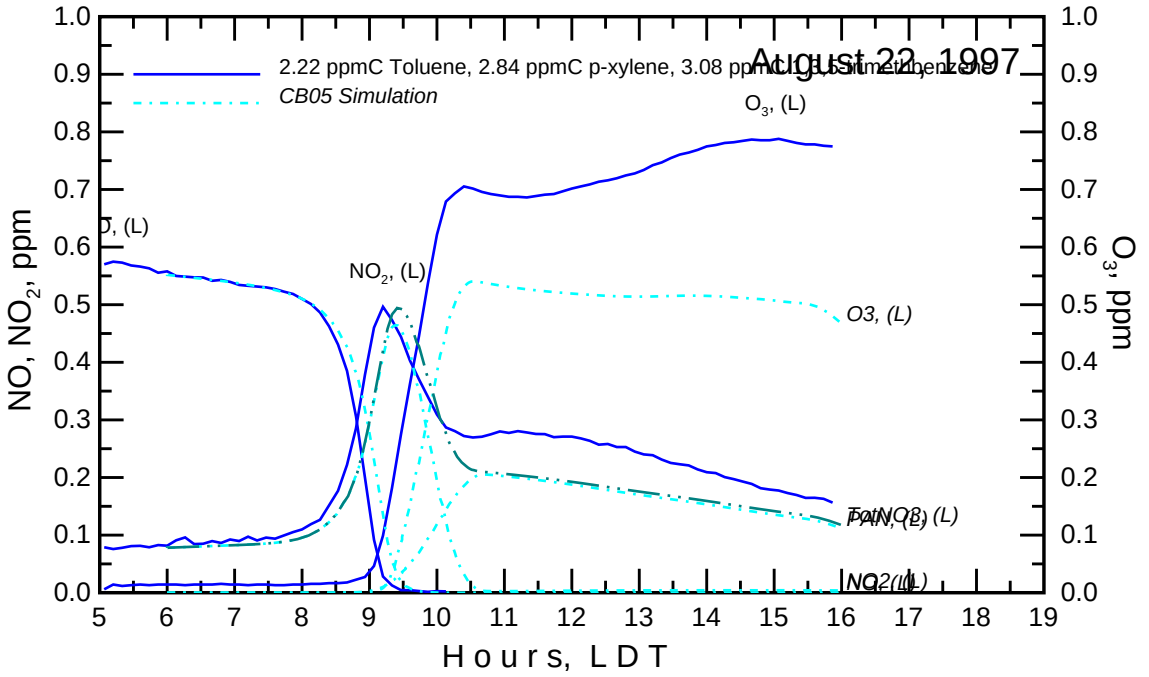

August 17, 1988
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


August 17, 1988
CCl4, (L)
CCl4, (R)
CCl4, relative
CCl4, relative
Hours, LDT

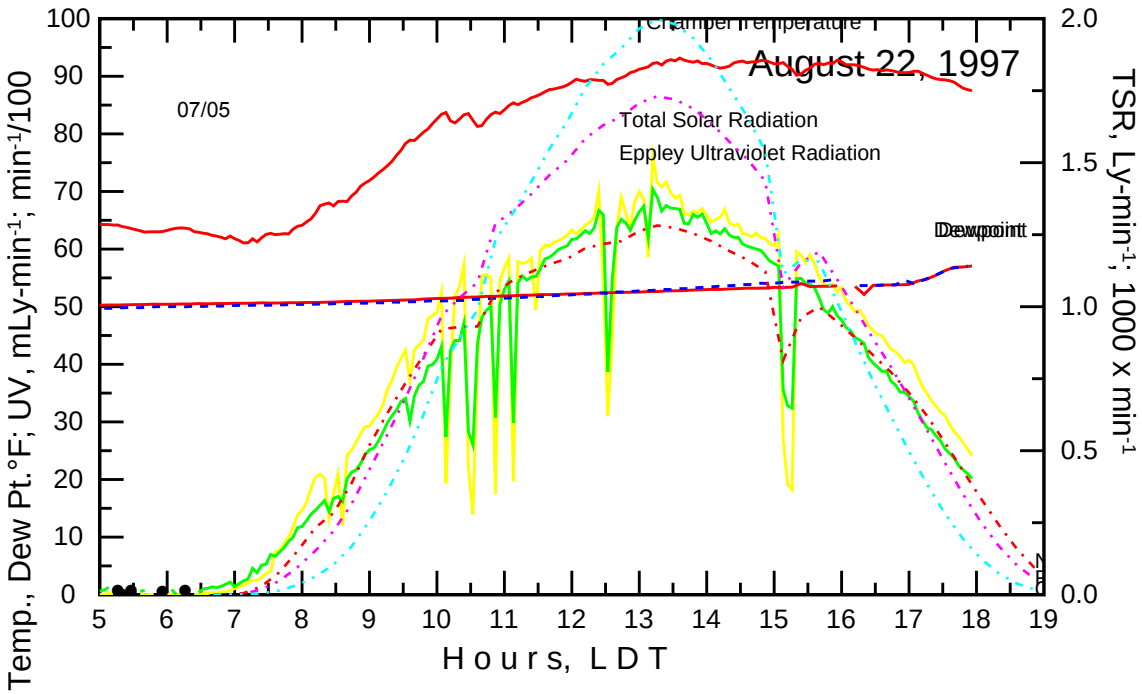

August 22, 1997
07/05
HCHO, (R)
TOL, (L)
FORM, (R)
ISOP, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

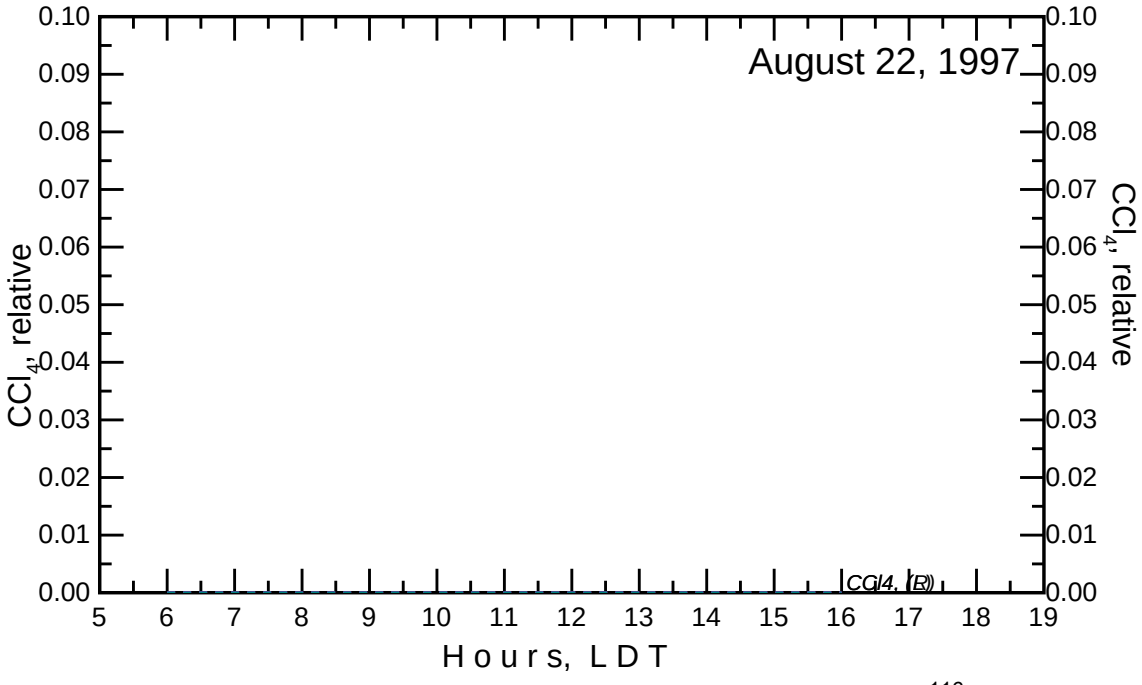

August 22, 1997
HCHO, (R)
FORM, (R)
TOL, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

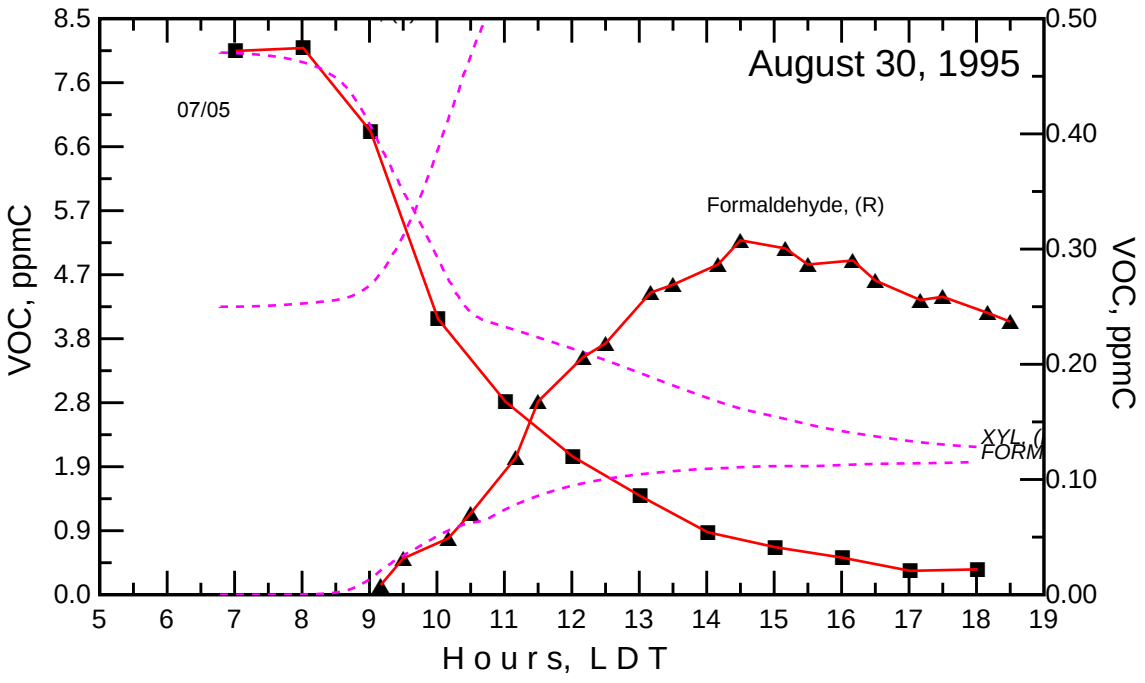


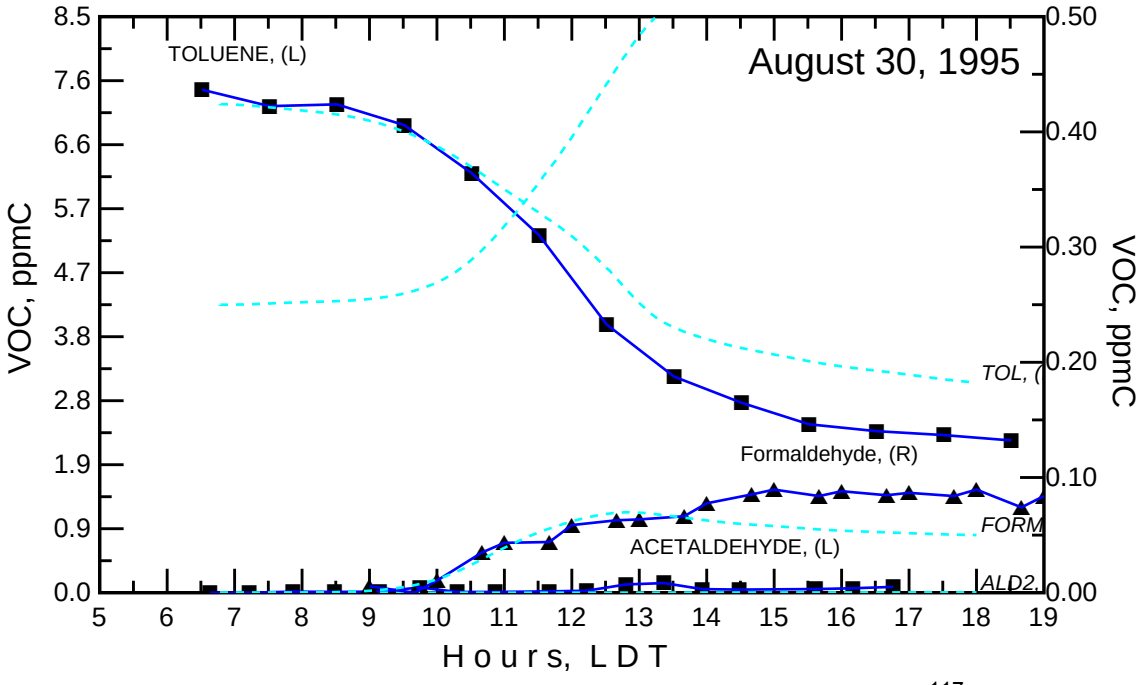


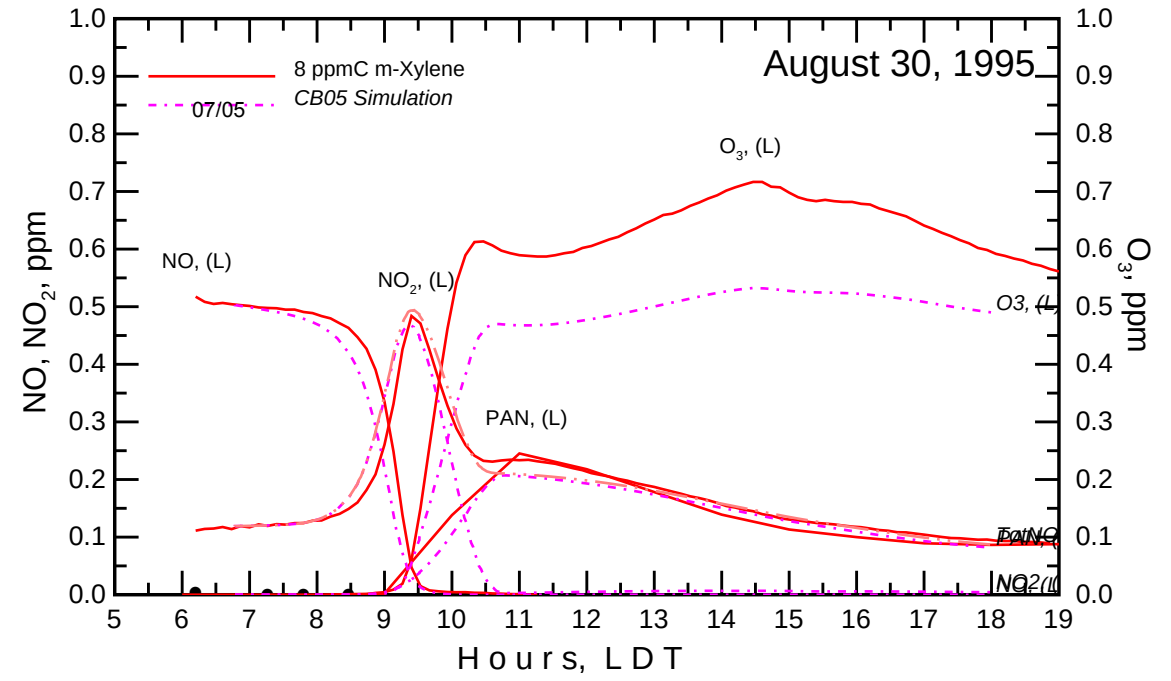
Toluene vs 1,3,5-trimethylbenzene, p-xylene and Toluene

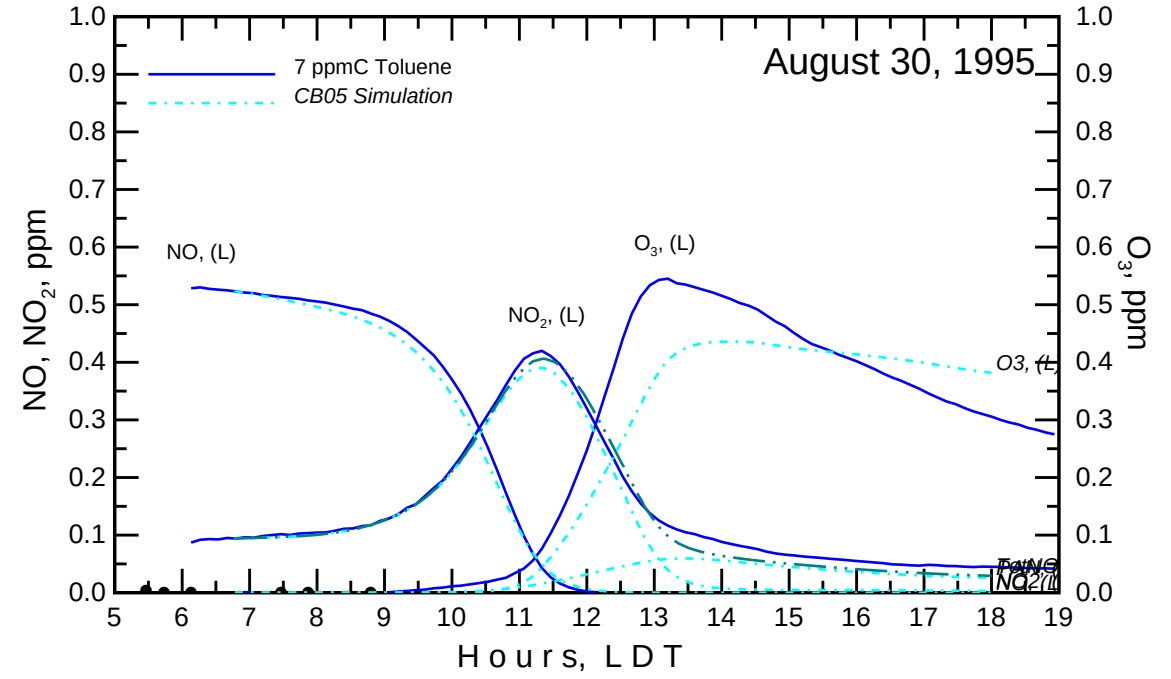

August 22, 1997
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


August 22, 1997
CCl4, relative
CCl4, relative
CCl4, (B)
Hours, LDT

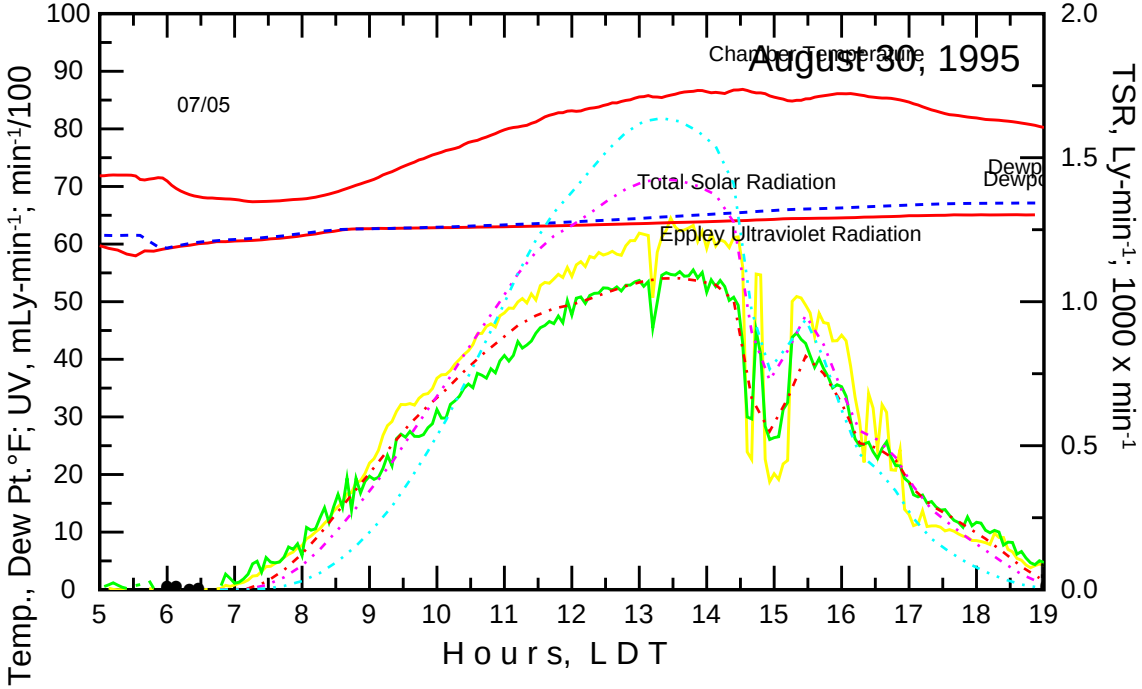

August 30, 1995
07/05
Formaldehyde, (R)
XYL, (
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT

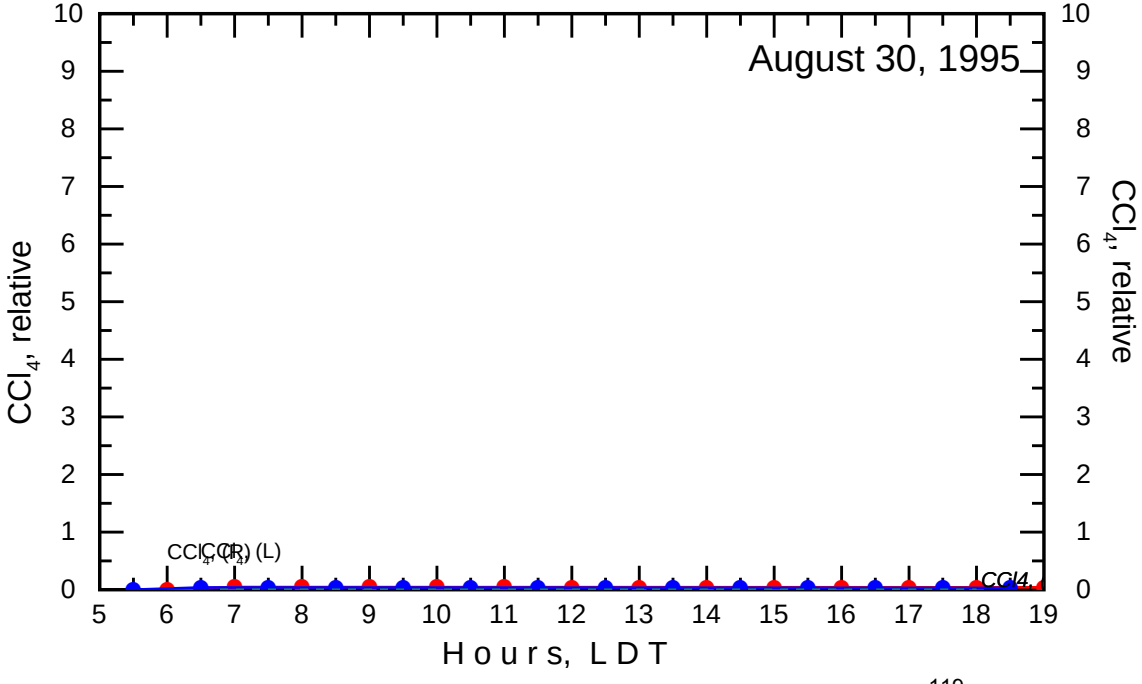

August 30, 1995
TOLUENE, (L)
TOL, (
Formaldehyde, (R)
FORM
ACETALDEHYDE, (L)
ALD2,
VOC, ppmC
VOC, ppmC
Hours, LDT

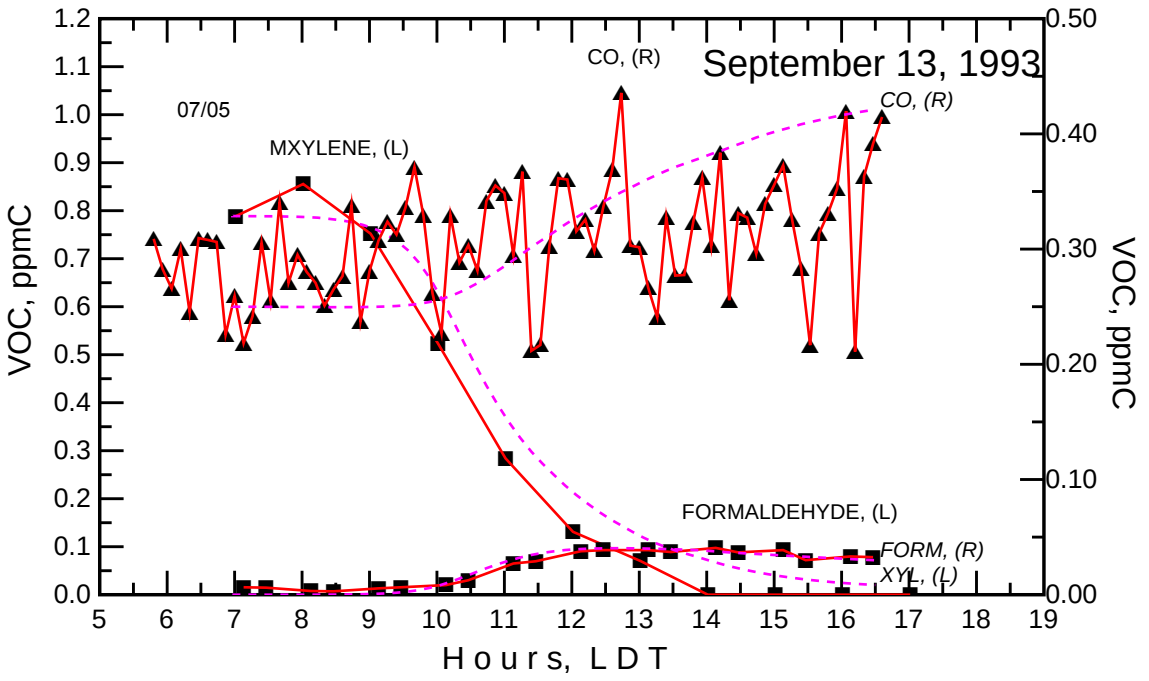


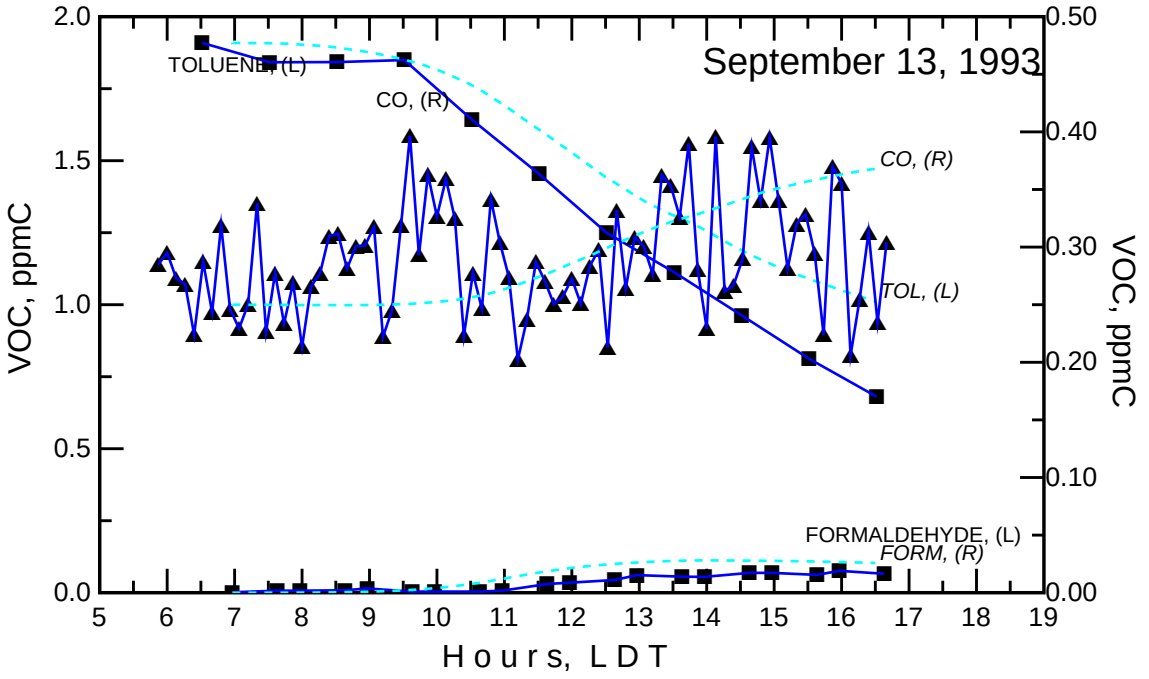


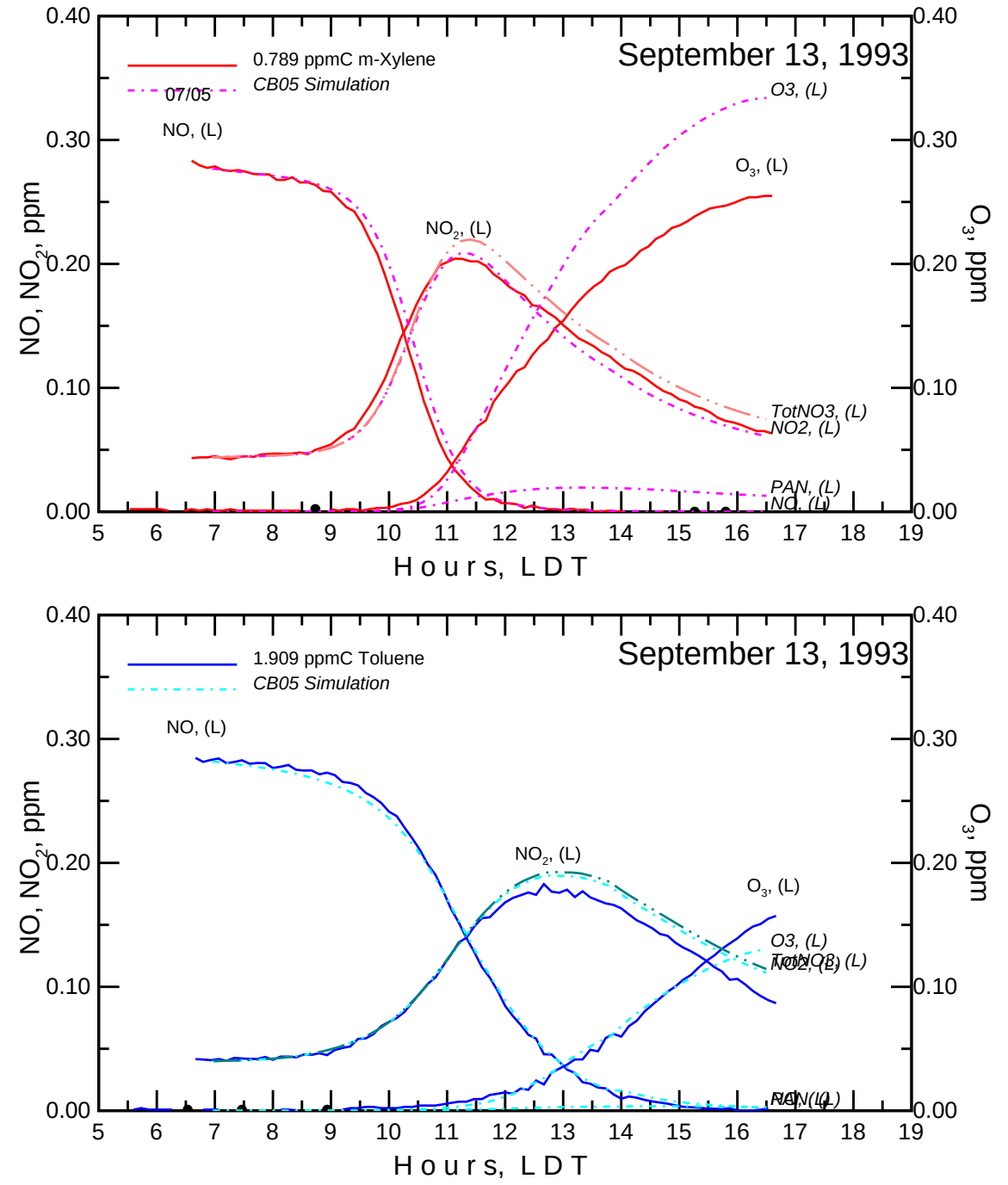
Toluene vs m-Xylene;


August 30, 1995
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

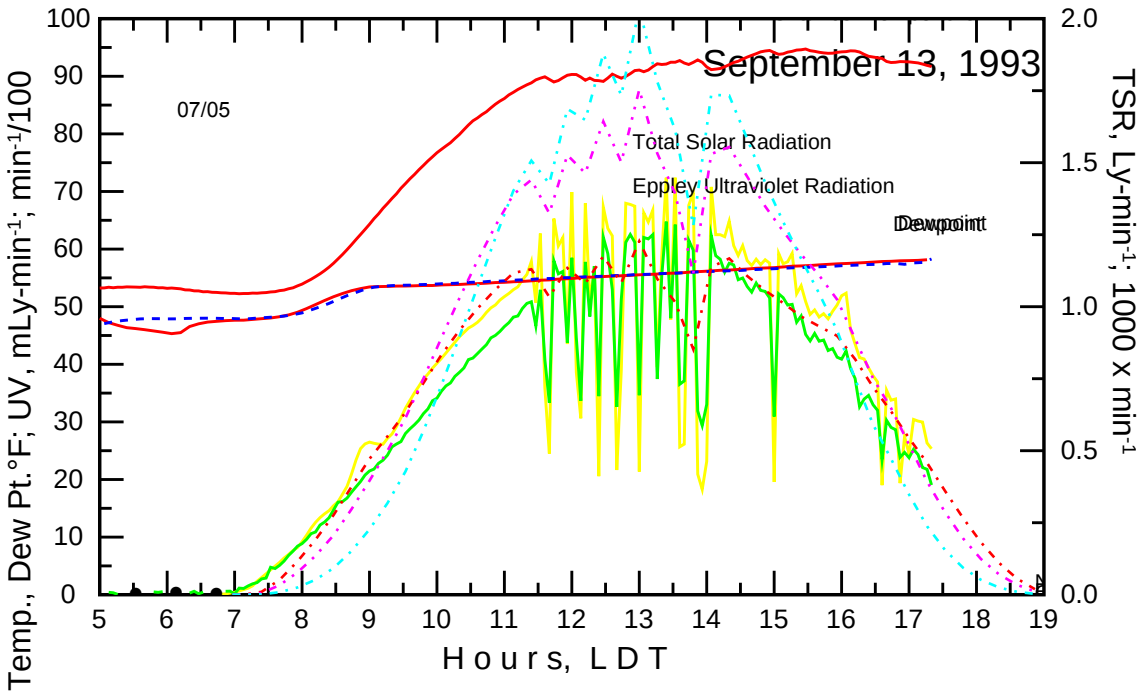

August 30, 1995
CCl4, (R) (L)
CCl4
CCl4, relative
Hours, LDT

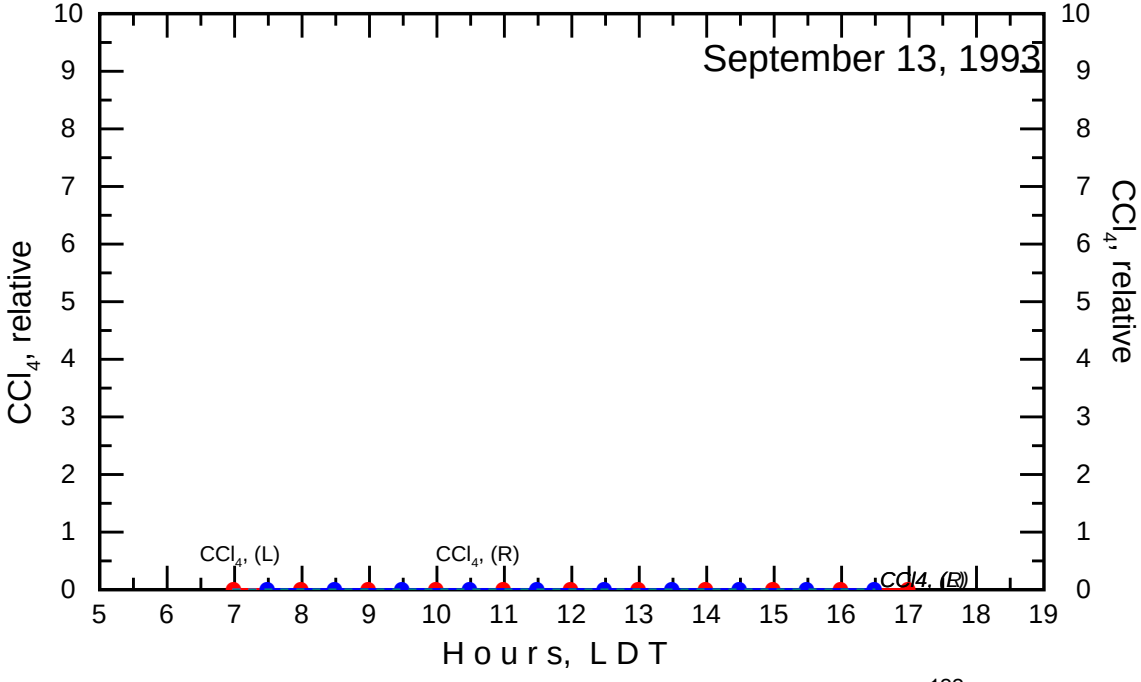

September 13, 1993
07/05
CO, (R)
MXYLENE, (L)
CO, (R)
FORMALDEHYDE, (L)
FORM, (R)
XYL, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

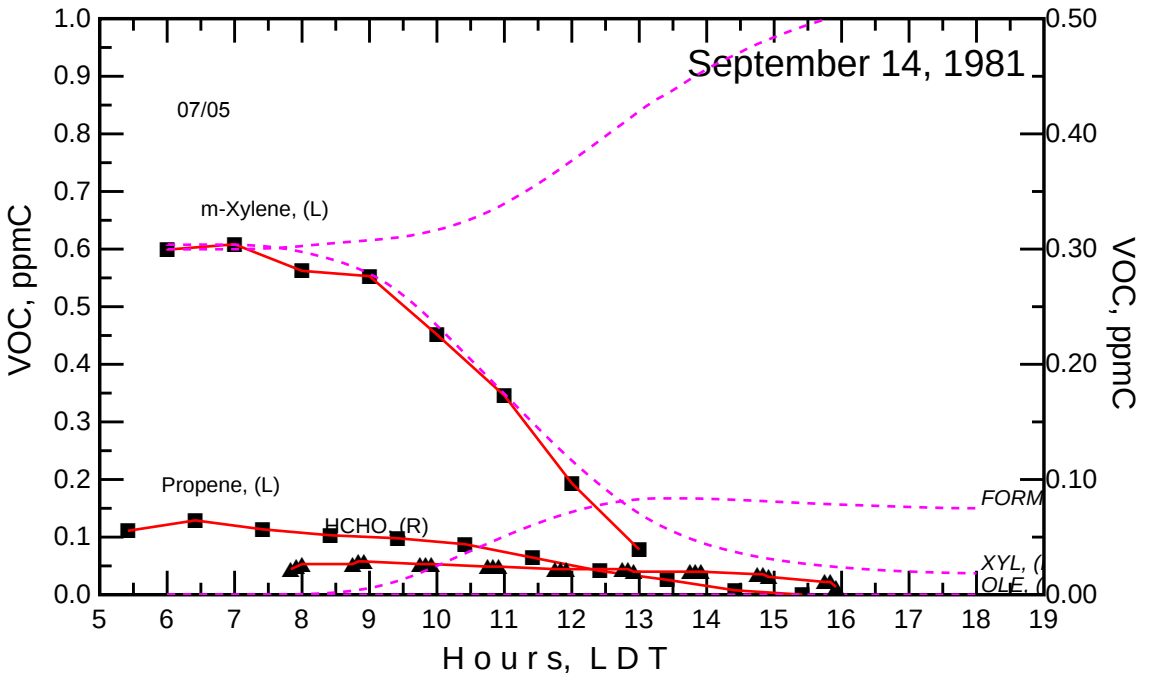

September 13, 1993
TOLUENE, (L)
CO, (R)
CO, (R)
TOL, (L)
FORMALDEHYDE, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT

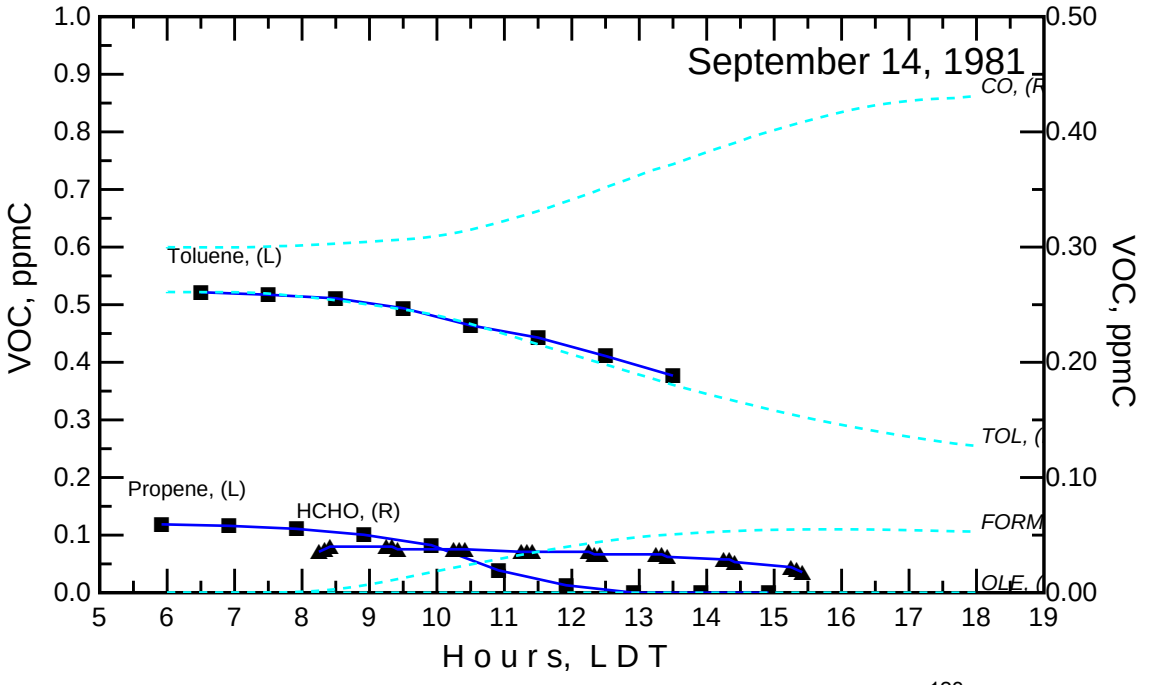


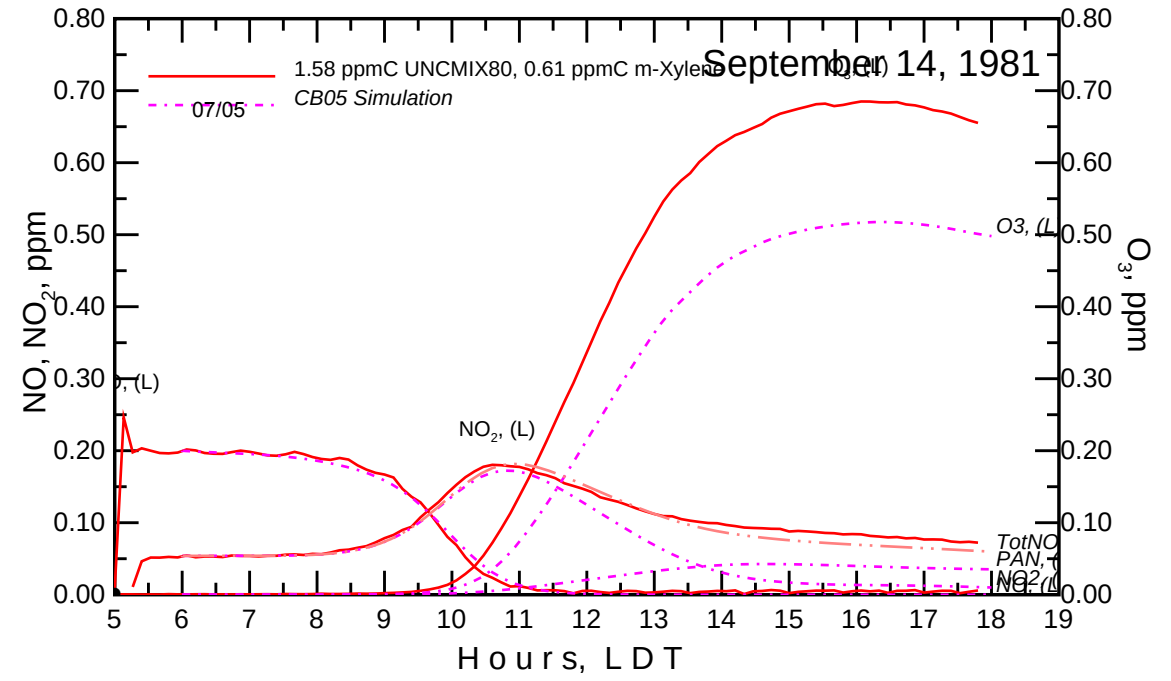
Toluene vs m-Xylene

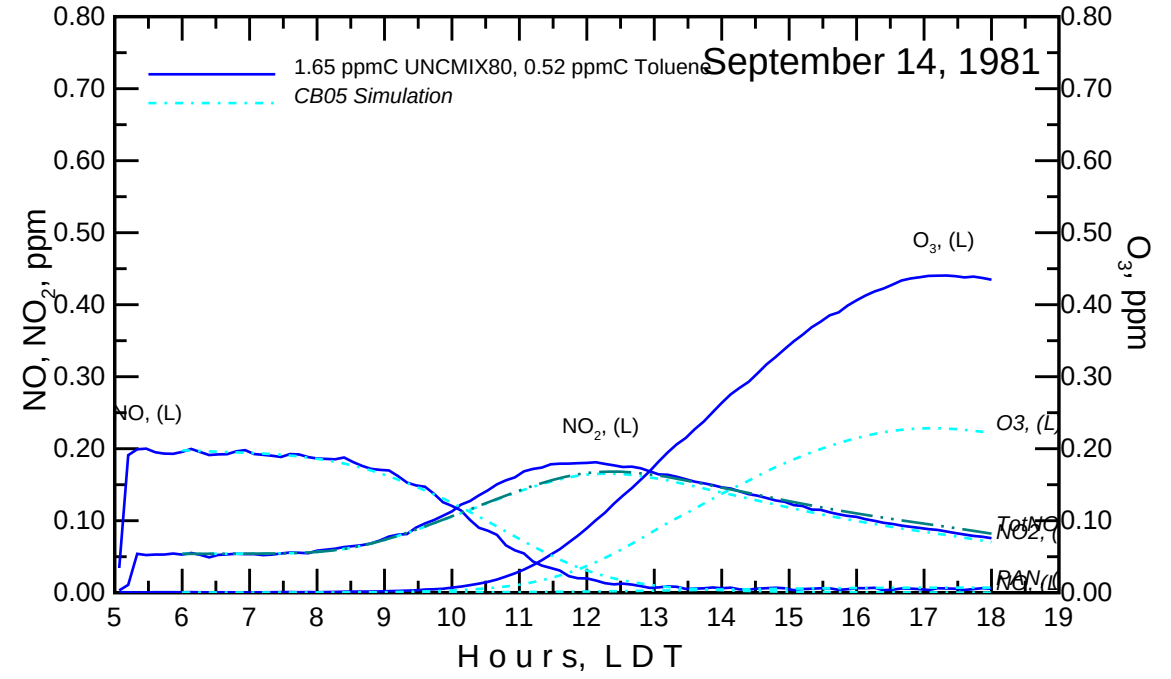

September 13, 1993
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

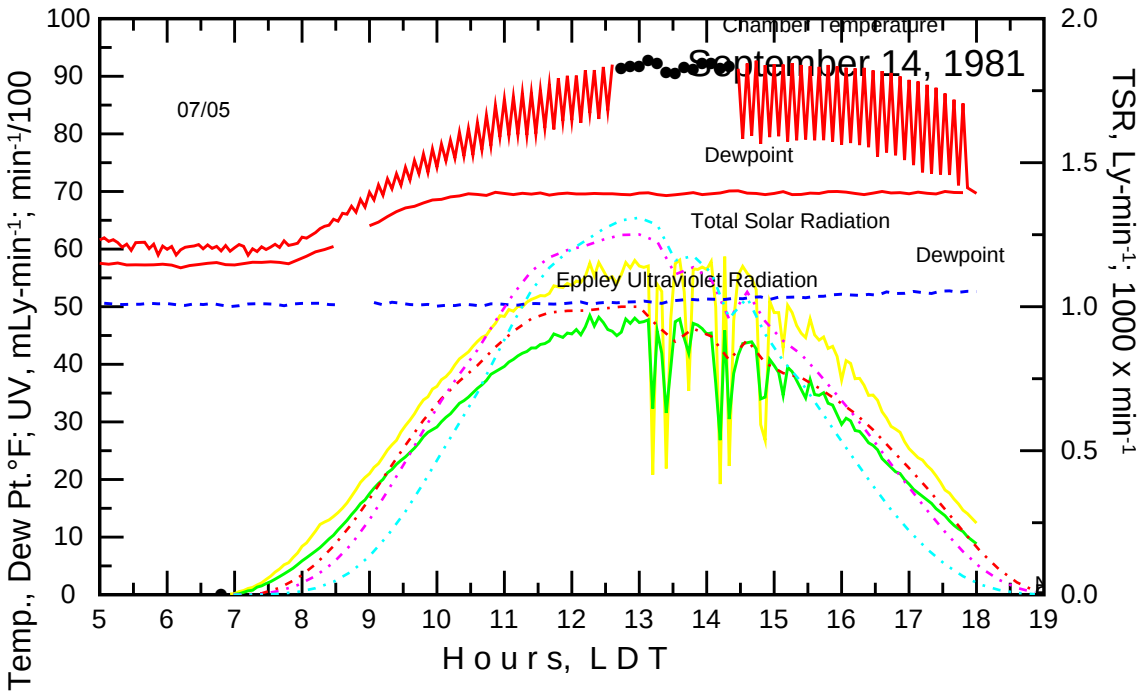

September 13, 1993
CCl4, relative
CCl4, (L)
CCl4, (R)
Hours, LDT

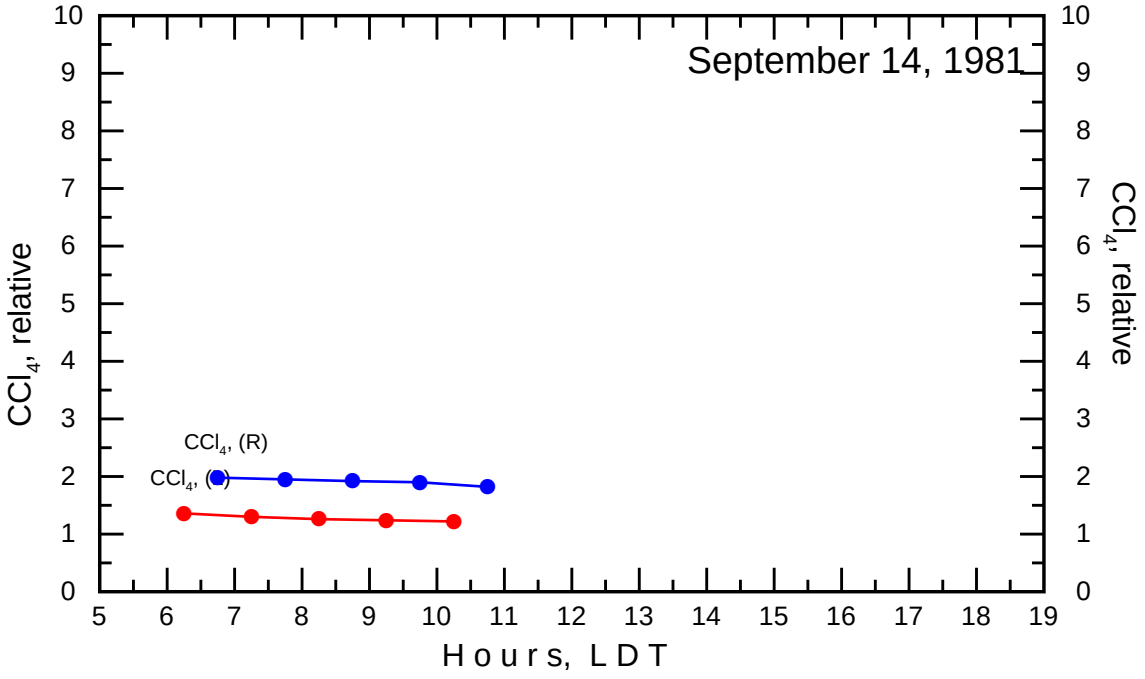

September 14, 1981
07/05
m-Xylene, (L)
Propene, (L)
HCHO, (R)
FORM
XYL, (
OLE, (
VOC, ppmC
VOC, ppmC
Hours, LDT

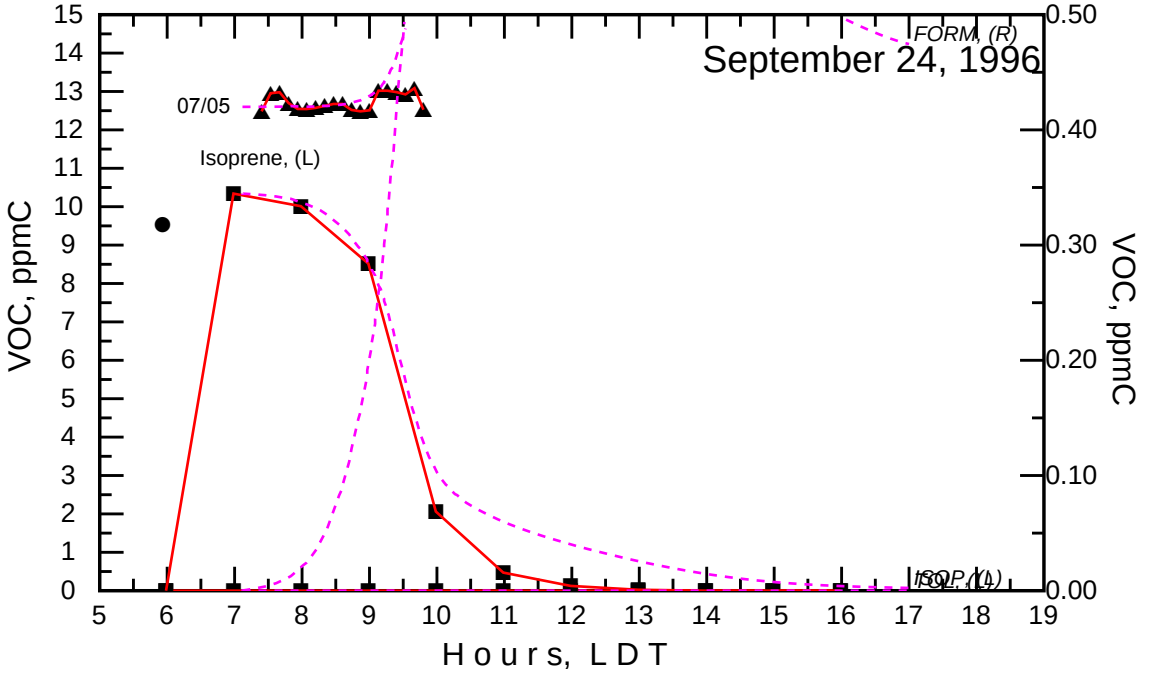

September 14, 1981
CO, (R
Toluene, (L)
Propene, (L)
HCHO, (R)
TOL, (
FORM
OLE, (
VOC, ppmC
VOC, ppmC
Hours, LDT

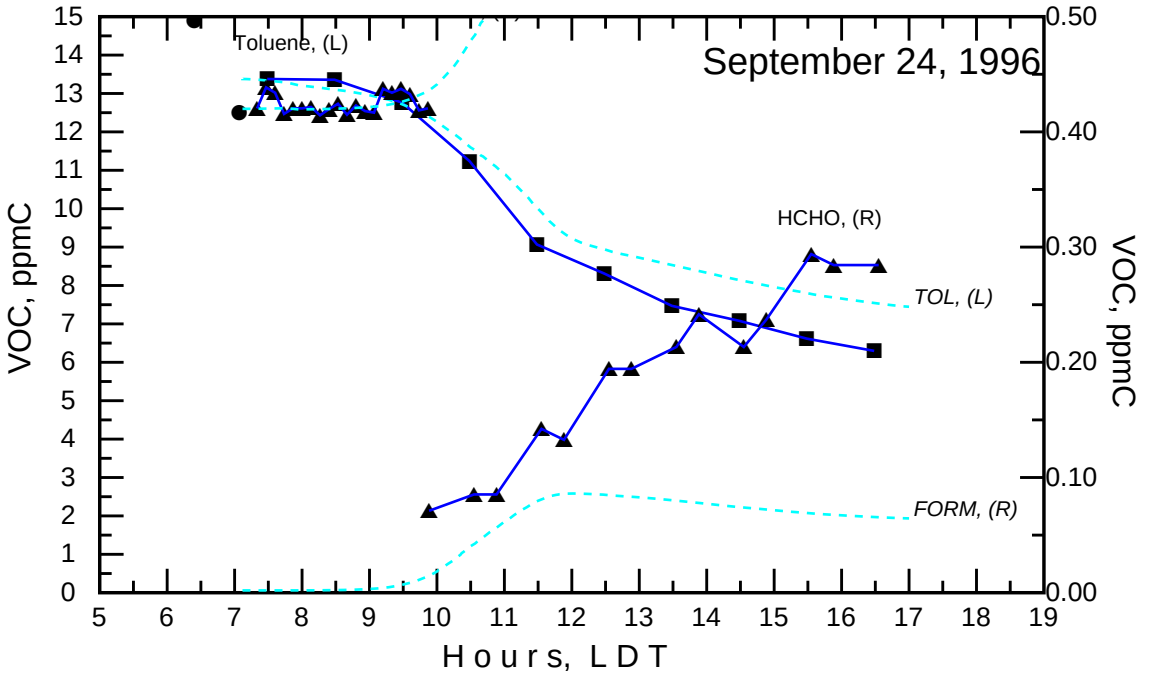

September 14, 1981
1.58 ppmC UNCMIX80, 0.61 ppmC m-Xylene
CB05 Simulation
07/05
NO, NO2, ppm
O3, ppm
NO2, (L)
O3, (L)
TotNO
PAN, (
Hours, LDT

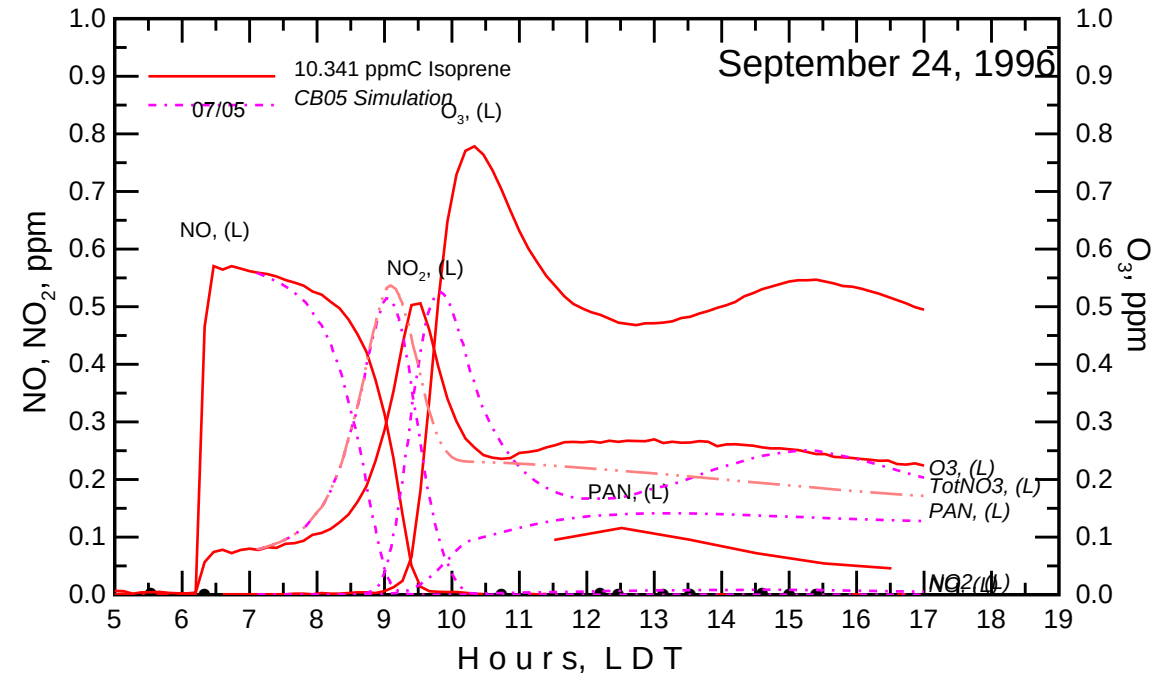

September 14, 1981
1.65 ppmC UNCMIX80, 0.52 ppmC Toluene
CB05 Simulation
NO, NO2, ppm
O3, ppm
O3, (L)
NO, (L)
NO2, (L)
O3, (L)
TotNO
PAN, (
Hours, LDT

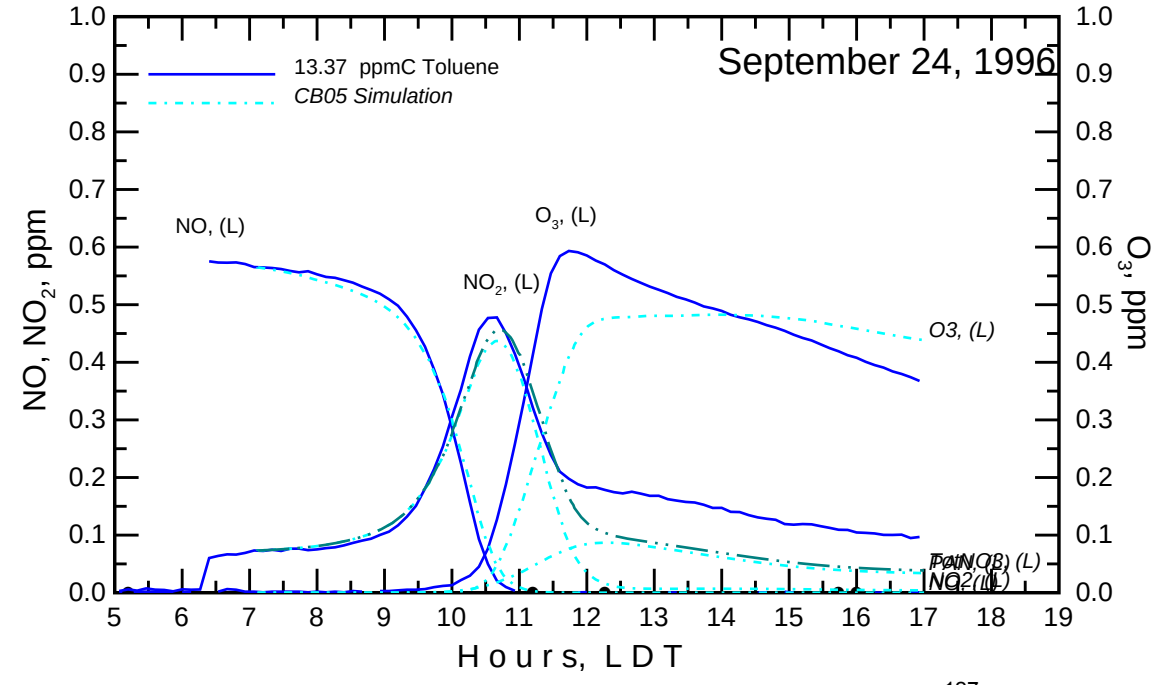

September 14, 1981
07/05
Chamber Temperature
Dewpoint
Total Solar Radiation
Dewpoint
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


September 14, 1981
CCl4, (R)
CCl4, (E)
CCl4, relative
CCl4, relative
Hours, LDT

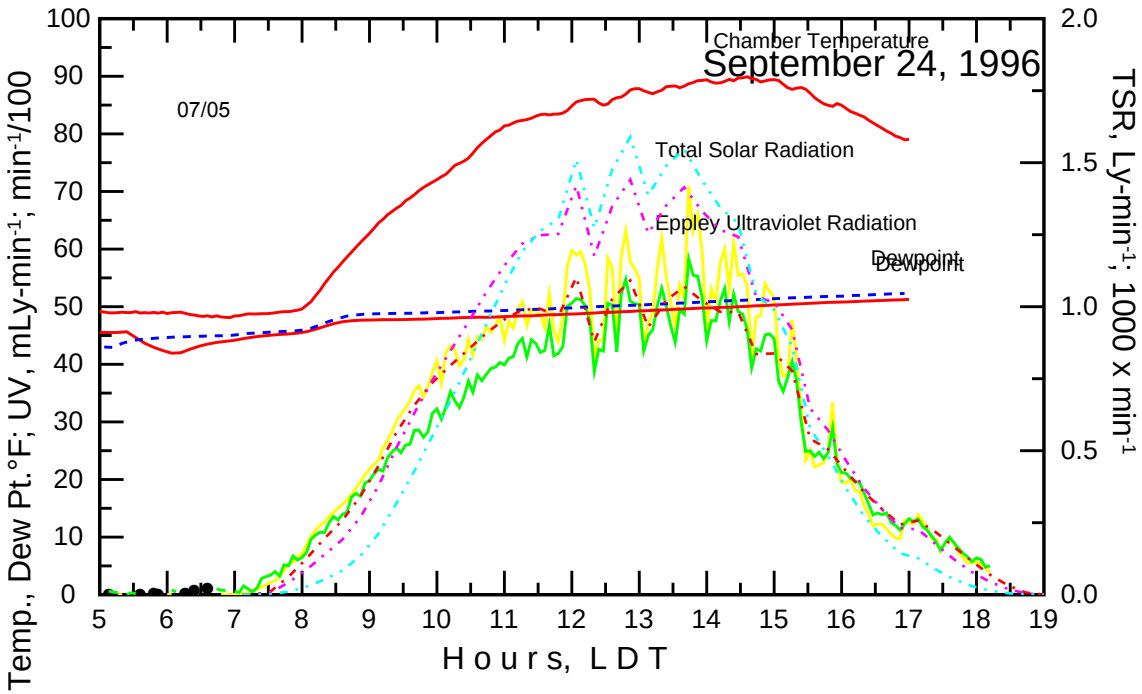

September 24, 1996
07/05
Isoprene, (L)
FORM, (R)
ISOP, (L)
TOL, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

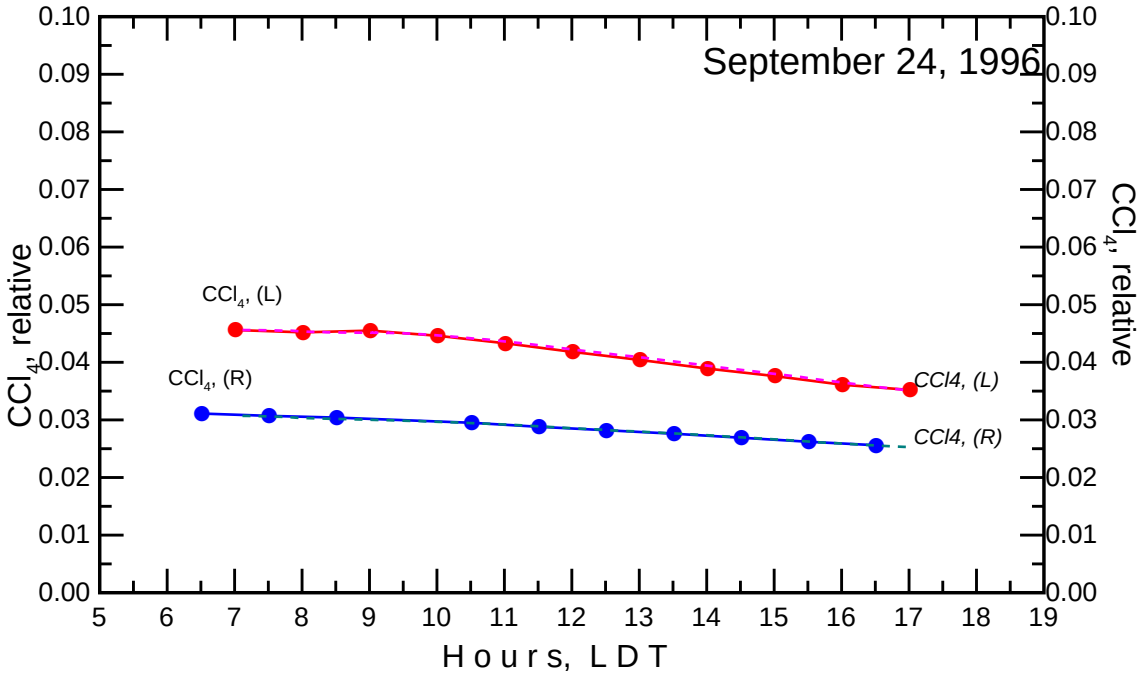

September 24, 1996
Toluene, (L)
HCHO, (R)
TOL, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT





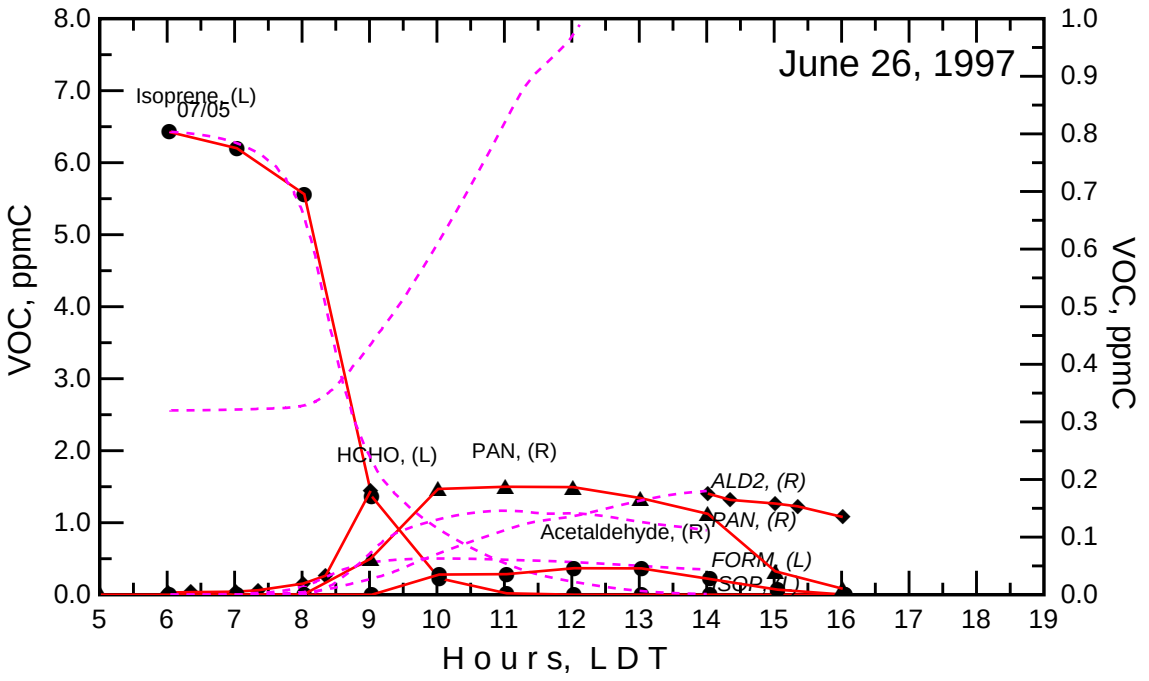
Toluene vs Isoprene

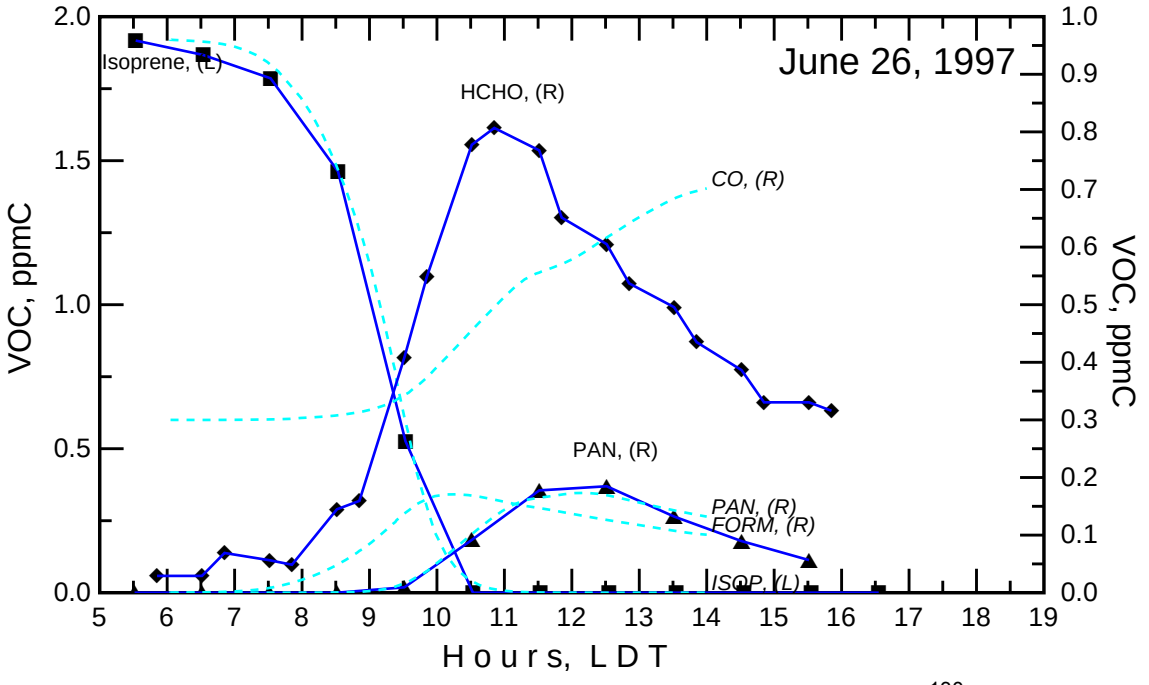

Chamber Temperature
September 24, 1996
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

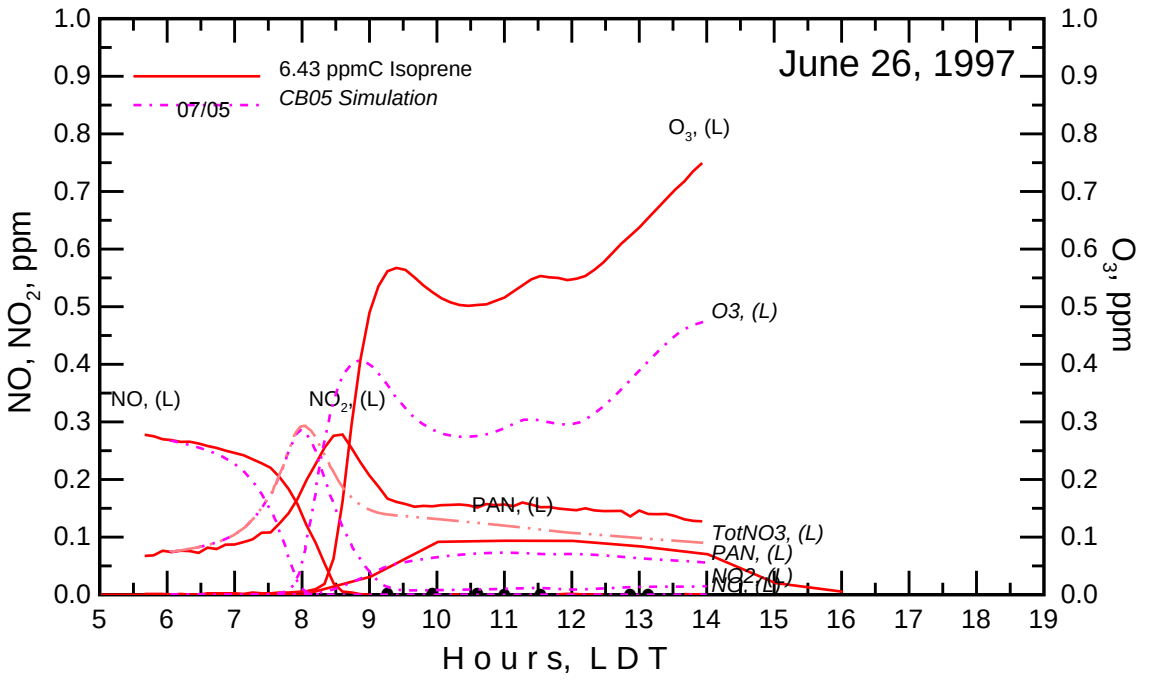

September 24, 1996
CCl4, (L)
CCl4, (R)
CCl4, (L)
CCl4, (R)
CCl4, relative
CCl4, relative
Hours, LDT

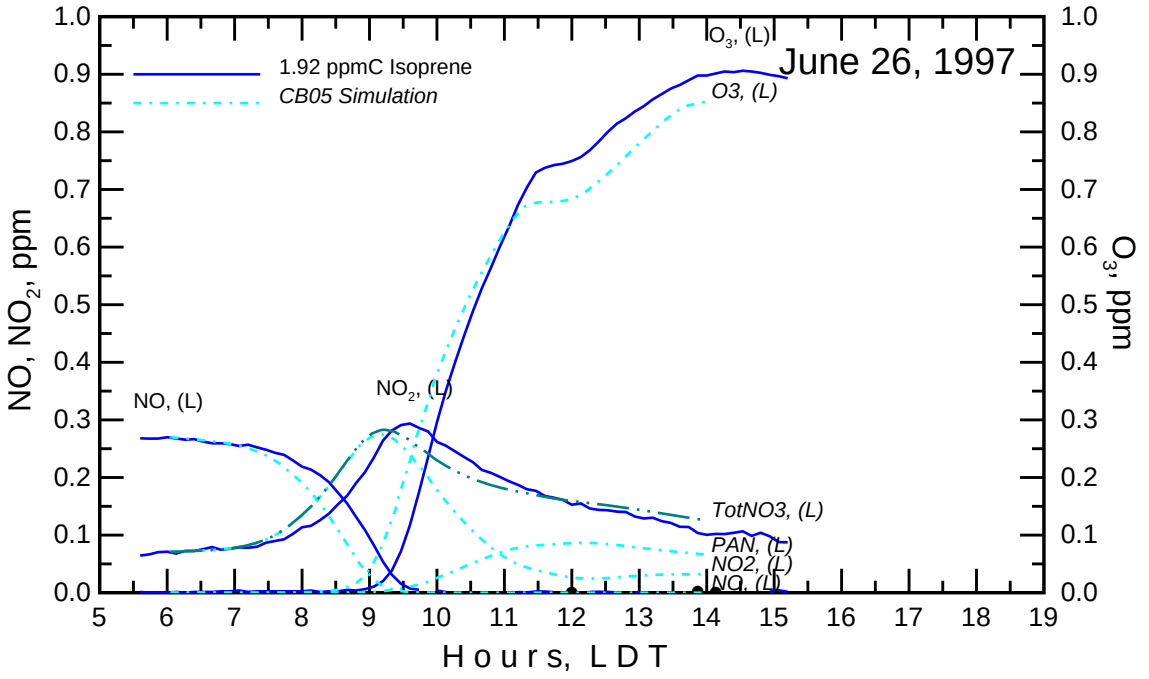
Isoprene (ISOP)

JN 26 97
AU 06 96
ST 11 99
ST 24 96

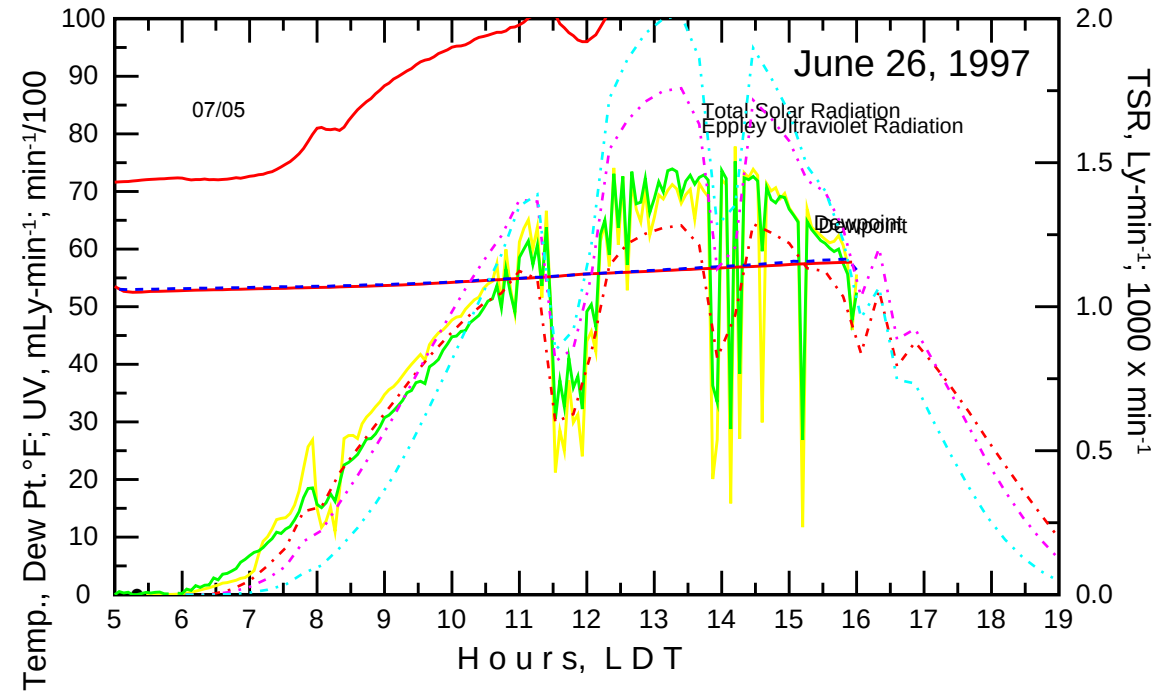

June 26, 1997
Isoprene, (L)
07/05
HCHO, (L)
PAN, (R)
ALD2, (R)
PAN, (R)
Acetaldehyde, (R)
FORM, (L)
ISOP, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT


June 26, 1997
Isoprene, (L)
HCHO, (R)
CO, (R)
PAN, (R)
PAN, (R)
FORM, (R)
ISOP, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT





Delta Isoprene


June 26, 1997
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
7
8
9
10
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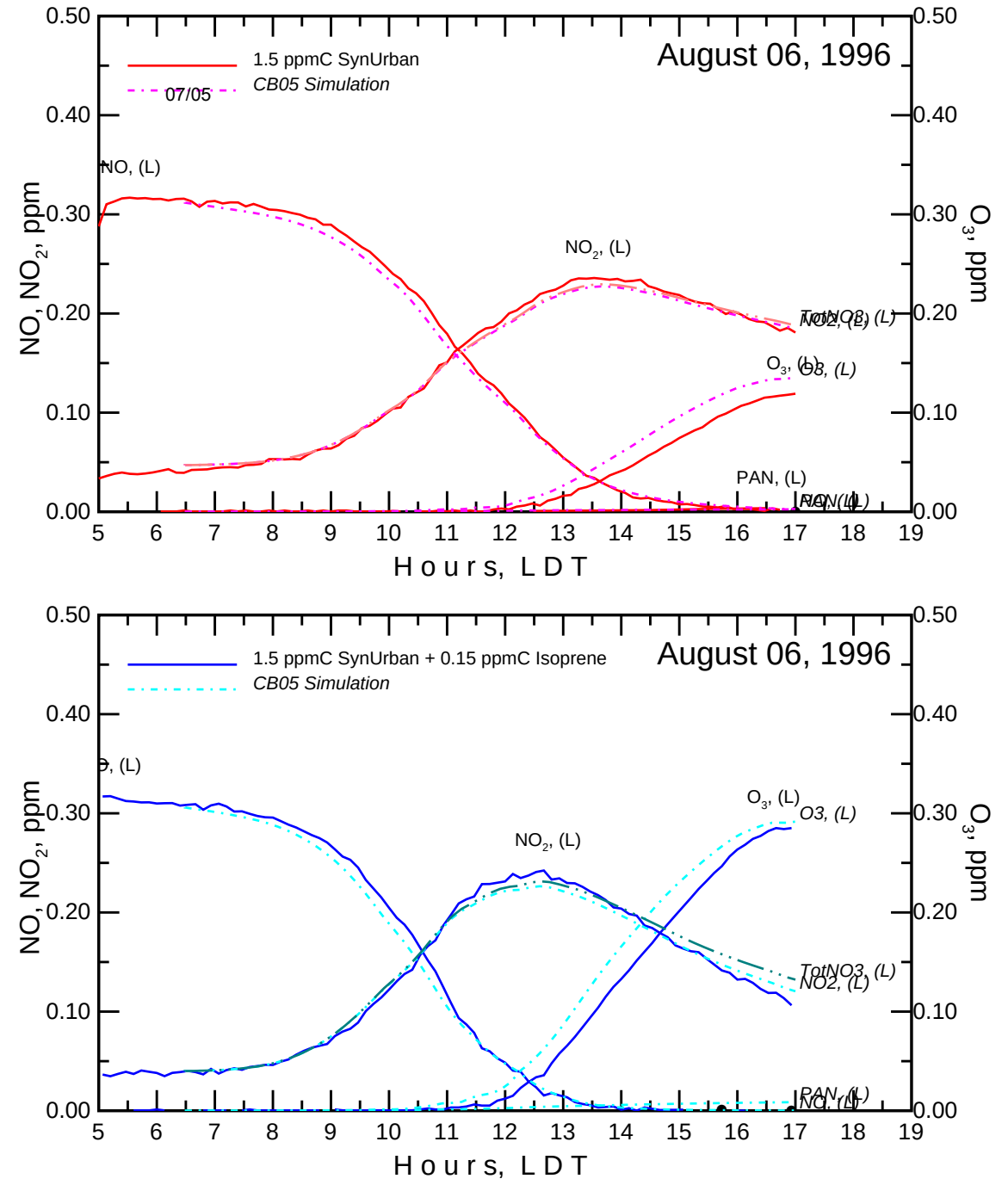
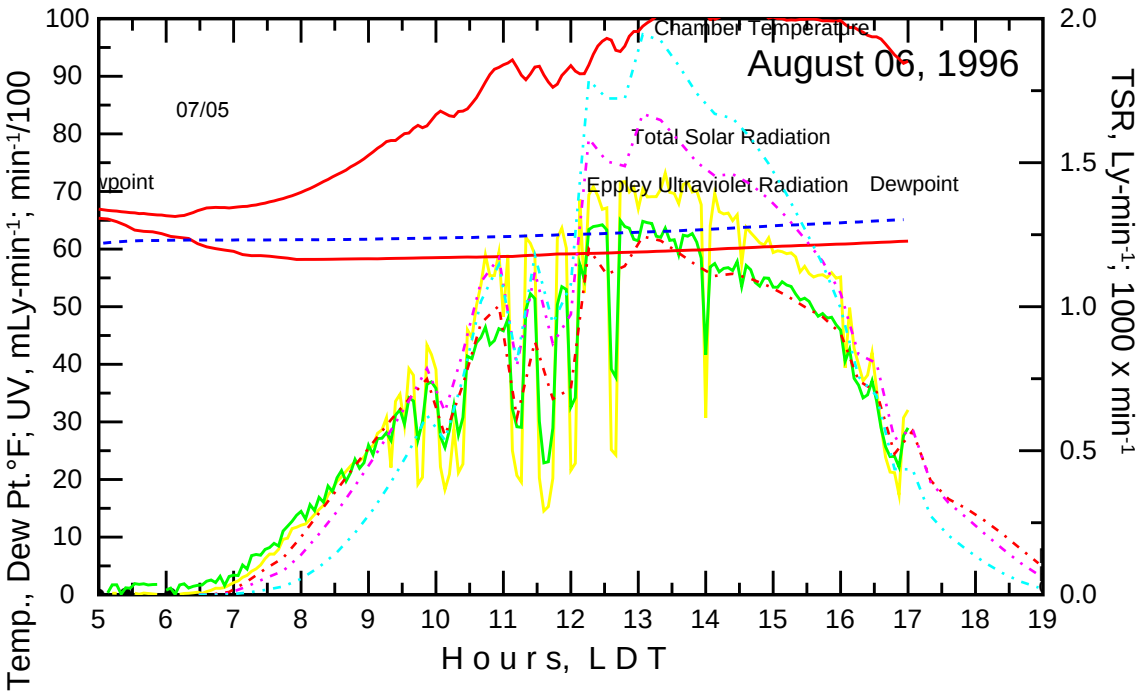
19



Matched SynUrban and NOx with Isoprene added BLUE


August 06, 1996
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
vpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
7
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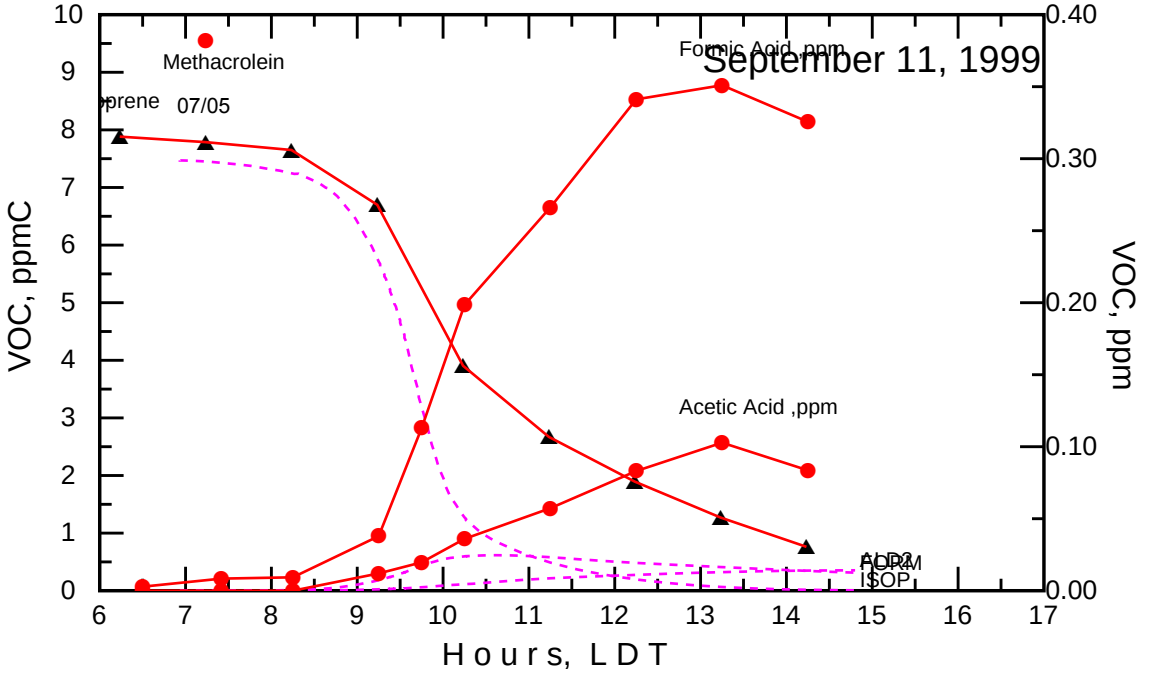
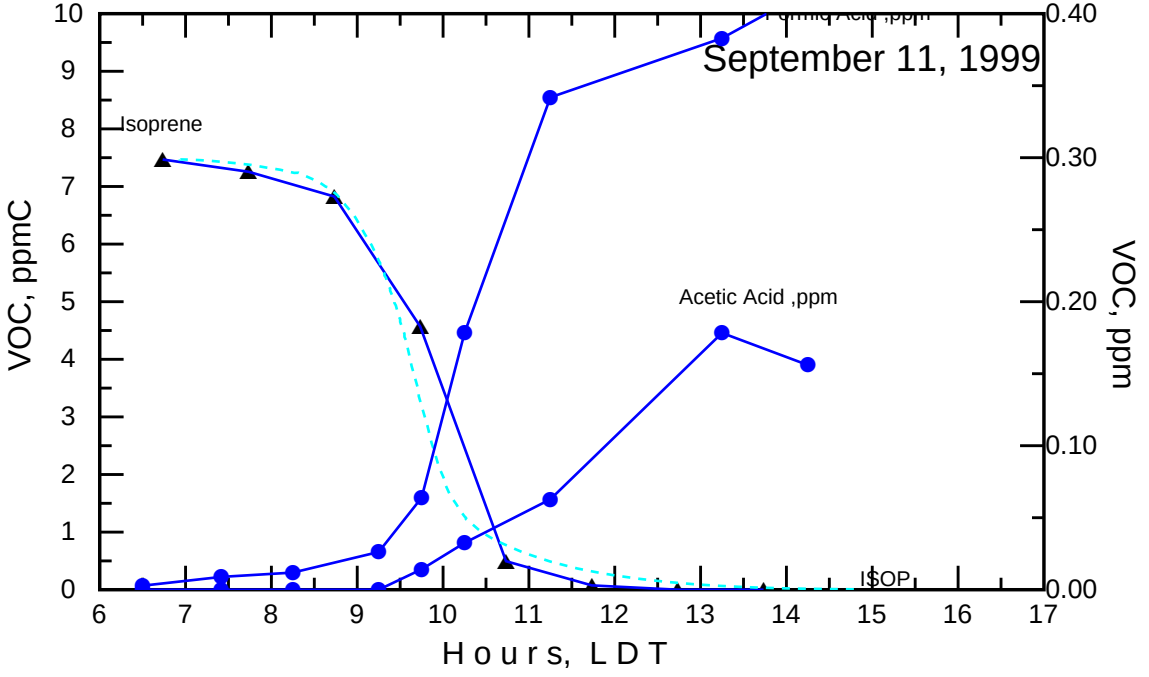
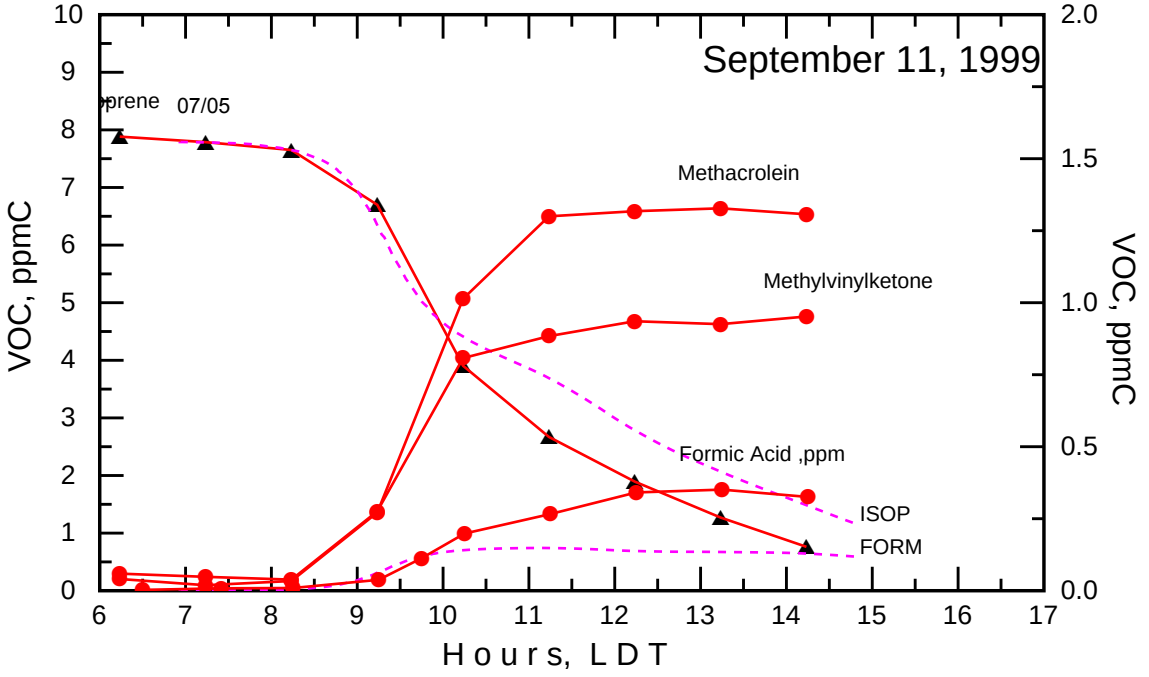
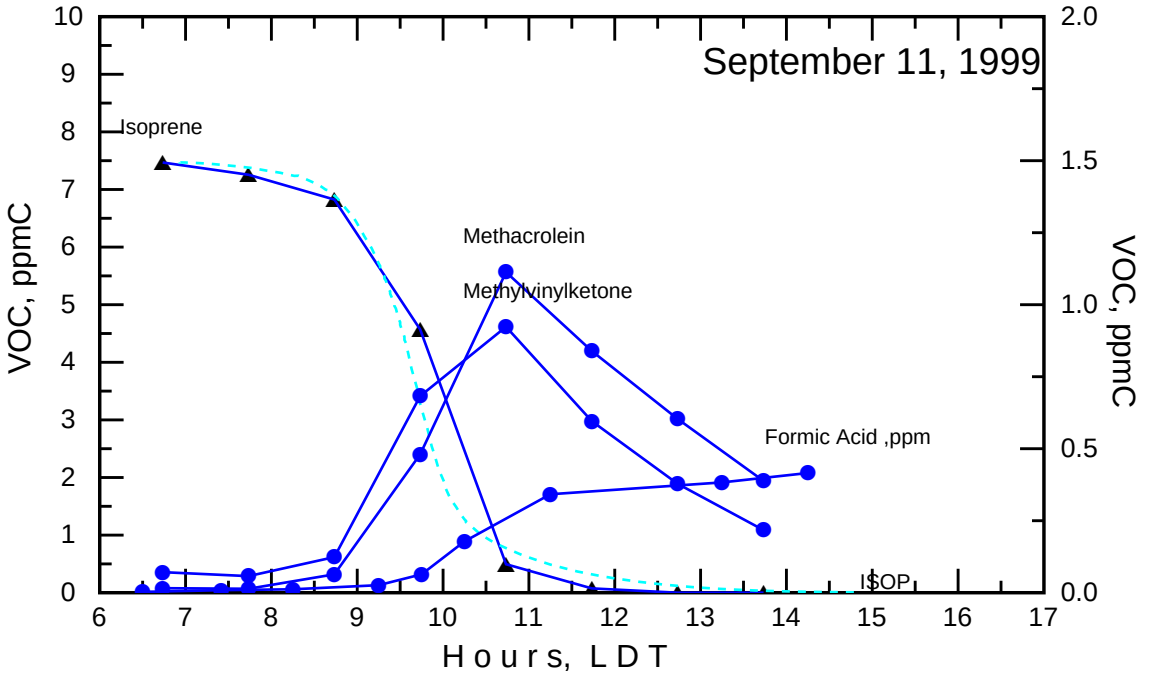
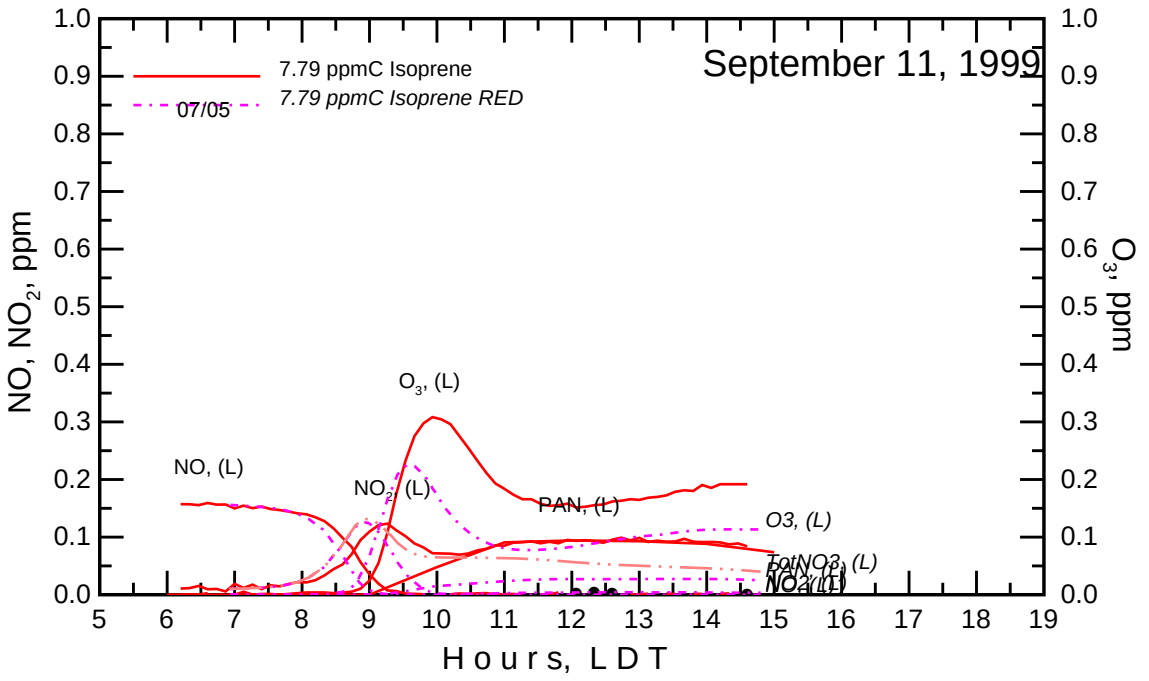
19

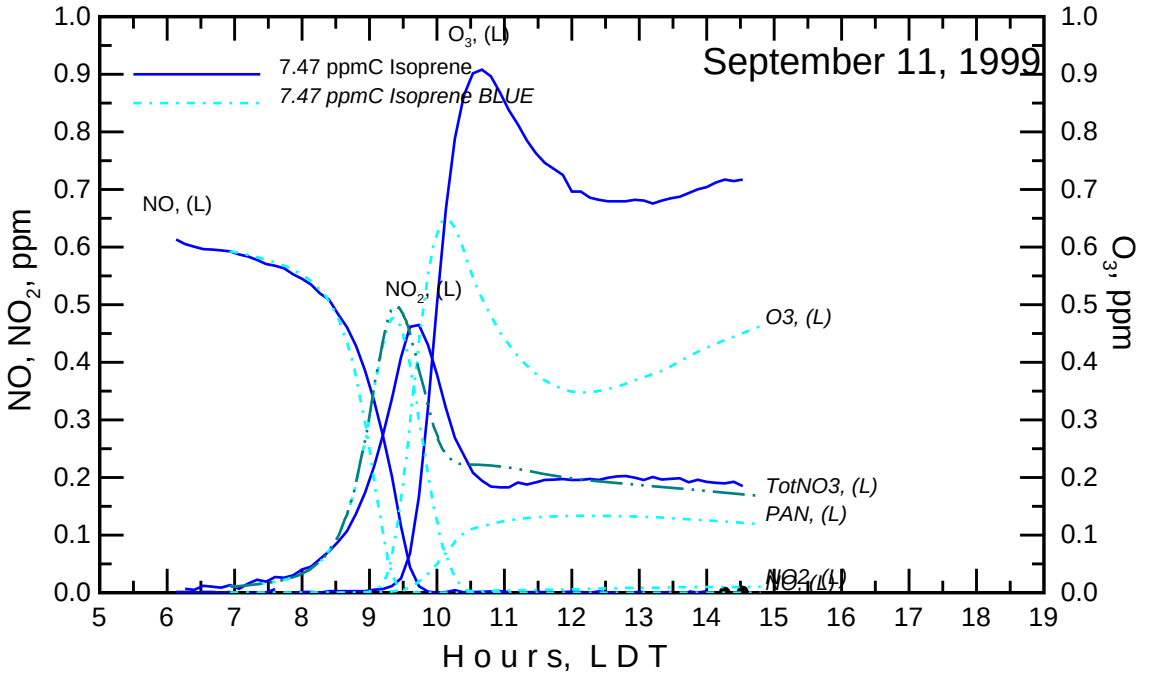

September 11, 1999
Methacrolein
Isoprene 07/05
Formic Acid ,ppm
Acetic Acid ,ppm
ALD2
ISOP
VOC, ppmC
VOC, ppm
Hours, LDT


September 11, 1999
Isoprene
Acetic Acid ,ppm
ISOP
VOC, ppmC
VOC, ppm
Hours, LDT

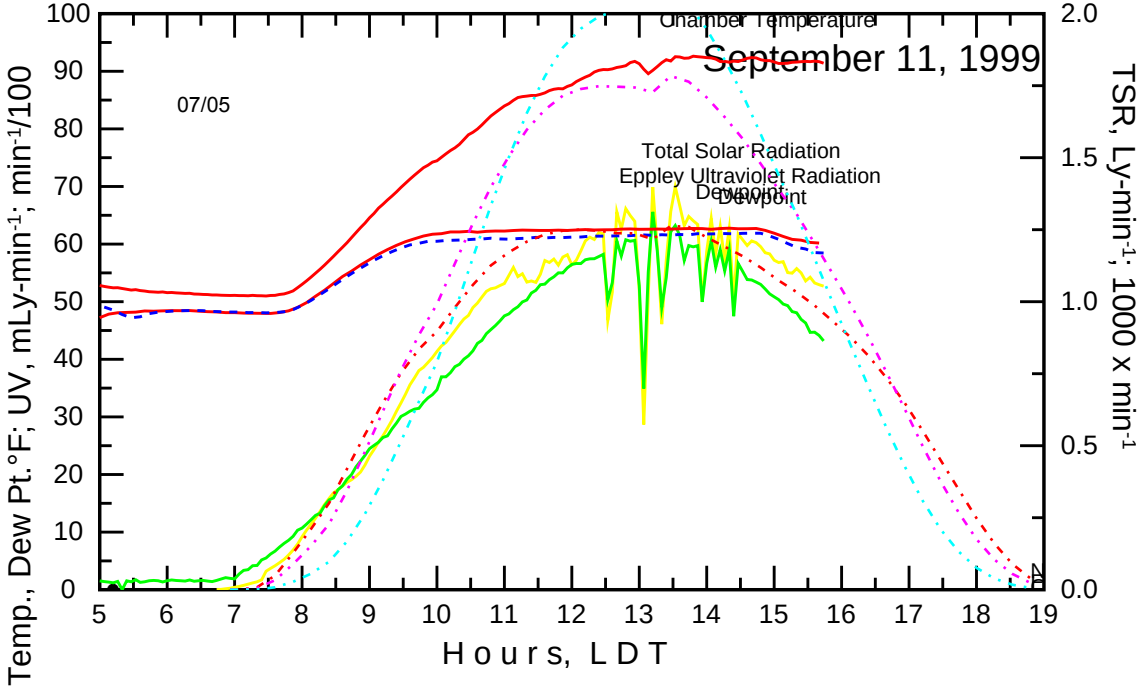

September 11, 1999
prene 07/05
Methacrolein
Methylvinylketone
Formic Acid ,ppm
ISOP
FORM
VOC, ppmC
VOC, ppmC
Hours, LDT

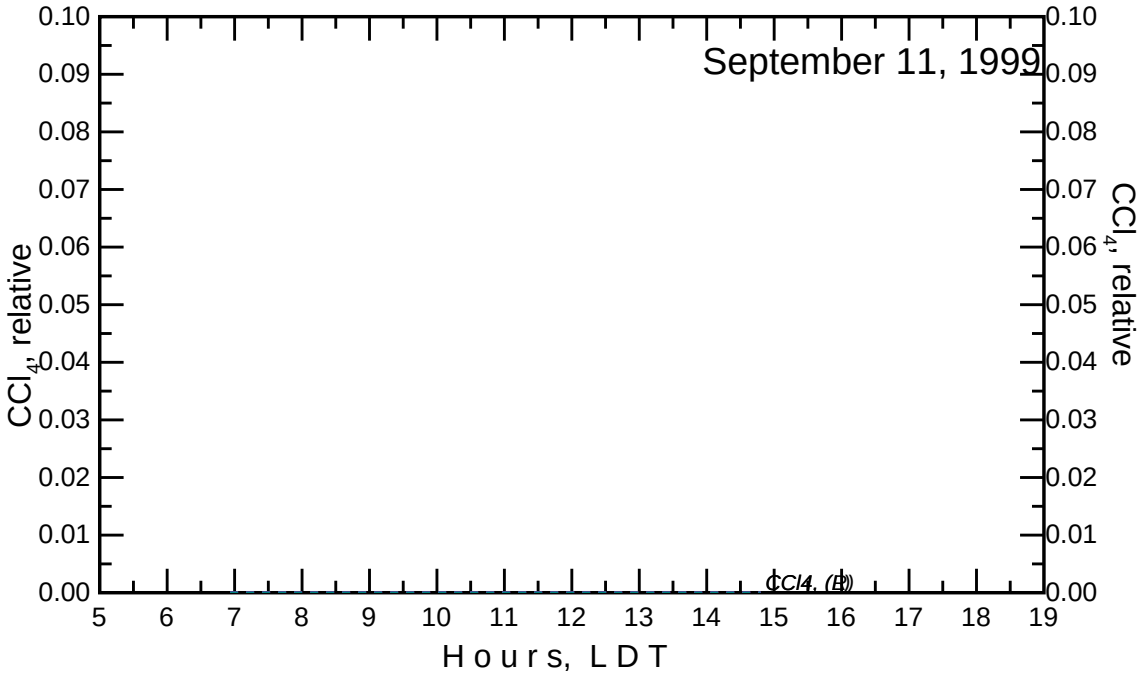

September 11, 1999
Isoprene
Methacrolein
Methylvinylketone
Formic Acid ,ppm
ISOP
VOC, ppmC
VOC, ppmC
Hours, LDT

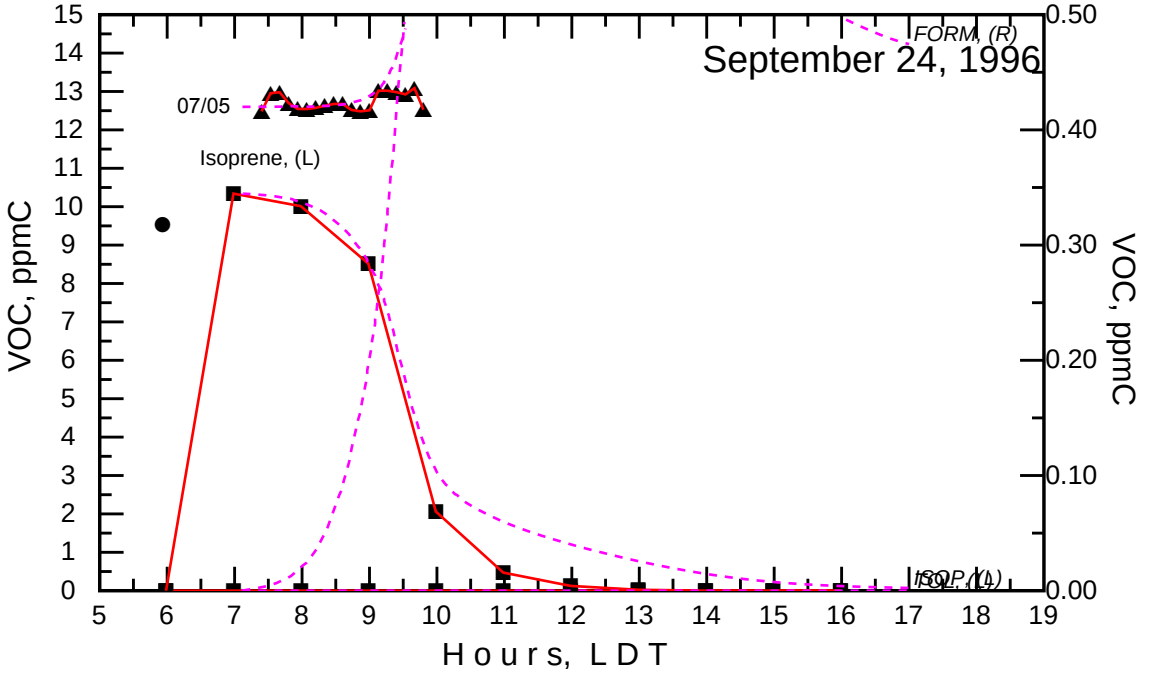


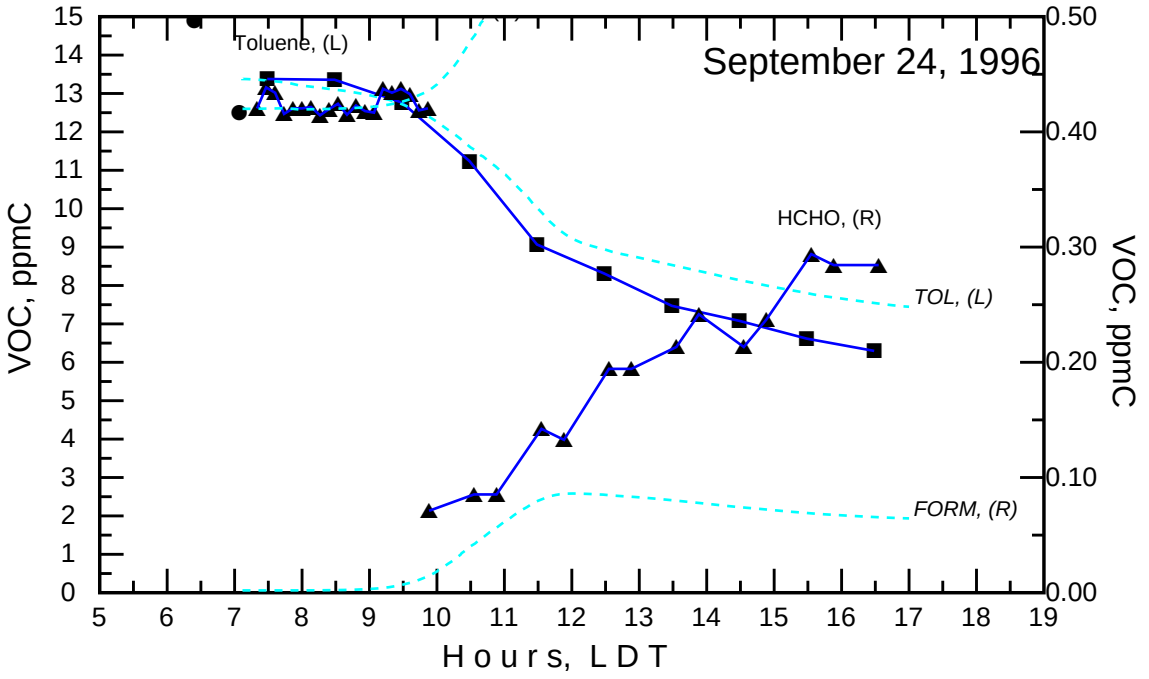


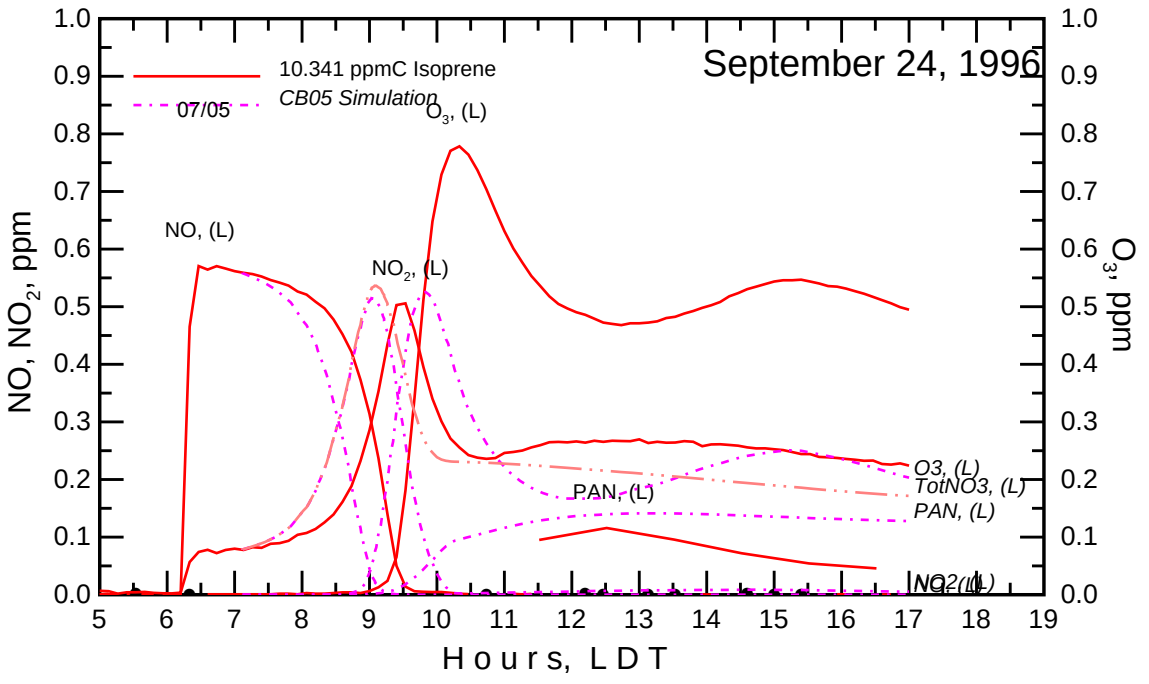
Matched Isoprene; Delta NOx

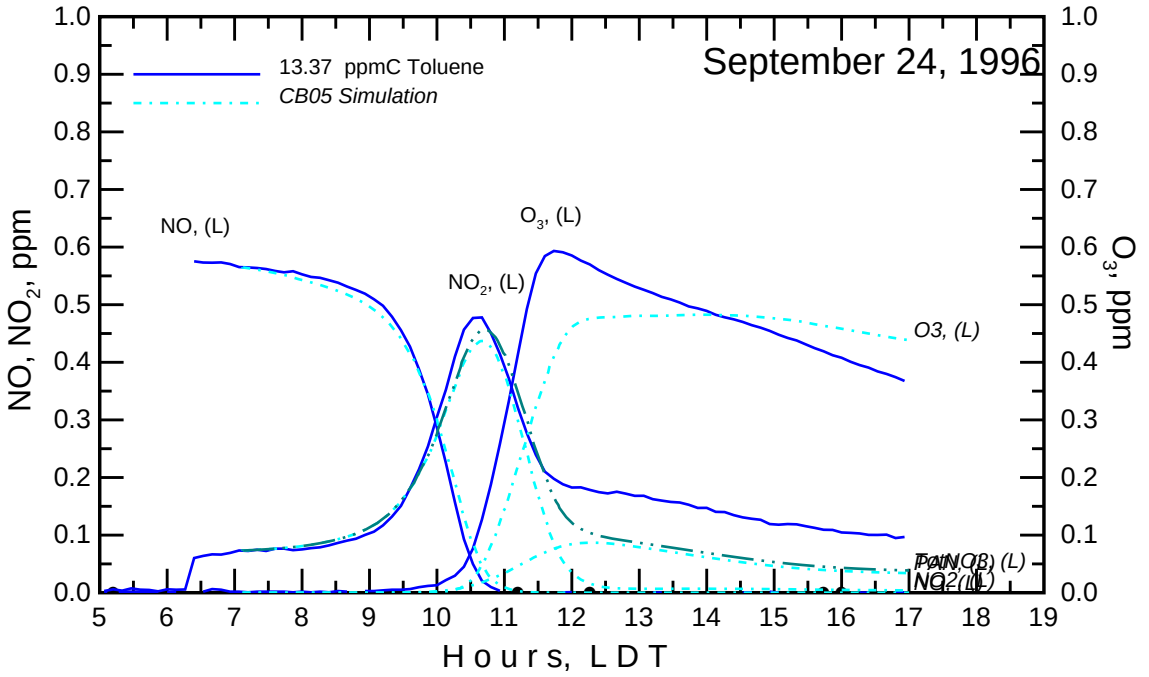

Chamber Temperature
September 11, 1999
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT


September 11, 1999
CCl4, relative
CCl4, relative
CCl4, (B)
Hours, LDT

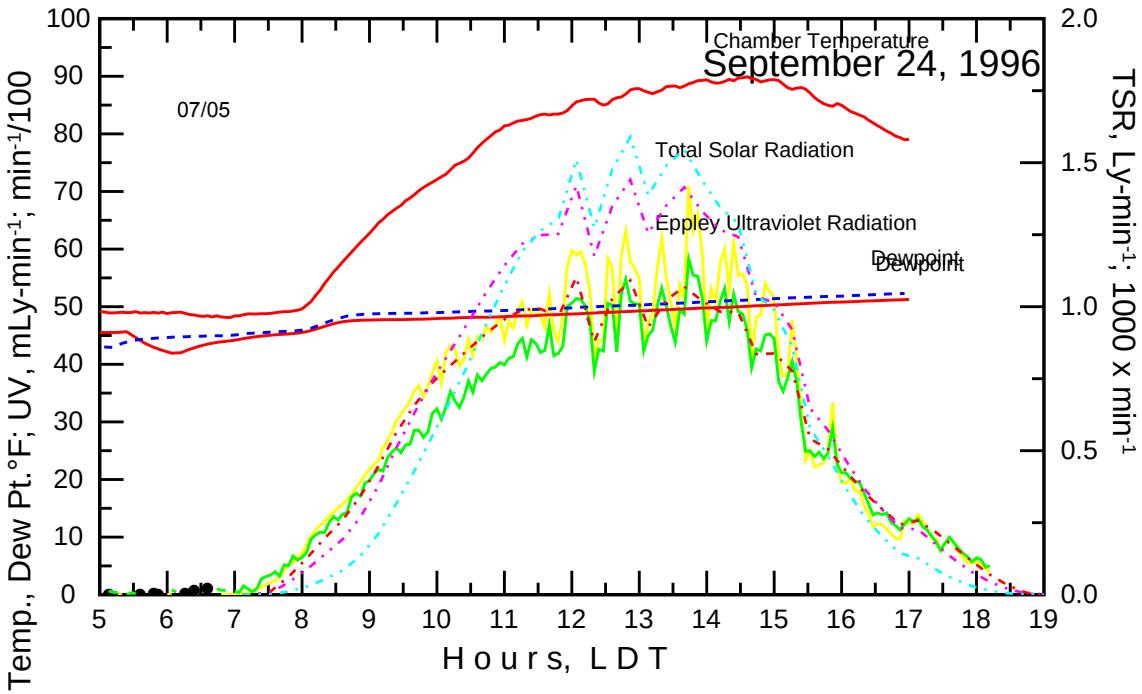

September 24, 1996
07/05
Isoprene, (L)
FORM, (R)
ISOP, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT

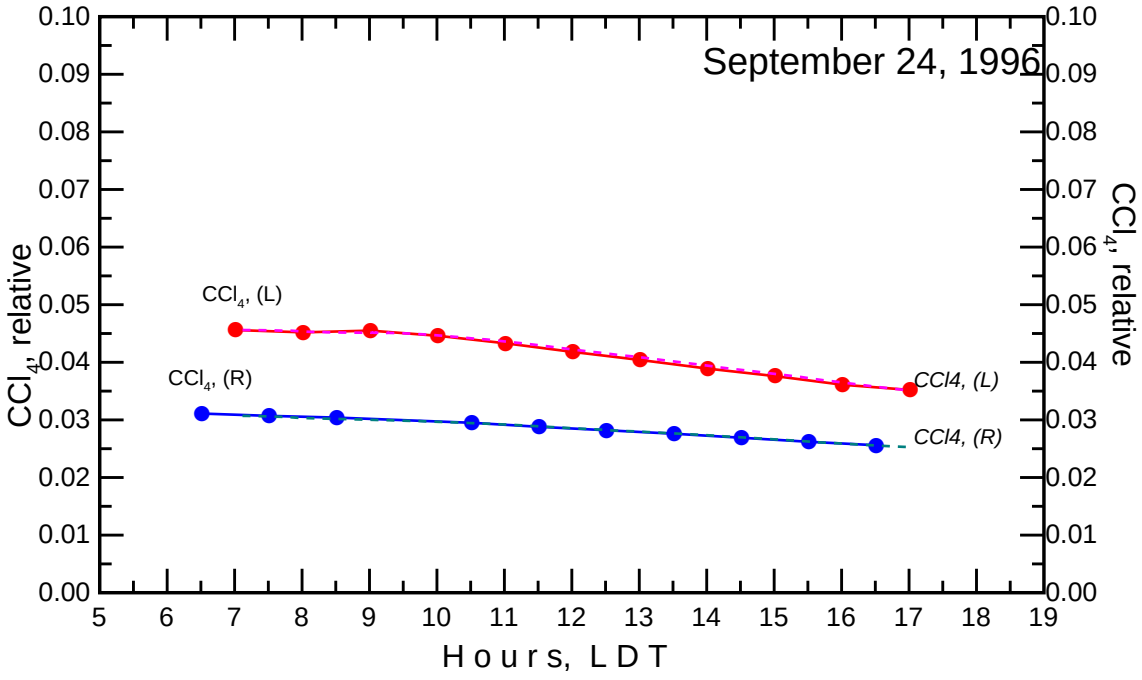

September 24, 1996
Toluene, (L)
HCHO, (R)
TOL, (L)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT





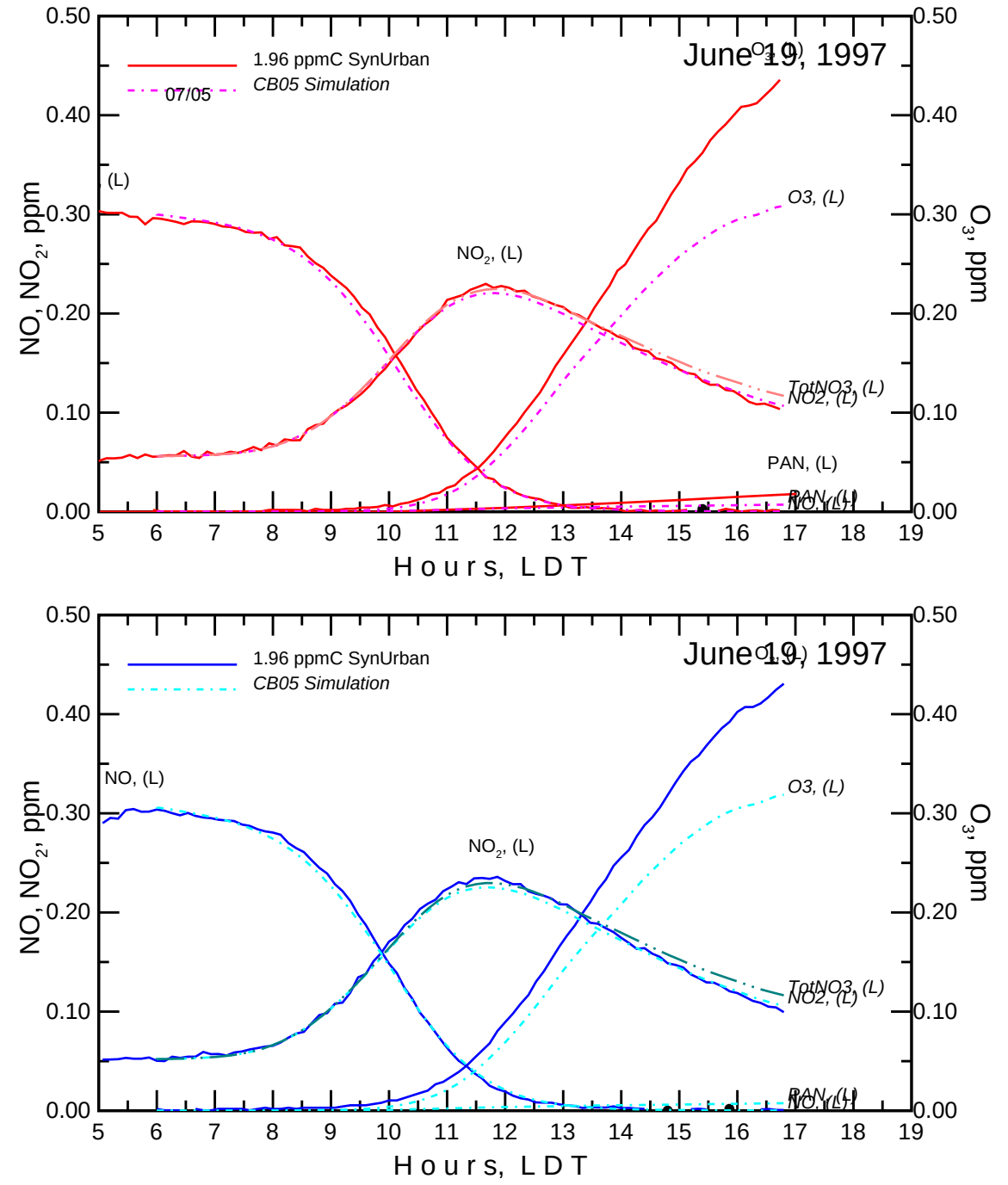
Toluene vs Isoprene


Chamber Temperature
September 24, 1996
07/05
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

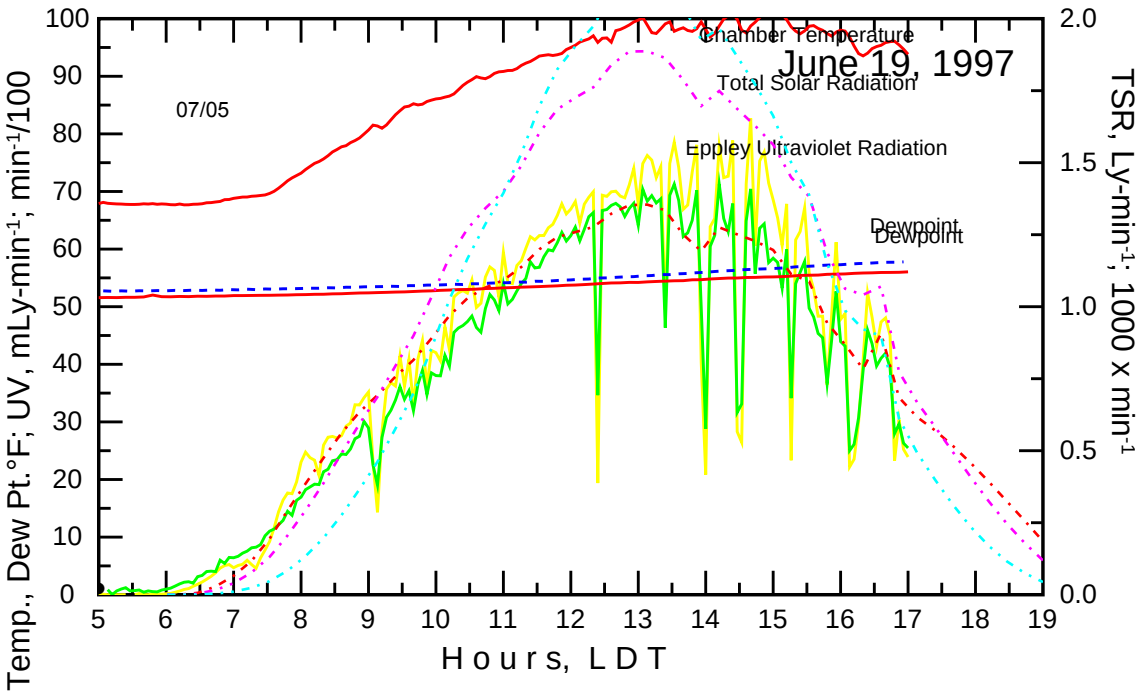

September 24, 1996
CCl4, (L)
CCl4, (R)
CCl4, (L)
CCl4, (R)
CCl4, relative
CCl4, relative
Hours, LDT

Urban Mixture

JN 19 97
AU 26 01
ST 10 99
ST 12 94
ST 14 00
ST 14 94
ST 15 94
ST 26 99



Matched SynUrban and NOx


June 19, 1997
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
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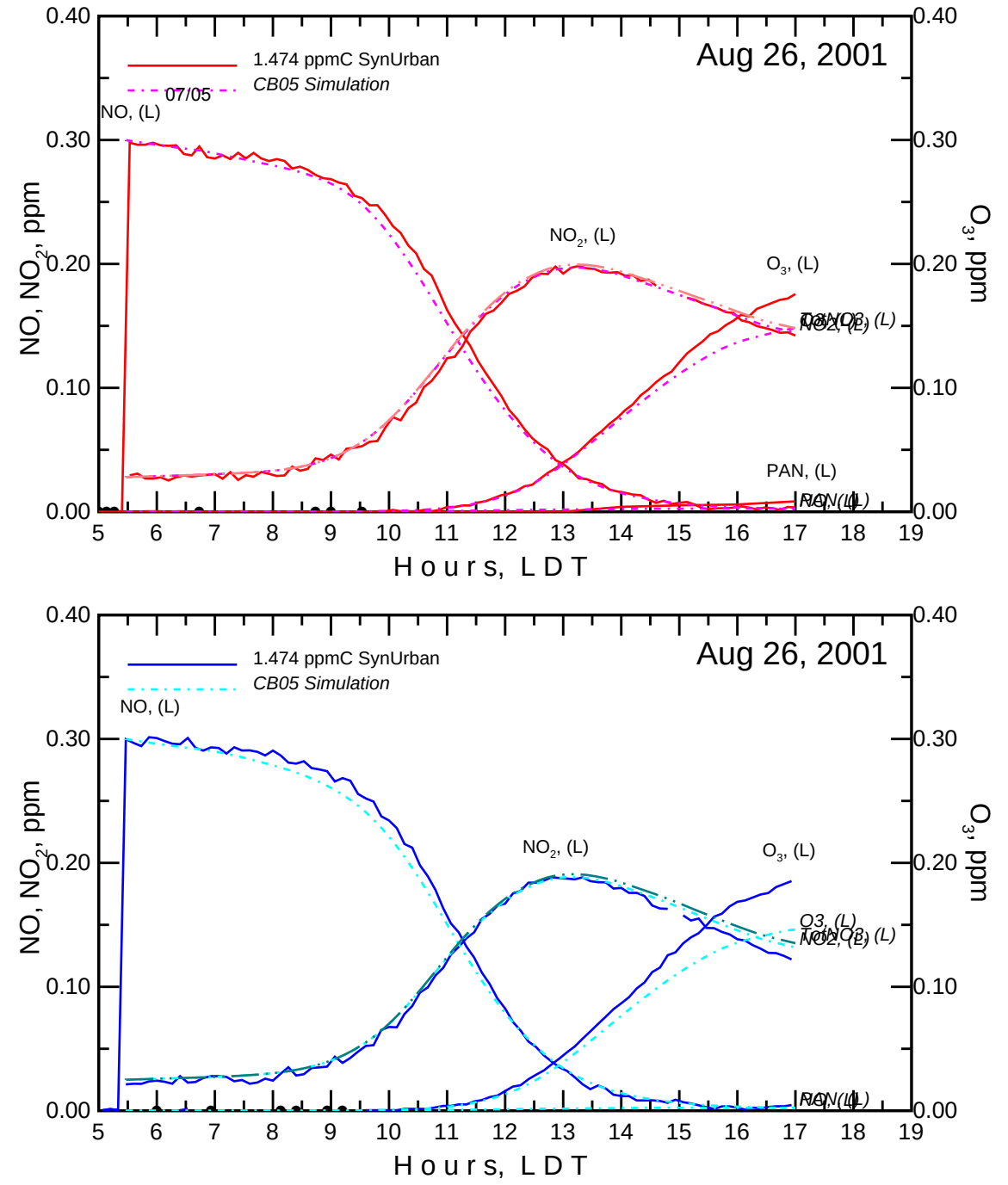
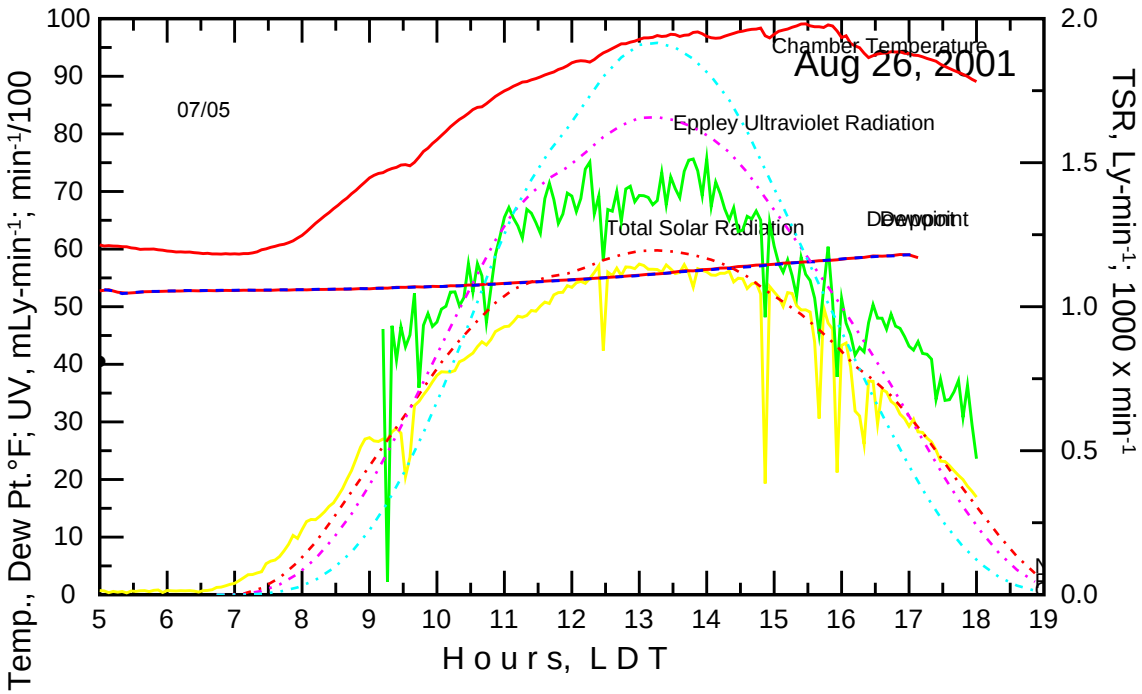
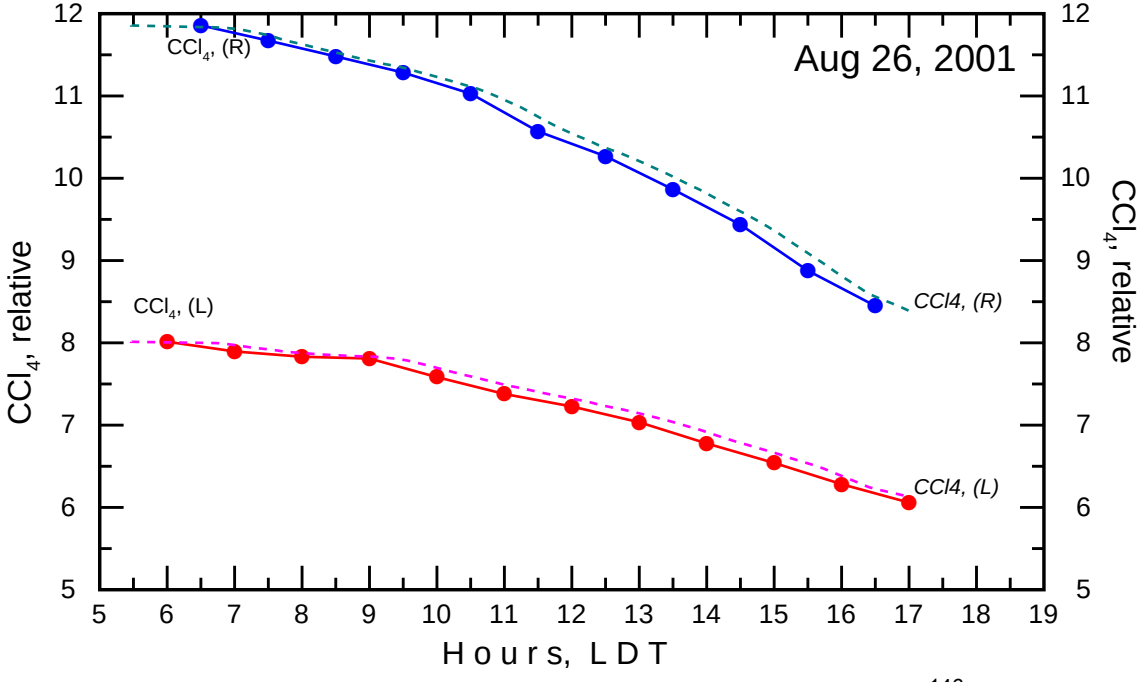
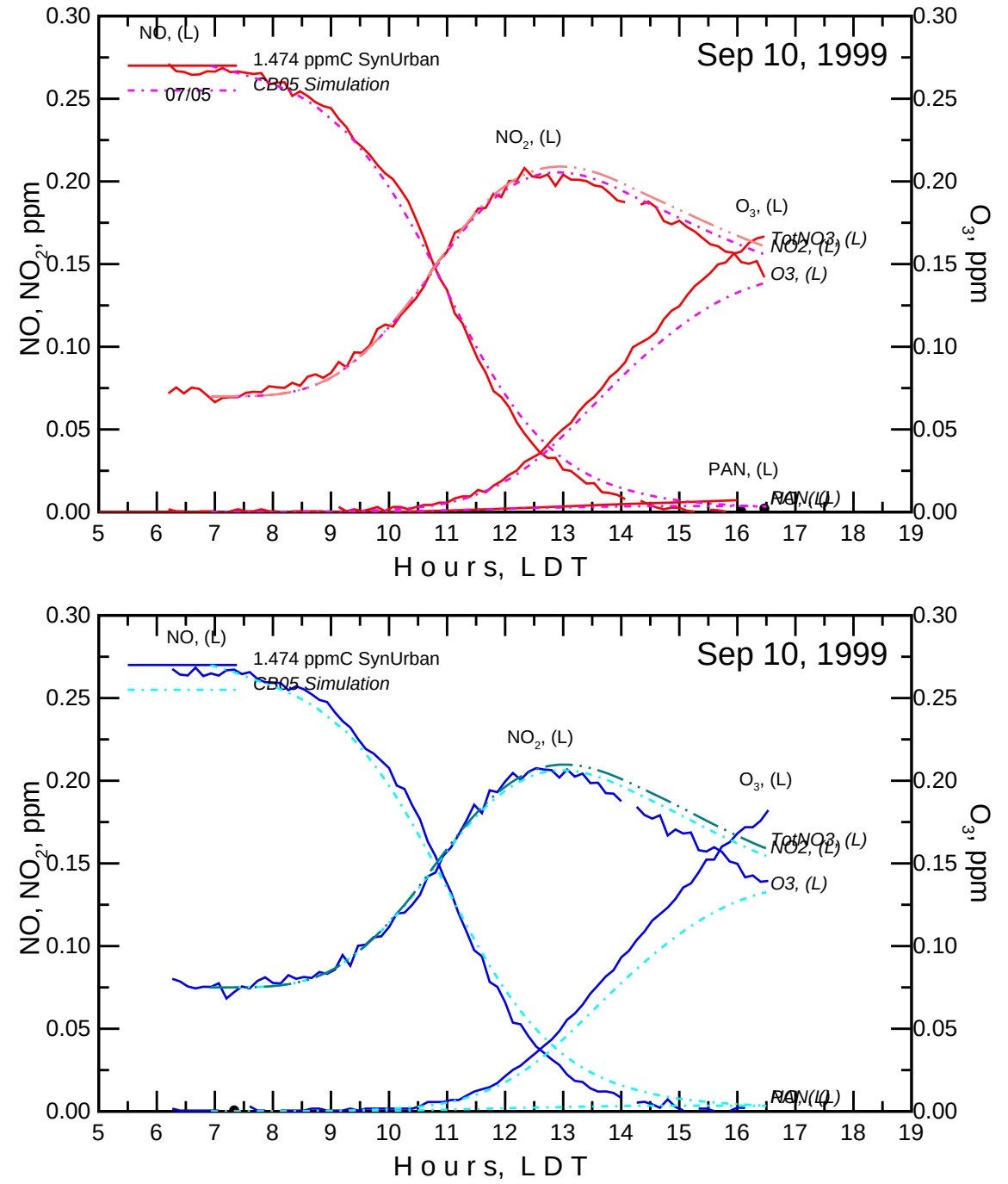


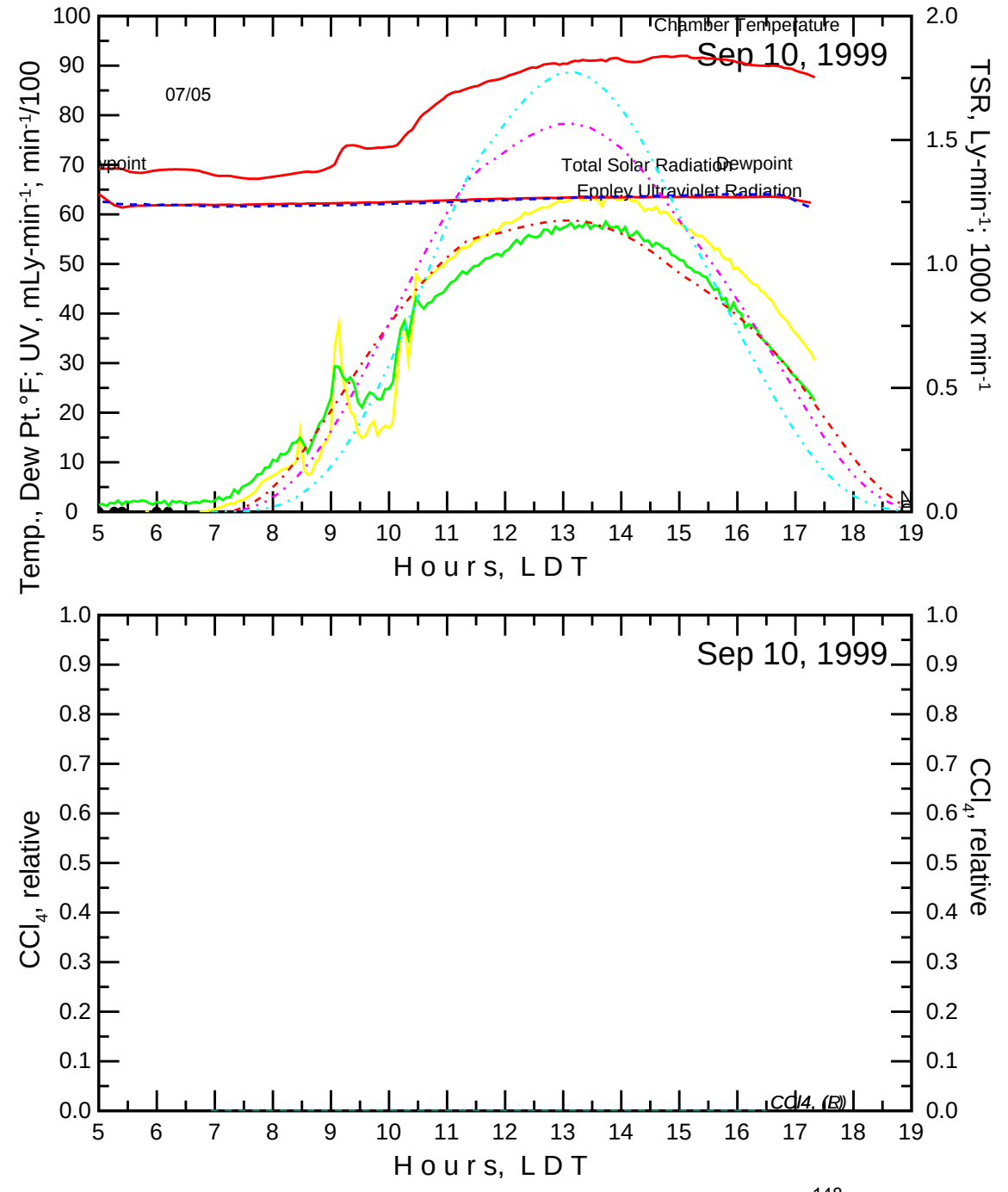
Matched SynUrban; Matched NOx

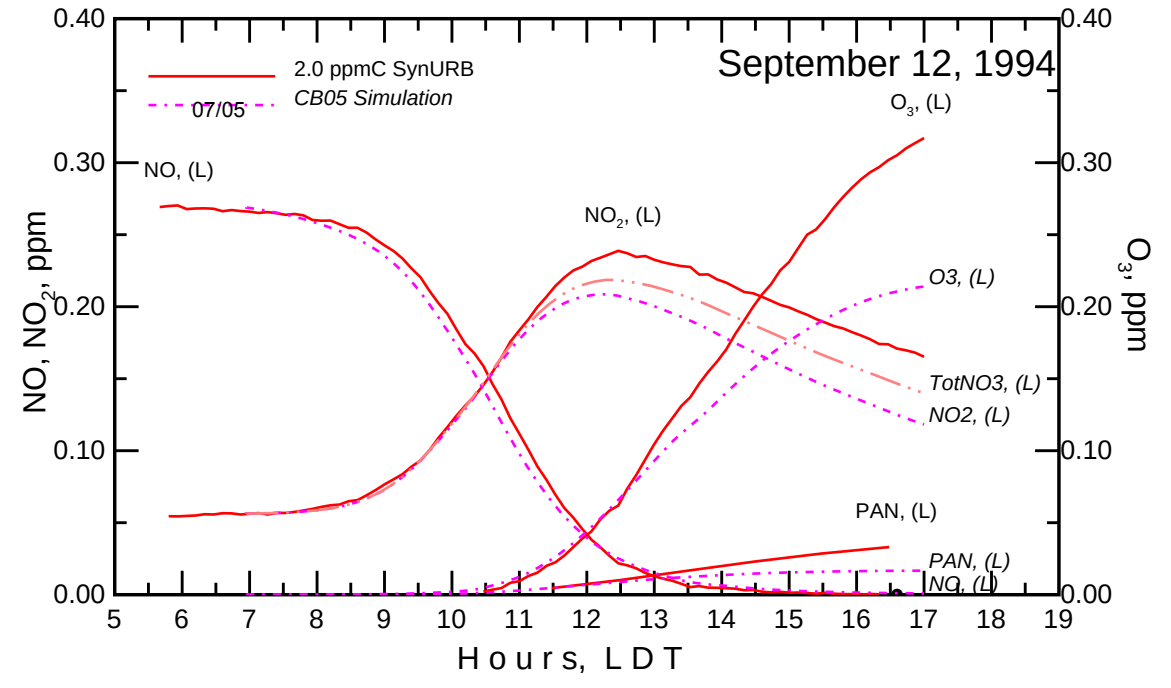

Aug 26, 2001
07/05
Chamber Temperature
Eppley Ultraviolet Radiation
Total Solar Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT

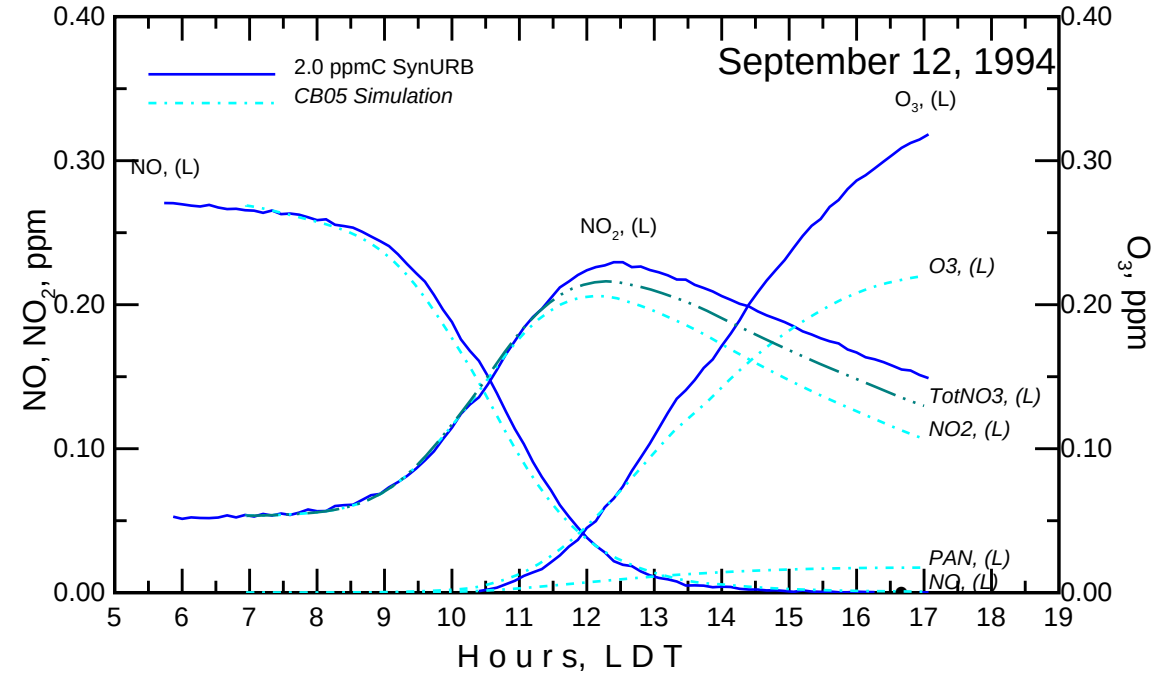

Aug 26, 2001
CCl4, (R)
CCl4, (L)
CCl4, relative
Hours, LDT



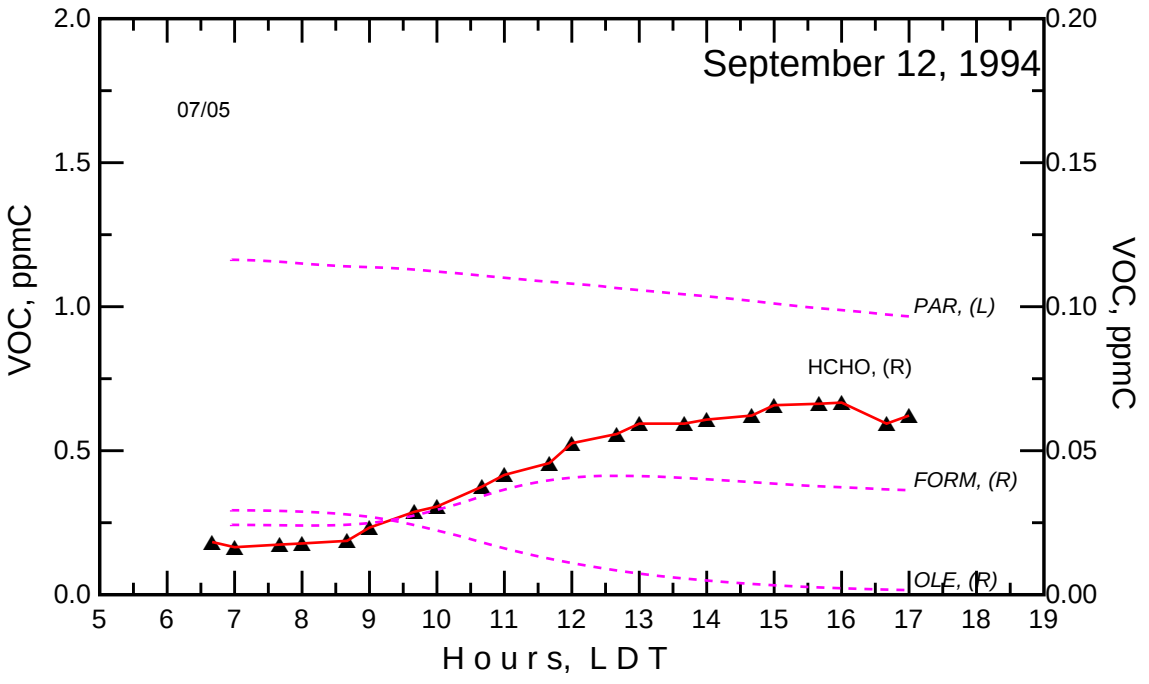
Matched SynUrban and NOx

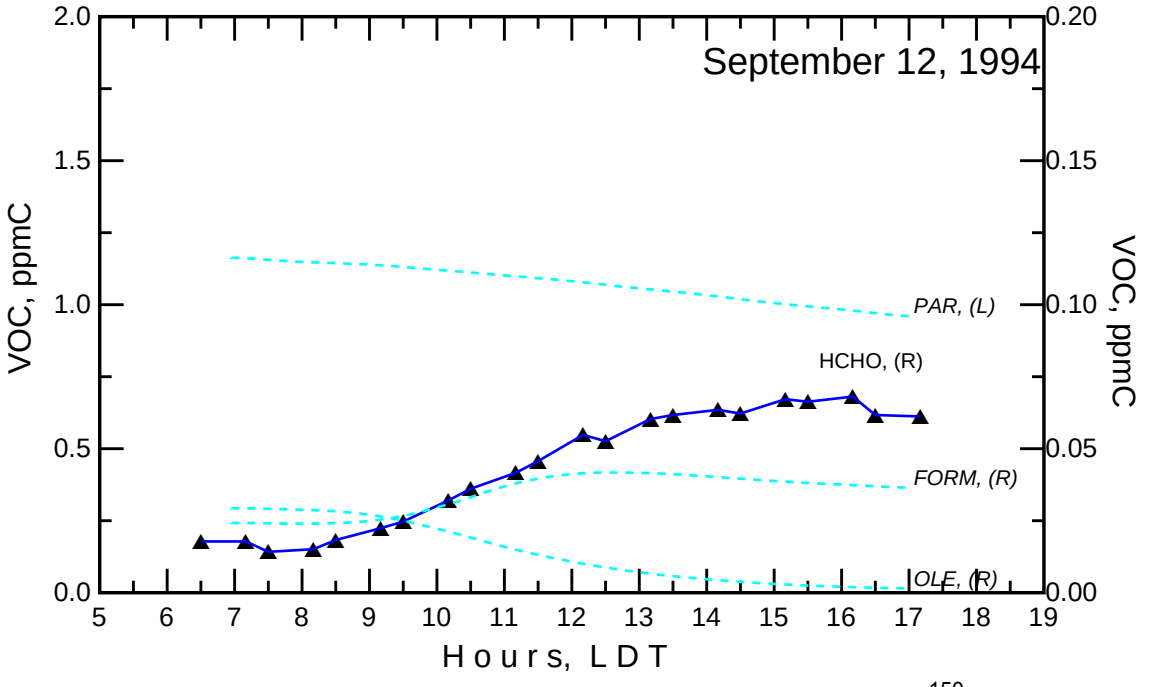

Chamber Temperature
Sep 10, 1999
07/05
Total Solar Radiation
Dewpoint
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
Sep 10, 1999
CCl4, relative
CCl4, (R)
Hours, LDT

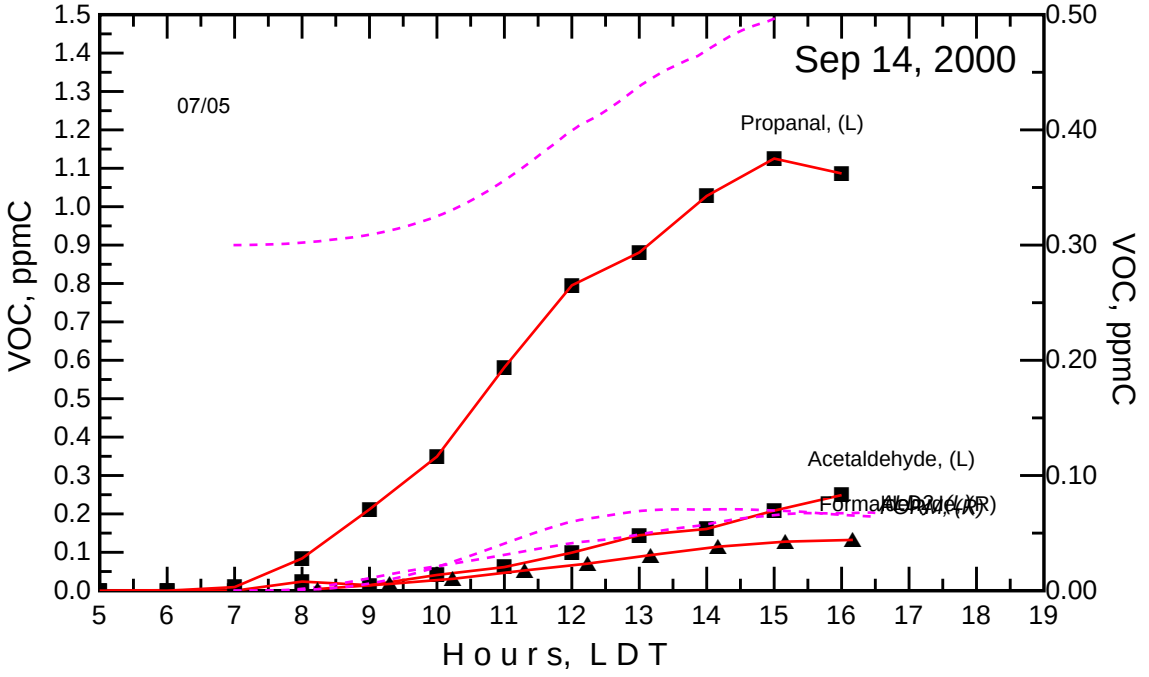


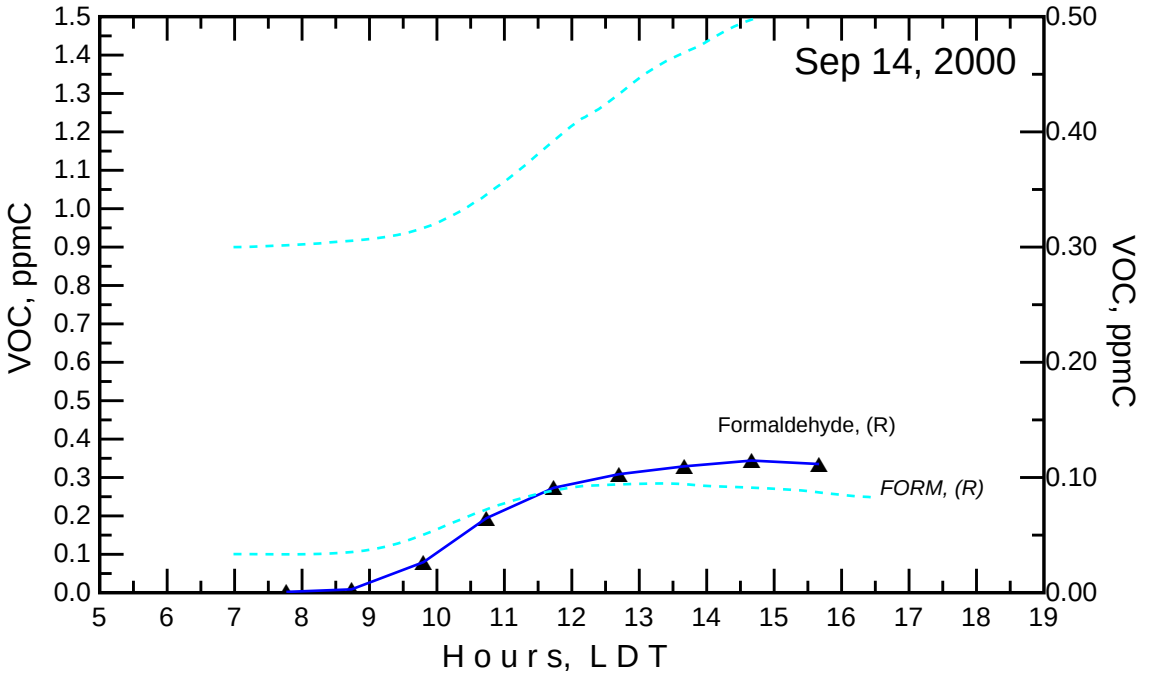


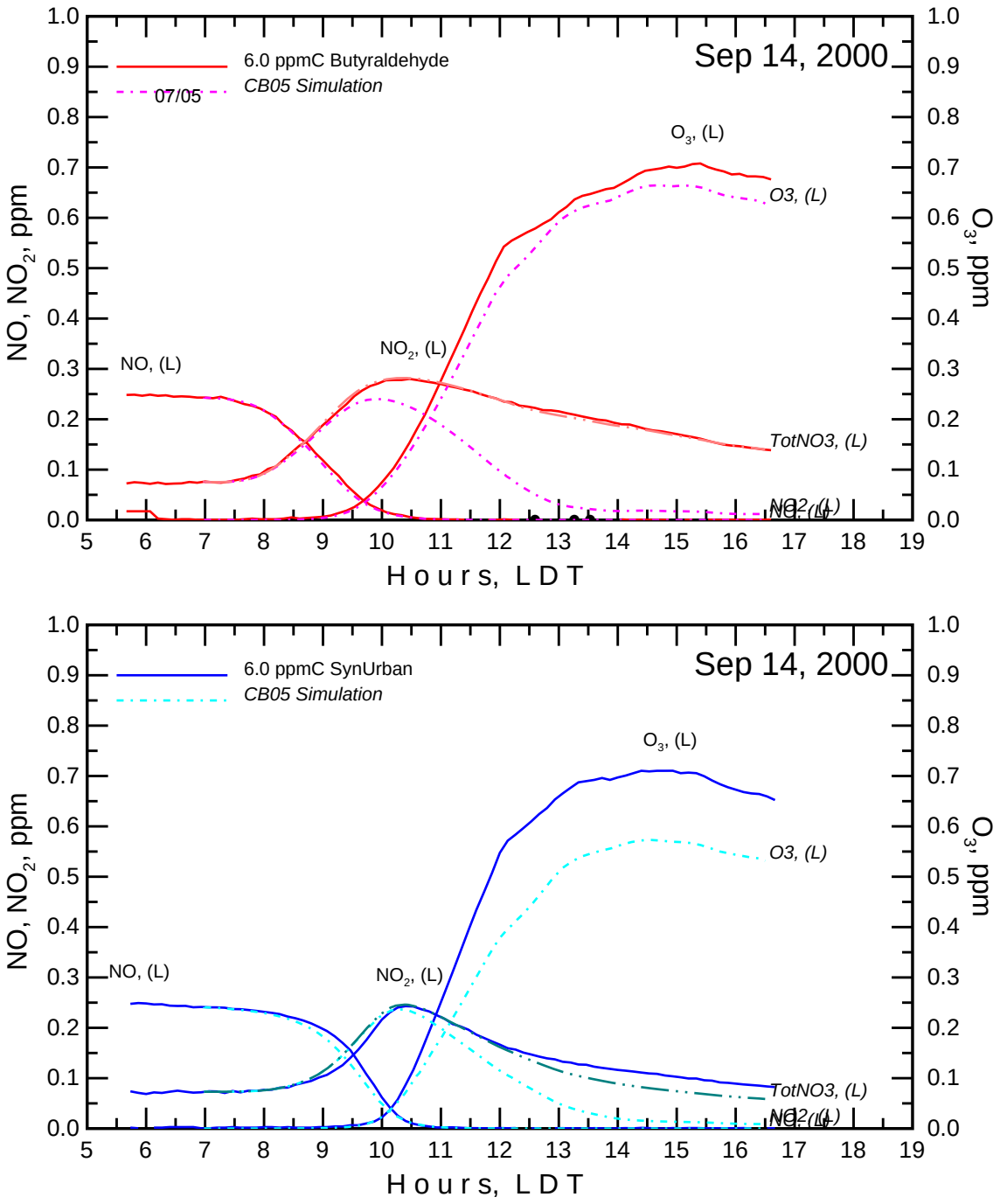
Matched SynURB


September 12, 1994
07/05
PAR, (L)
HCHO, (R)
FORM, (R)
OLE, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT
2.0
1.5
1.0
0.5
0.0
0.20
0.15
0.10
0.05
0.00
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

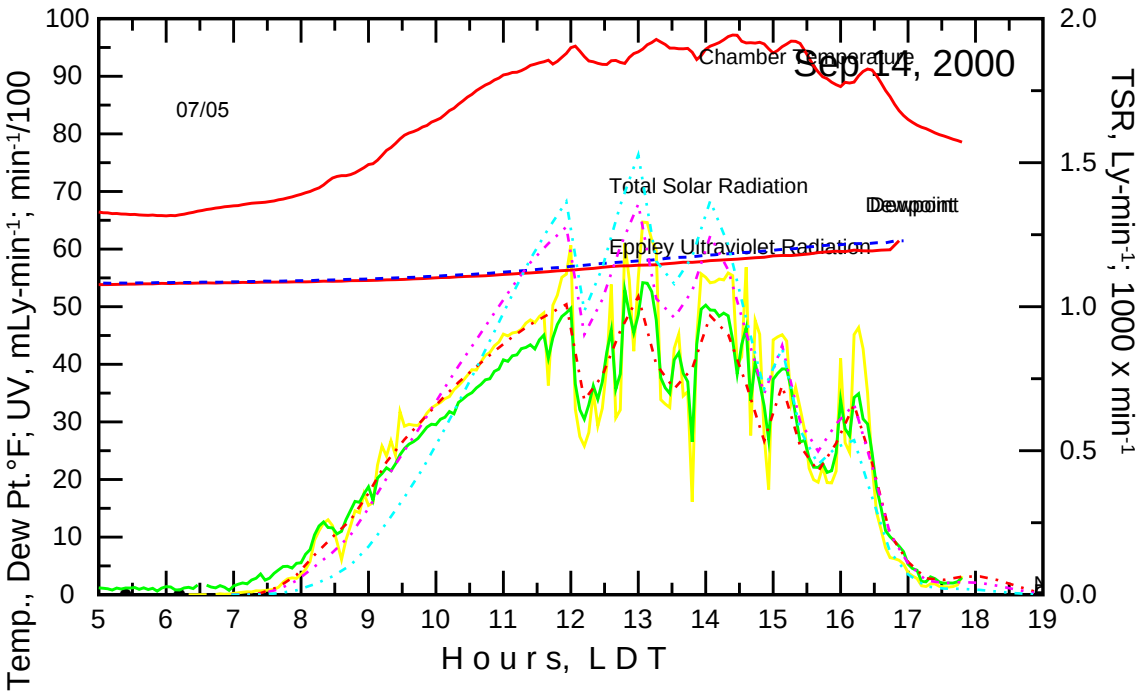

September 12, 1994
PAR, (L)
HCHO, (R)
FORM, (R)
OLE, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT
2.0
1.5
1.0
0.5
0.0
0.20
0.15
0.10
0.05
0.00
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19


Sep 14, 2000
07/05
Propanal, (L)
Acetaldehyde, (L)
VOC, ppmC
VOC, ppmC
Hours, LDT


Sep 14, 2000
Formaldehyde, (R)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT



Butyraldehyde vs SynUrban; matched NOx


Sep 14, 2000
07/05
Chamber Temperature
Total Solar Radiation
Dewpoint
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
0
10
20
30
40
50
60
70
80
90
100
0.0
0.5
1.0
1.5
2.0
5
6
7
8
9
10
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14
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16
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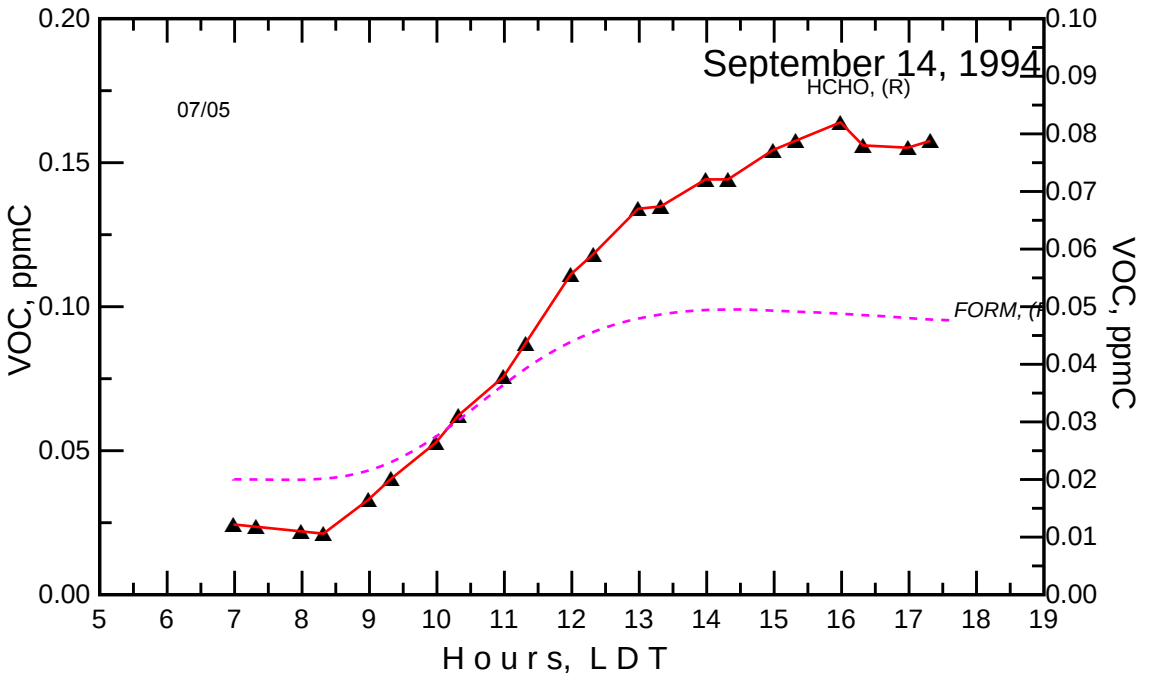
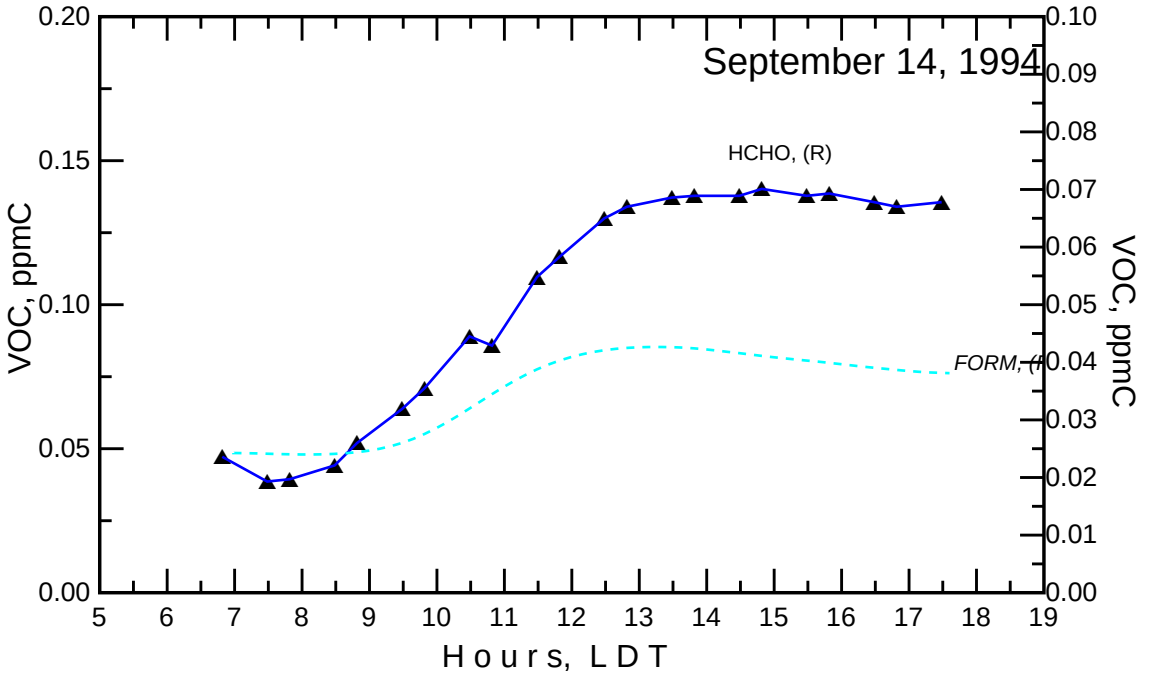
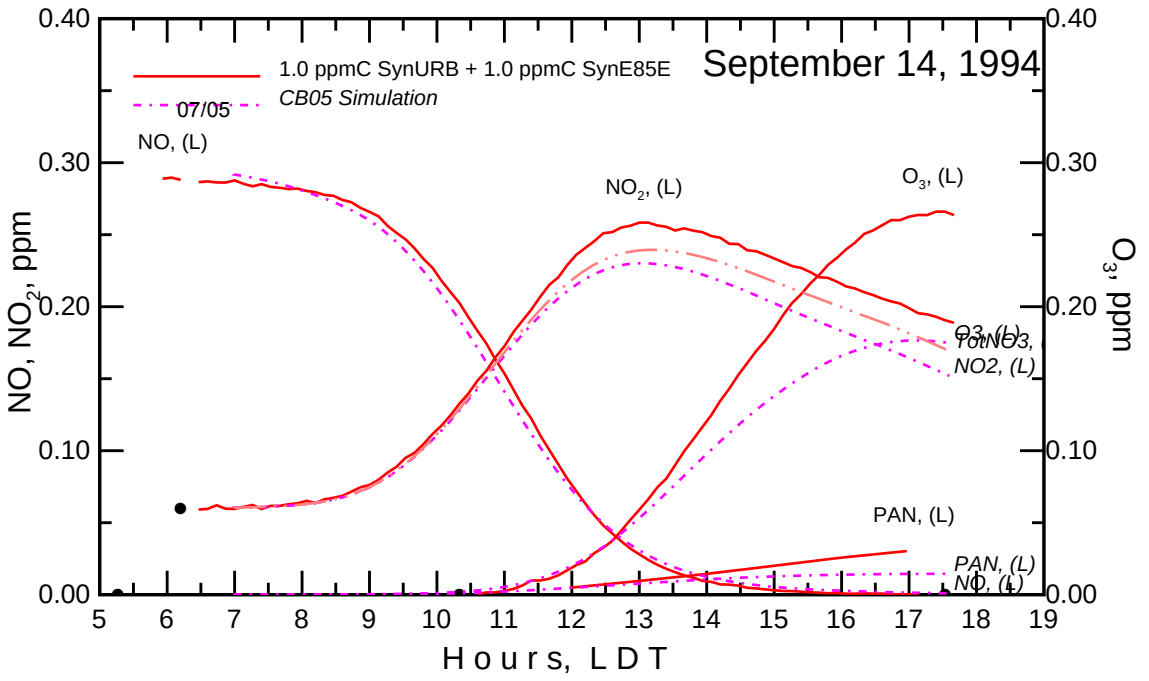
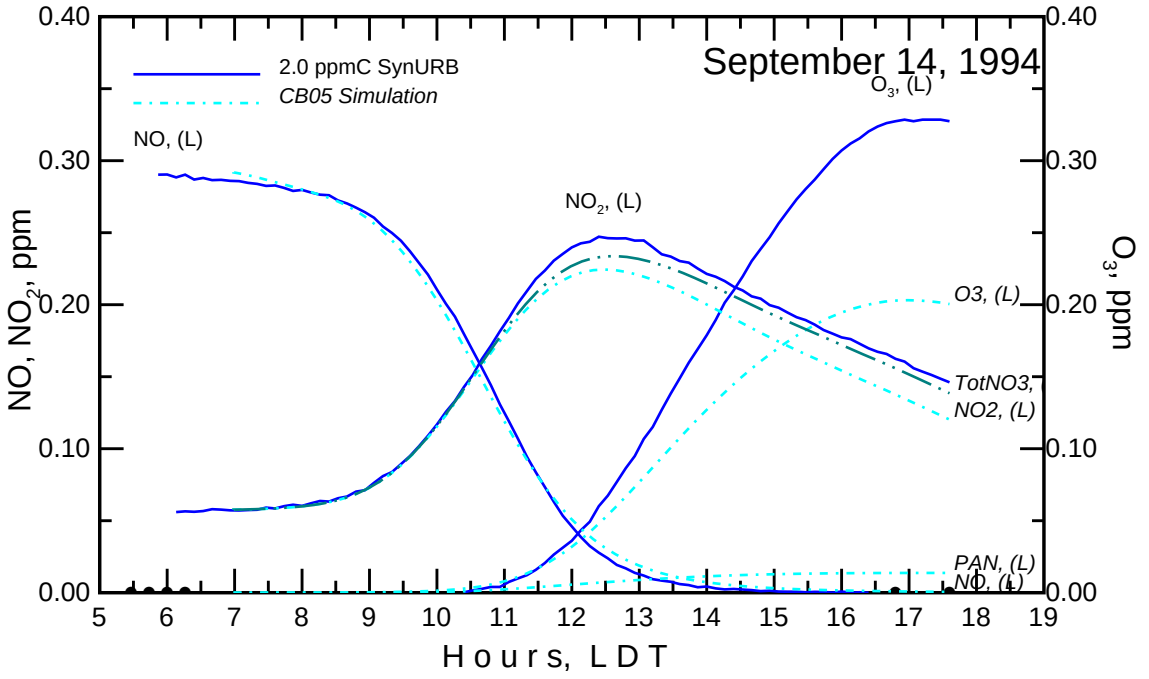
18
19

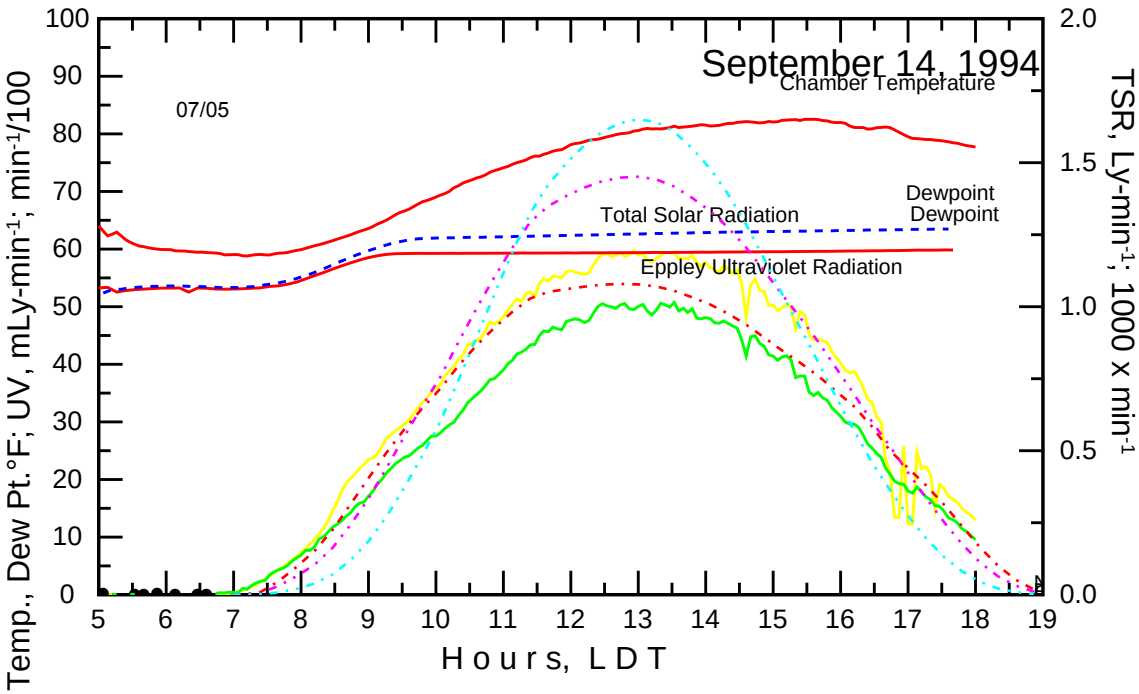

September 14, 1994
07/05
HCHO, (R)
FORM, (R)
VOC, ppmC
VOC, ppmC
0.20
0.15
0.10
0.05
0.00
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
Hours, LDT


September 14, 1994
HCHO, (R)
FORM, (R)
VOC, ppmC
VOC, ppmC
0.20
0.15
0.10
0.05
0.00
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
Hours, LDT





SynURB vs SynURB/SynE85


September 14, 1994
07/05
Chamber Temperature
Dewpoint
Dewpoint
Total Solar Radiation
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
100
90
80
70
60
50
40
30
20
10
0
2.0
1.5
1.0
0.5
0.0
5
6
7
8
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11
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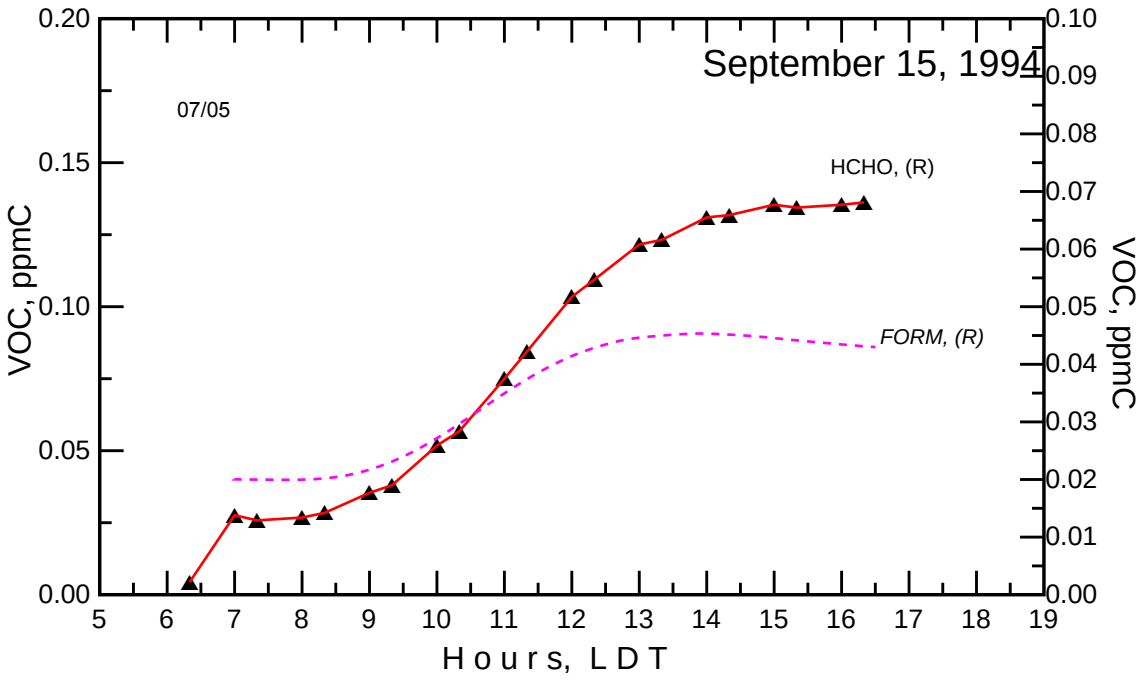
18
19


September 15, 1994
07/05
HCHO, (R)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT
0.00
0.05
0.10
0.15
0.20
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.10
5
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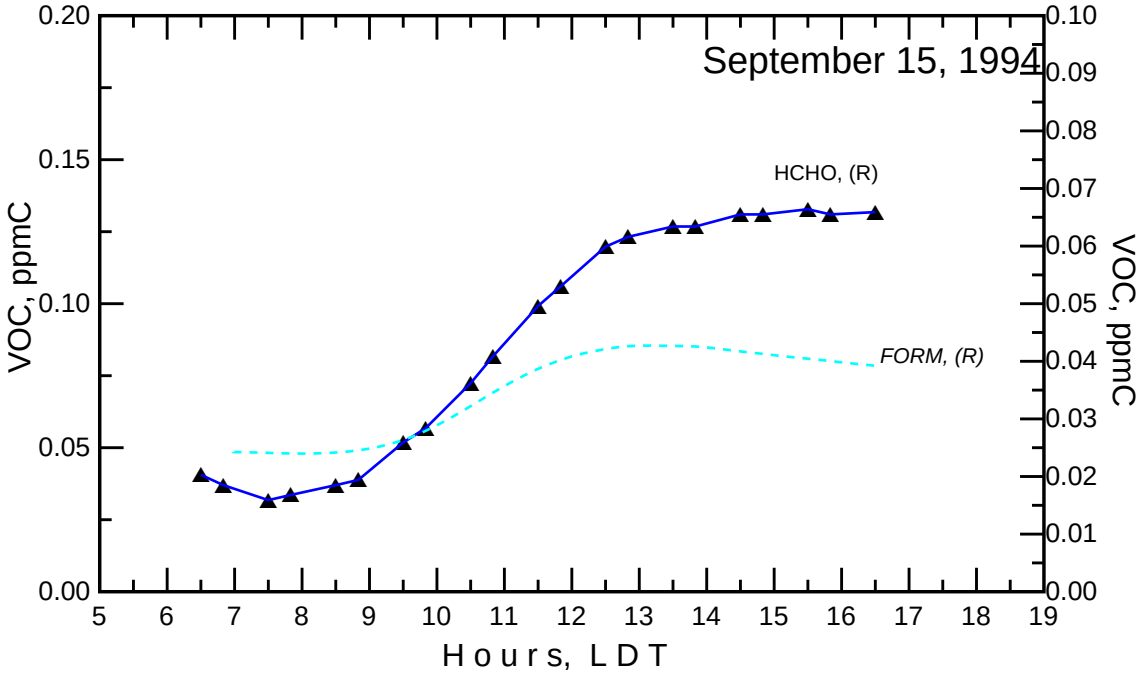
September 15, 1994
HCHO, (R)
FORM, (R)
VOC, ppmC
VOC, ppmC
Hours, LDT
0.00
0.05
0.10
0.15
0.20
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.10
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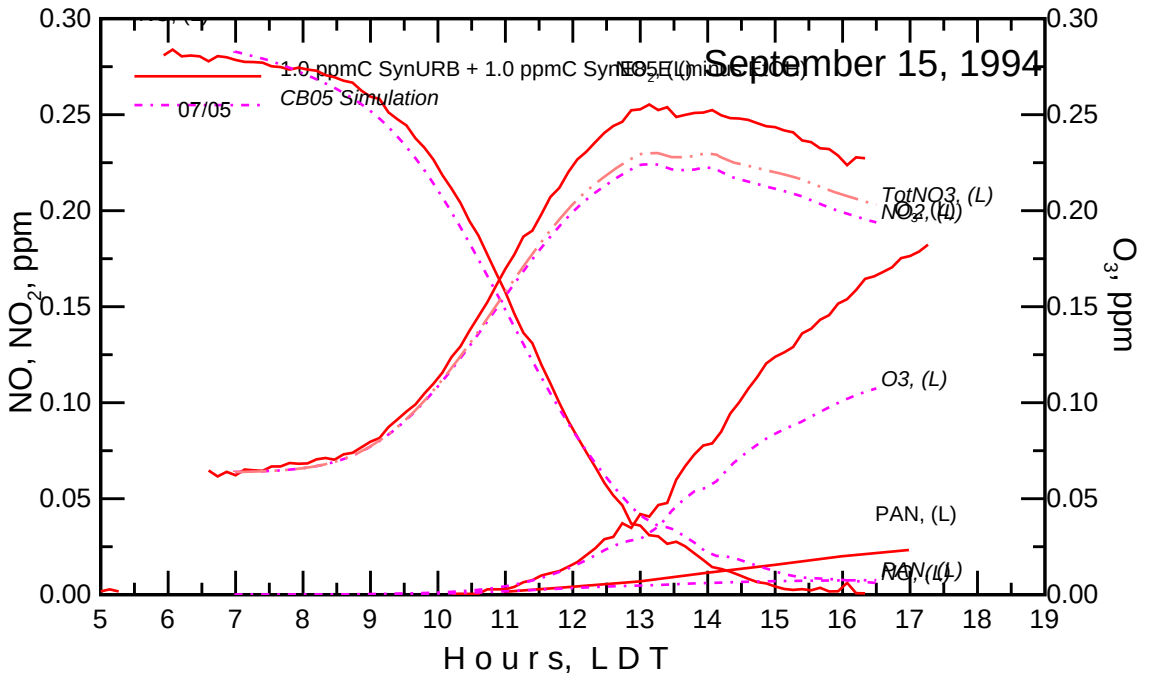
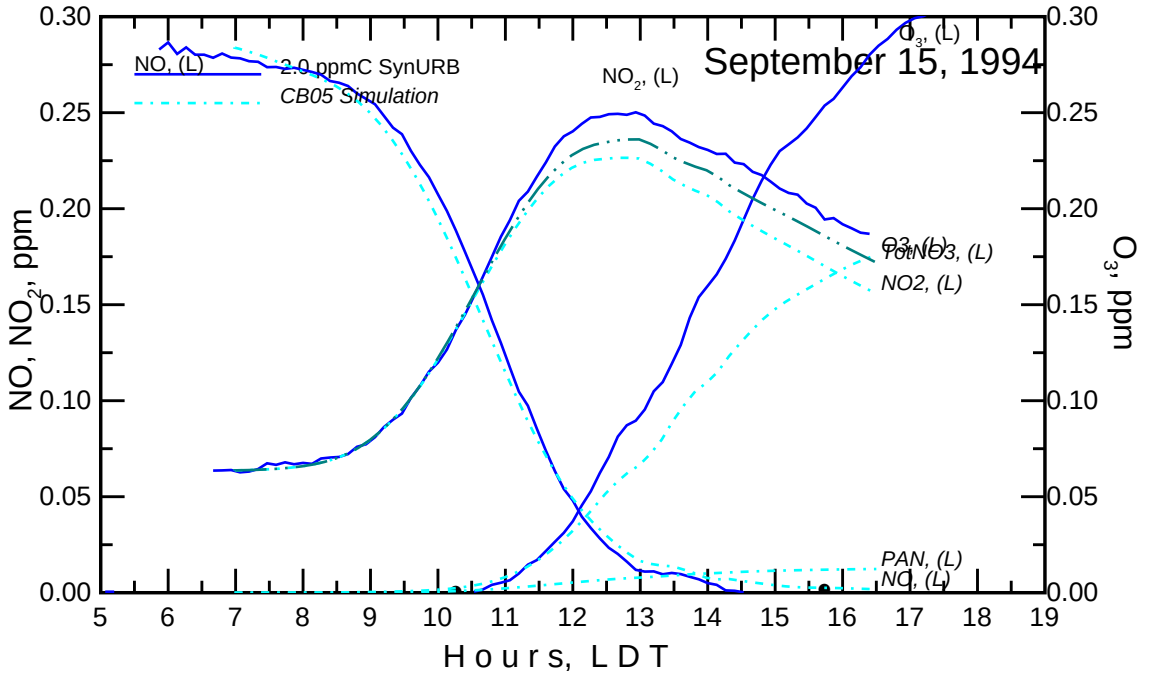
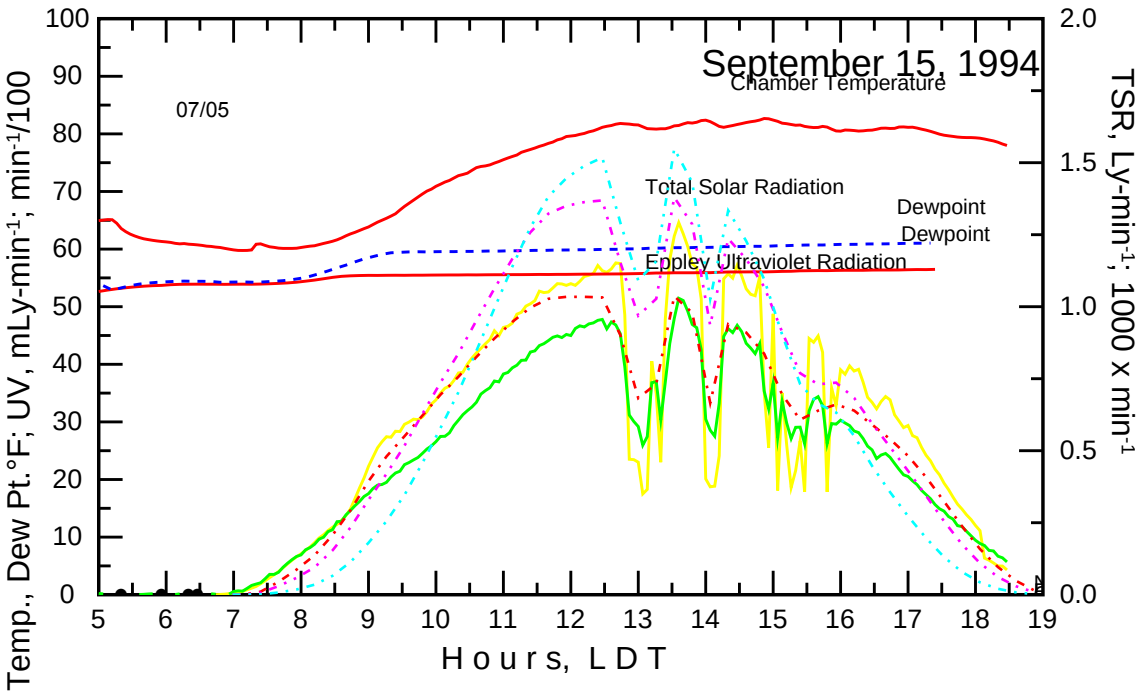




SynURB vs SynURB/SynE85 (no EtOH)


September 15, 1994
07/05
Chamber Temperature
Total Solar Radiation
Dewpoint
Dewpoint
Eppley Ultraviolet Radiation
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
100
90
80
70
60
50
40
30
20
10
0
2.0
1.5
1.0
0.5
0.0
5
6
7
8
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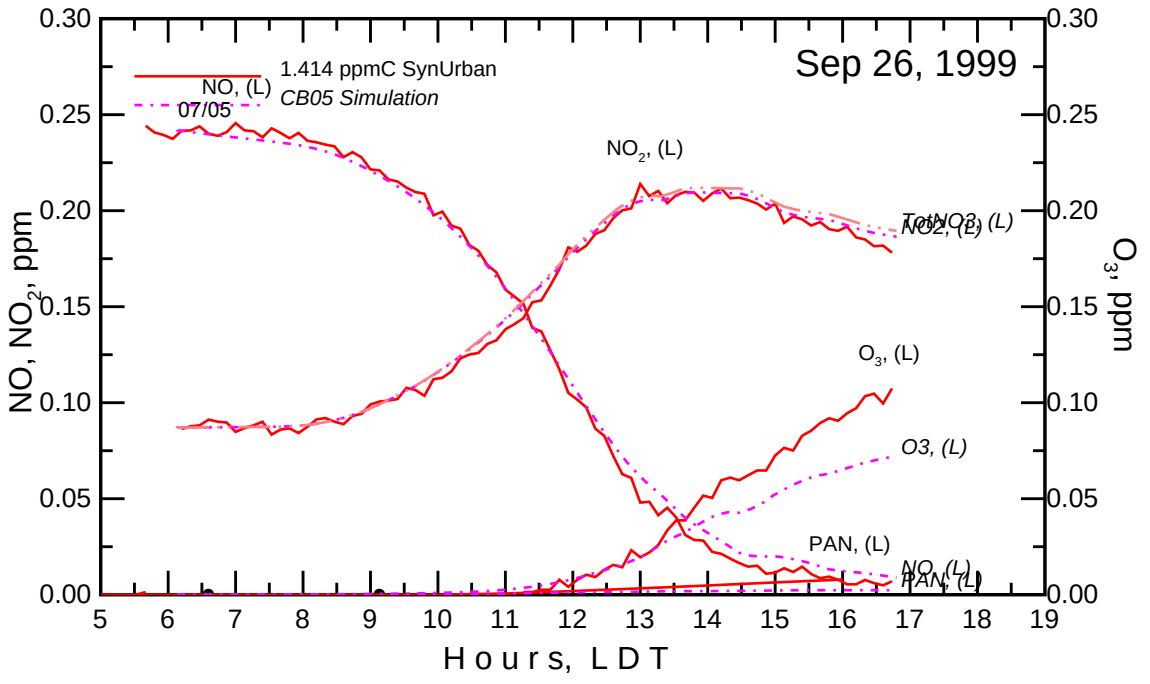
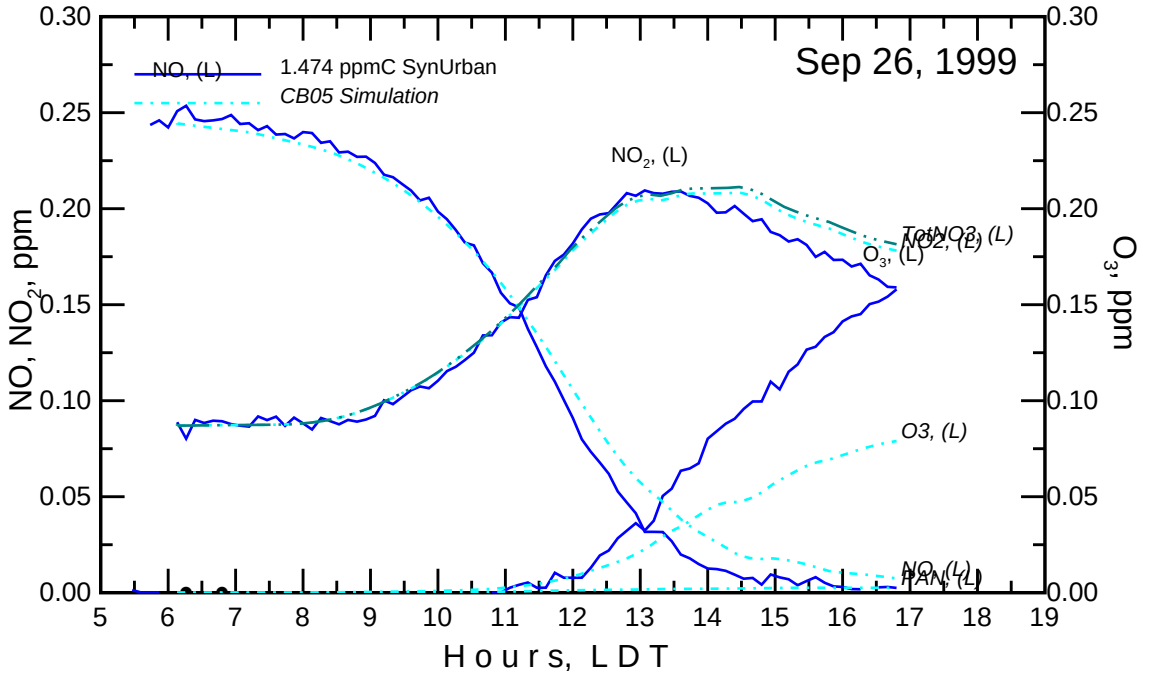
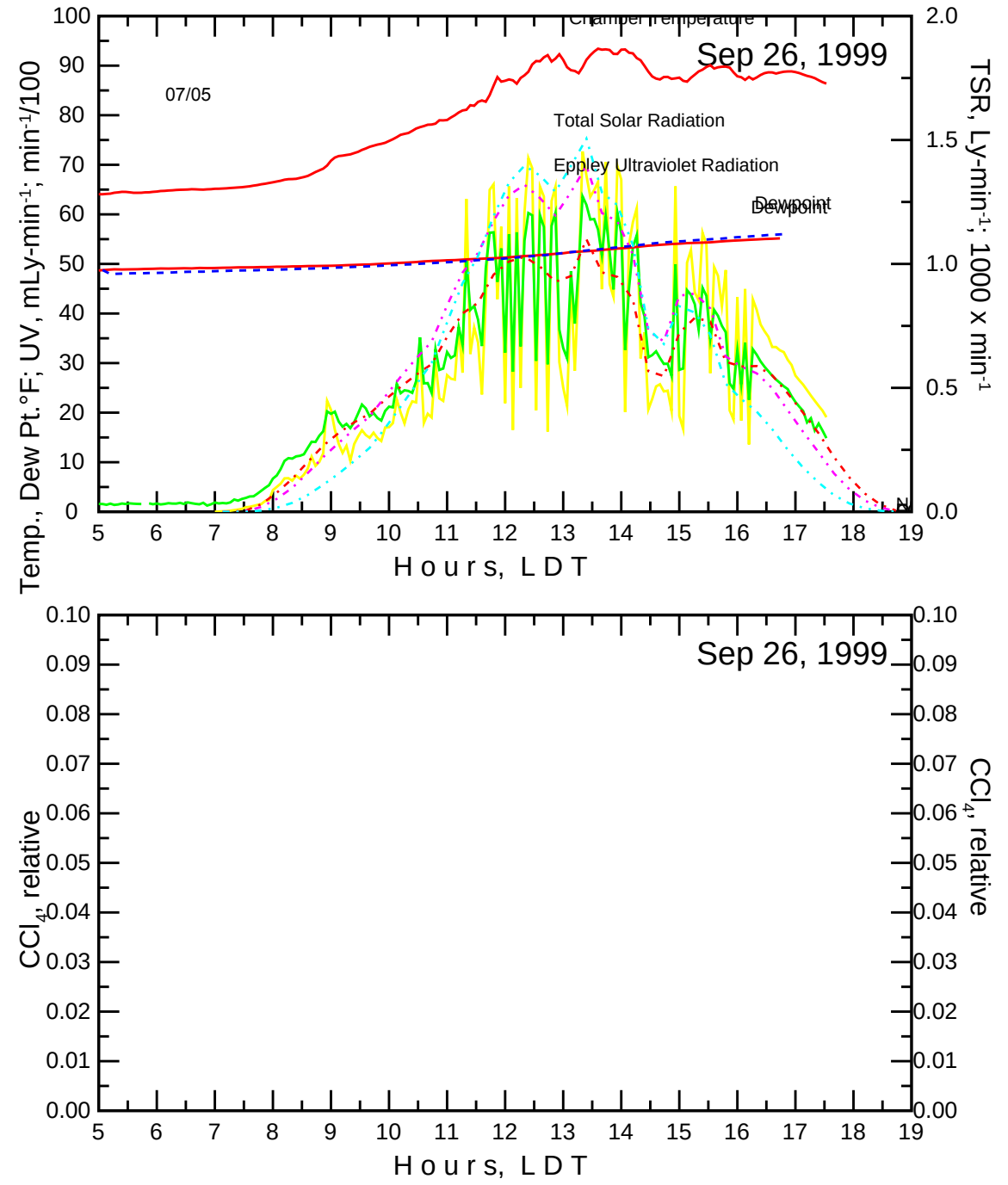




4% SynUrban Difference; Matched NOx


Sep 26, 1999
07/05
Chamber Temperature
Total Solar Radiation
Eppley Ultraviolet Radiation
Dewpoint
Temp., Dew Pt. °F; UV, mLy-min-1; min-1/100
TSR, Ly-min-1; 1000 x min-1
Hours, LDT
Sep 26, 1999
CCl4, relative
CCl4, relative
Hours, LDT