

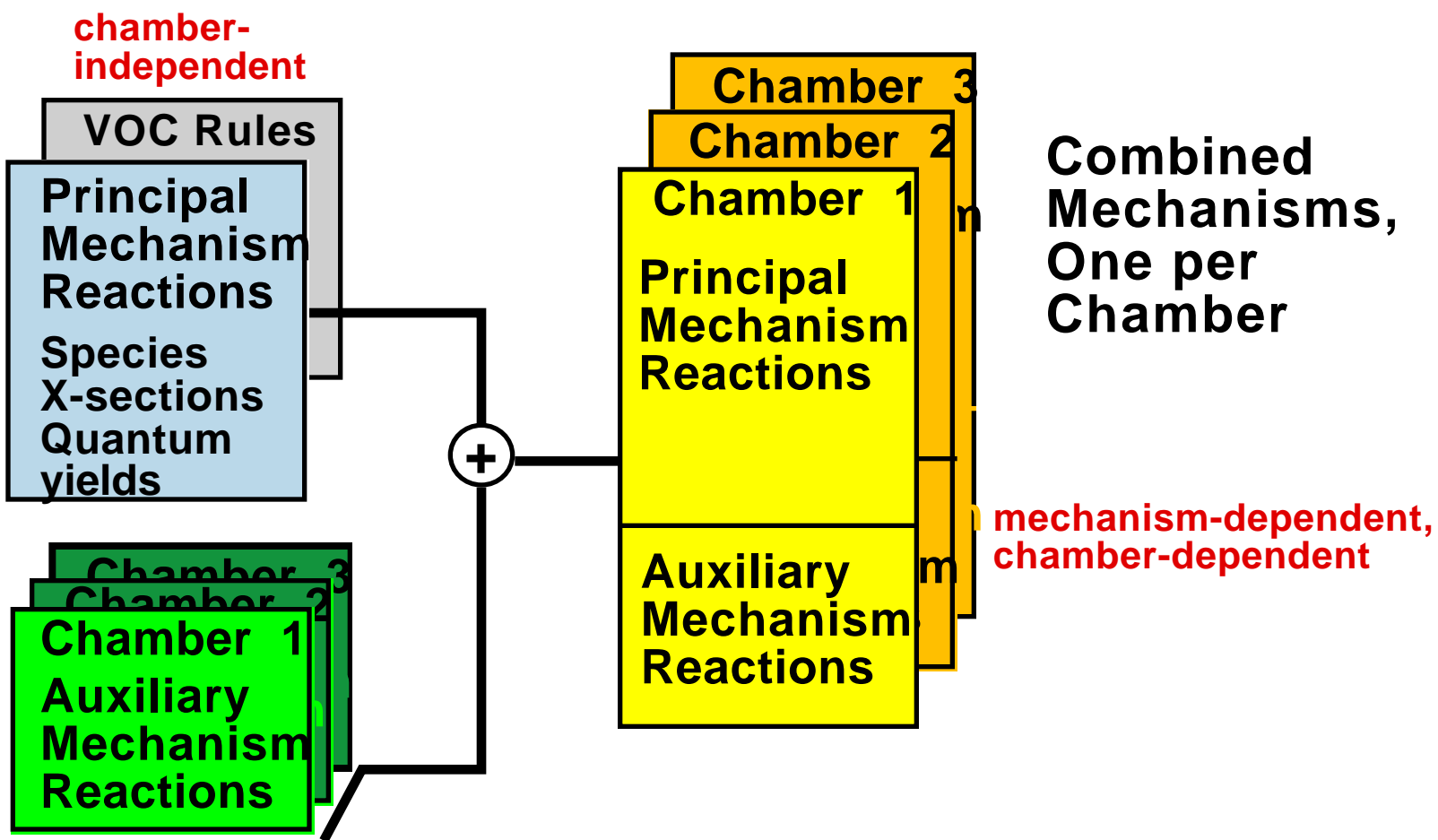
Auxiliary Mechanism (Wall Model)

UNC Outdoor Chamber



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Sciences and Engineering
School of Public Health
University of North Carolina

Principal & Aux Mechanisms



chamber-dependent

UNCAuxMech93.RXN

```
/*
*   UNC Chamber Dependent Reactions
*   Units are molecules/cc/secs ( 6/15/93, HEJ )
***/
```

SCALARS

```
WALLOH =2.5E-3, // scale factors, not rates
WALLNO2 =2.0E-3;
```

```
R[Wal I NO2a] = NO2 -hv-> HONO @ j [NO2_to_03P] * WALLOH ;
R[Wal I NO2b] = NO2 ----> 0.50*HONO + 0.50*WHNO3 @ 1.0E-19;
// 1.6E-4 /ppm-min

R[Wal I NO2c] = WHNO3 -hv-> NO2 @ j [NO2_to_03P] * WALLNO2;
```

UNCAux93.react

```
// Ambient Air background (all runs)
```

```
INJECT
```

```
{
```

```
  1790 PPB CH4
```

```
  580 PPB H2
```

```
}
```

```
// Seasonal ly variable Biogenic VOCs
```

```
INJECT
```

```
{
```

```
  0.140 PPM BVOC
```

```
}
```

```
// Provide initial HONO.
```

```
INJECT
```

```
{
```

```
  4.0 PPB HONO
```

```
}
```

```
// set the wall conditions
```

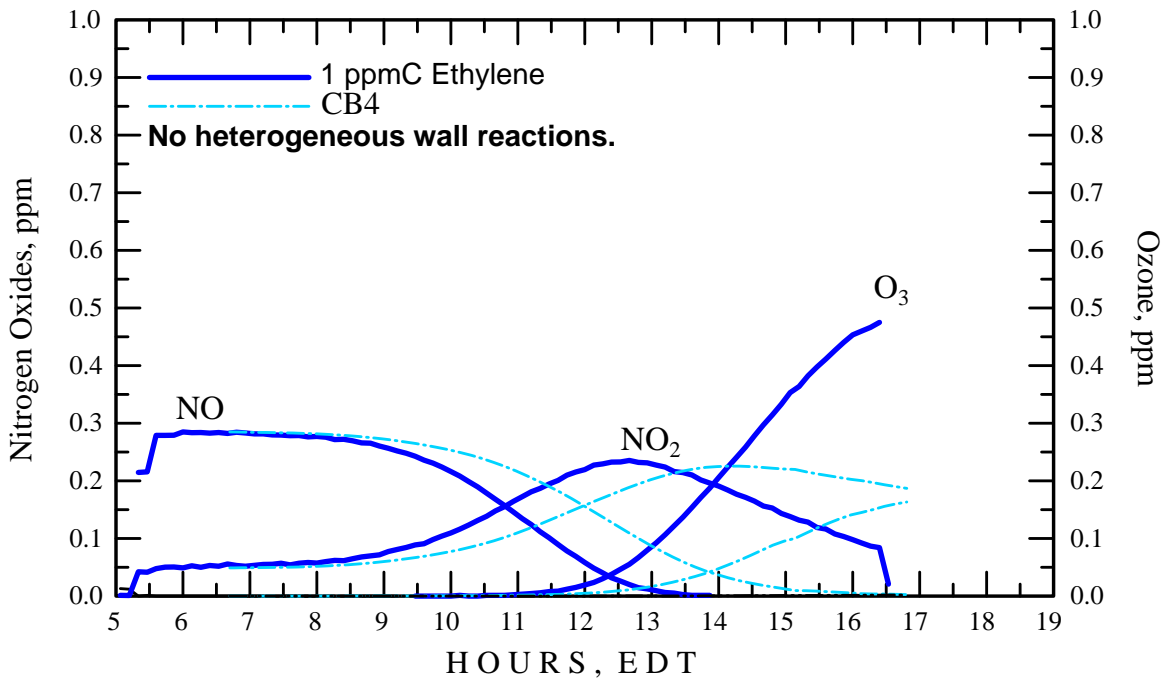
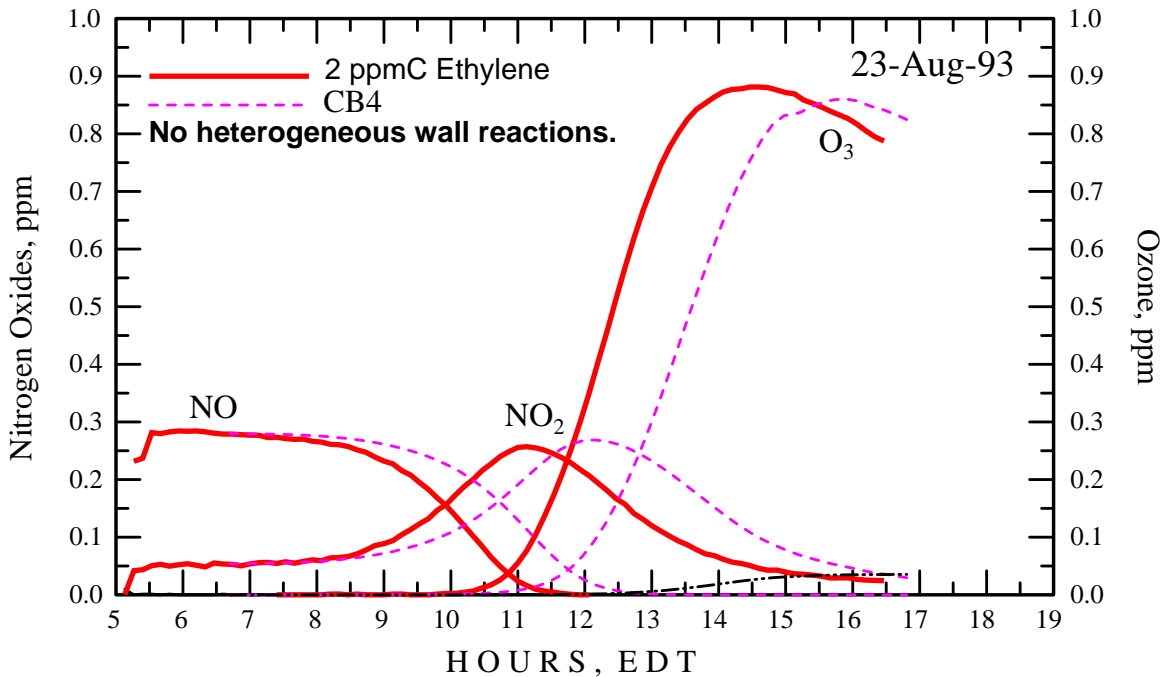
```
// NO2 -hv--> HONO @ j[N02_to_03P] * sf_HONO_walI_src
```

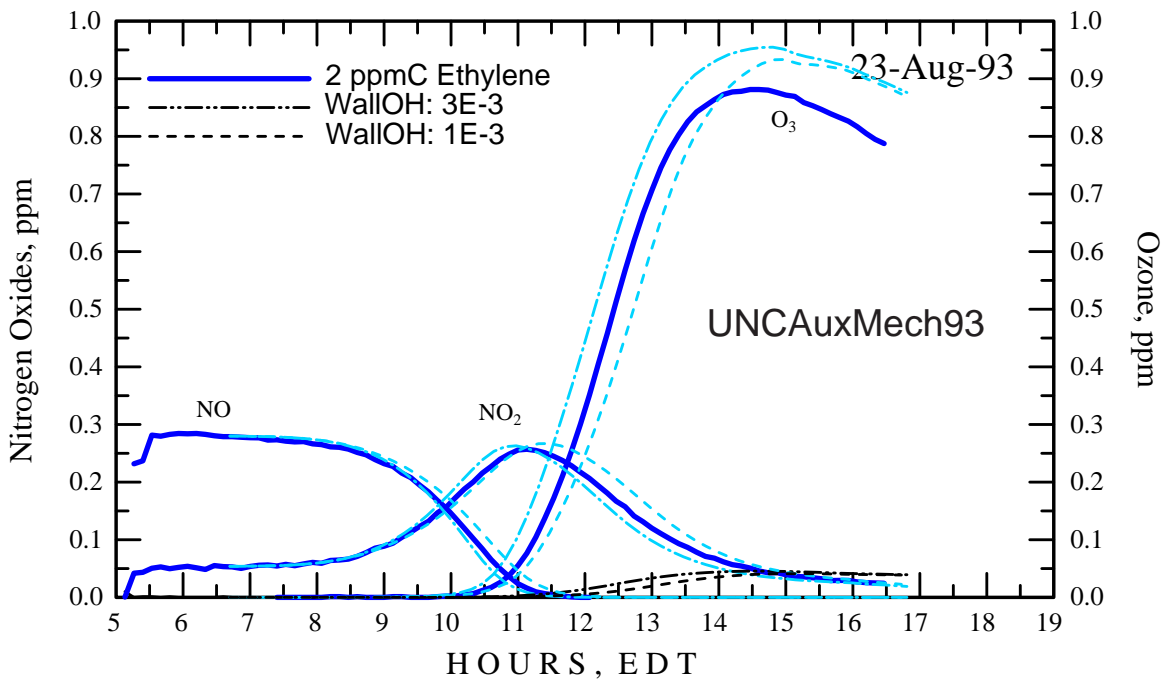
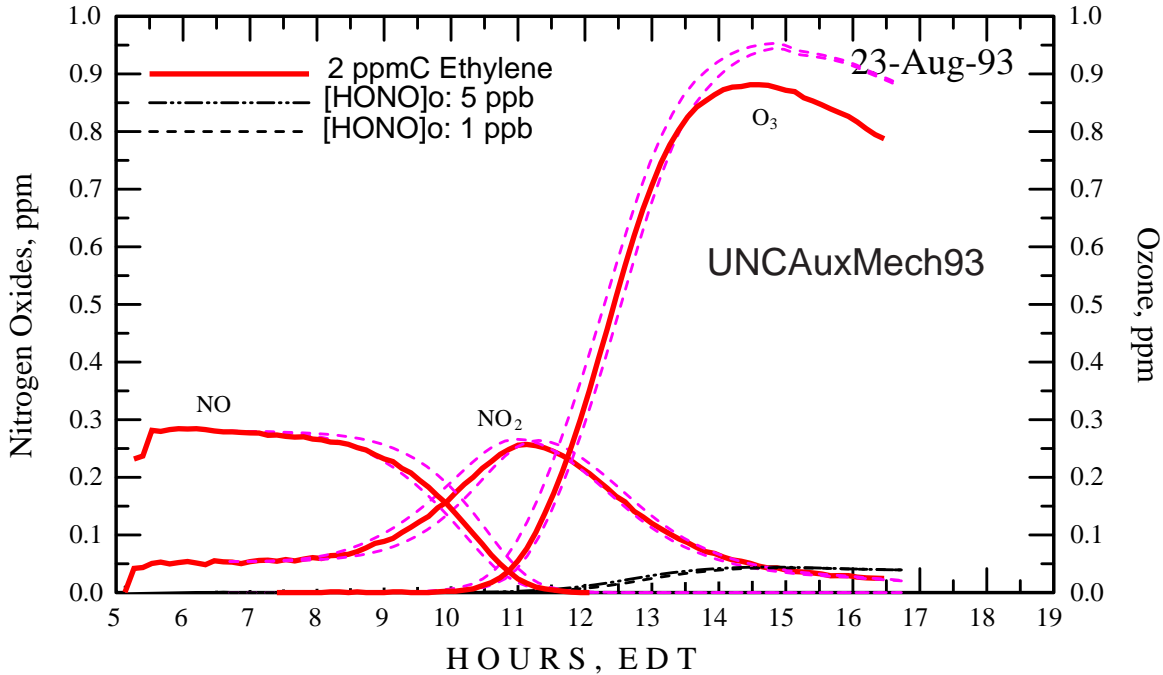
```
VARIABLES
```

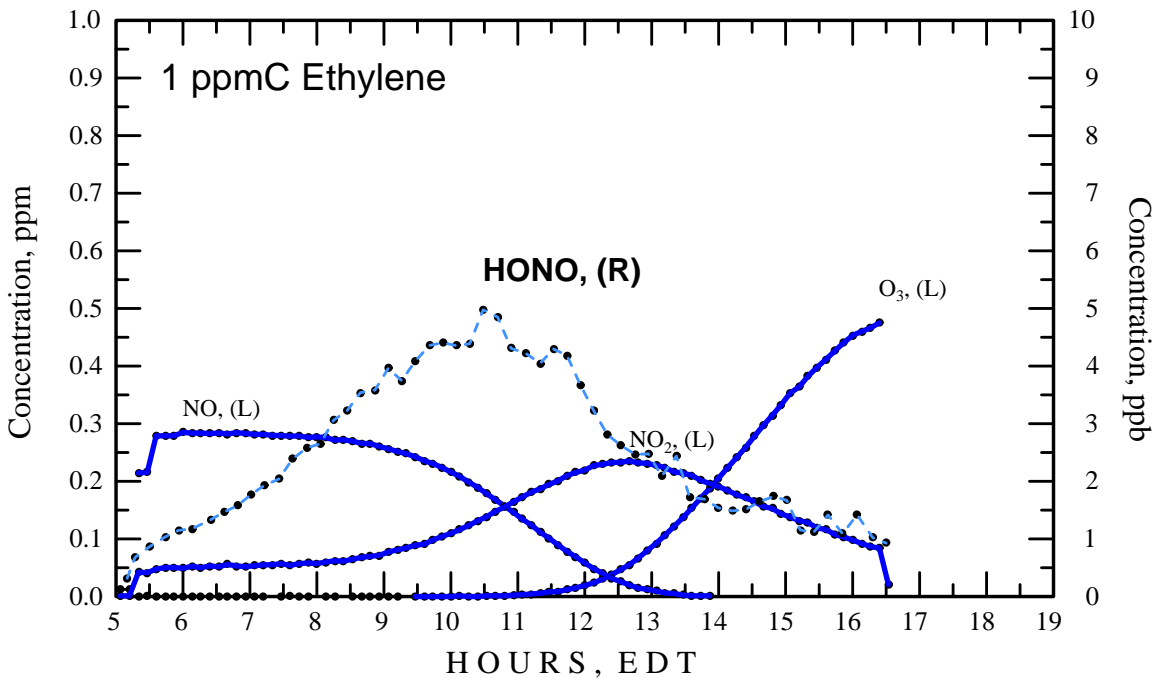
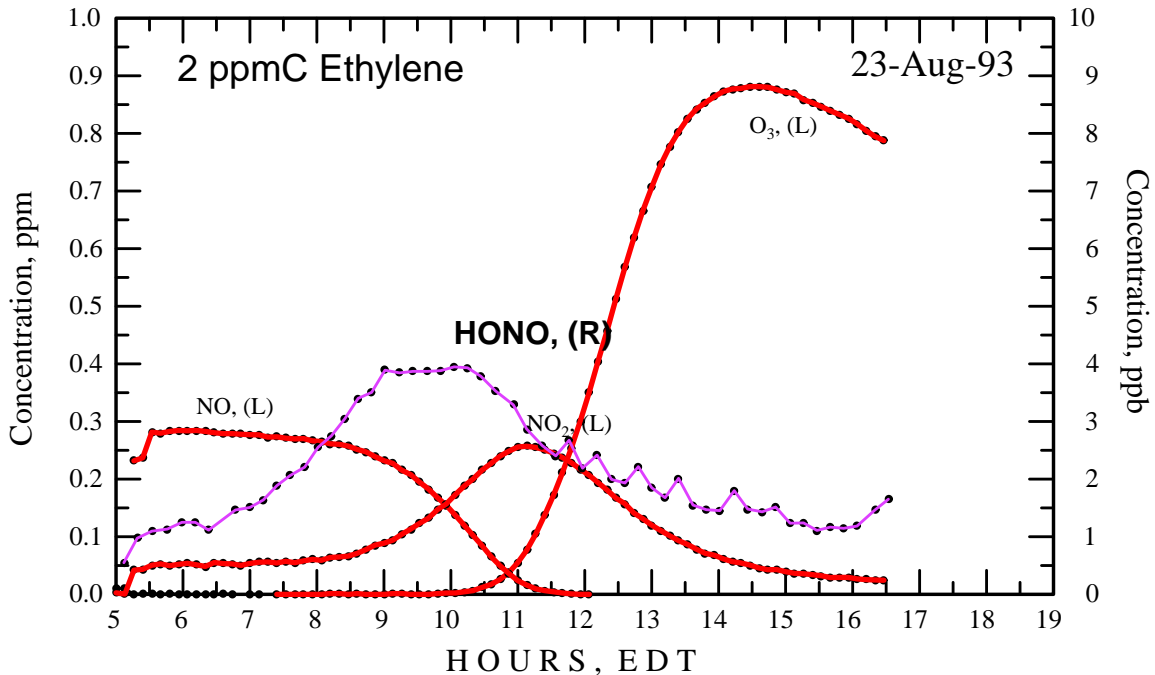
```
{
```

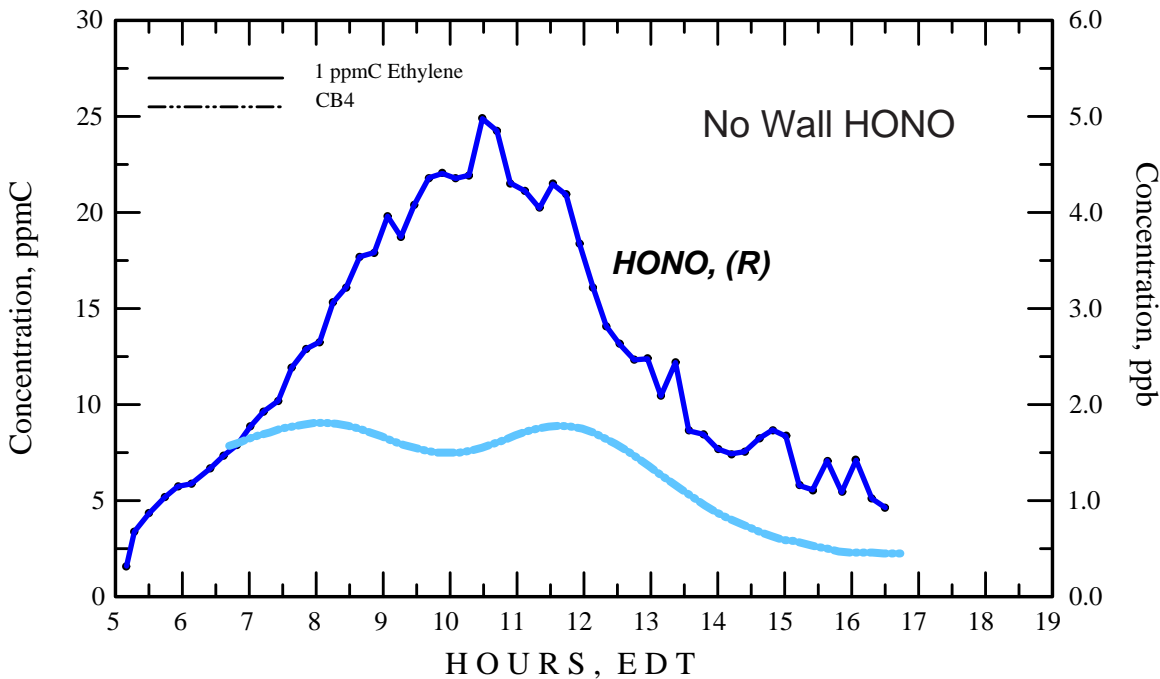
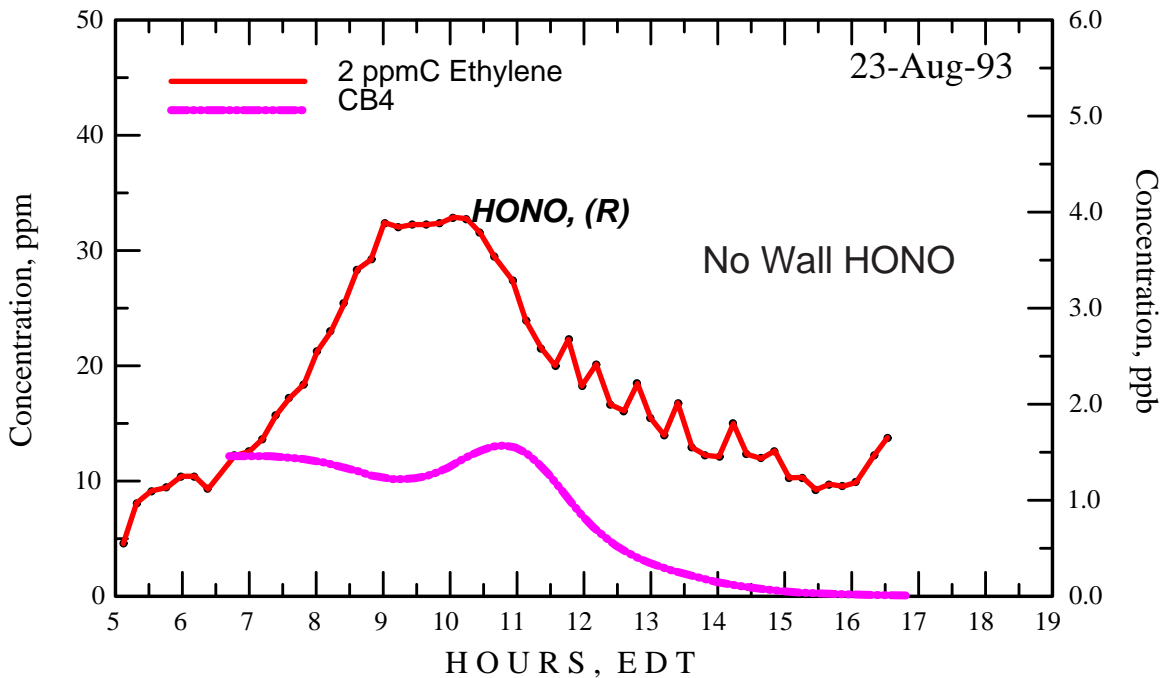
```
  sf_HONO_walI_src = 1.8E-3
```

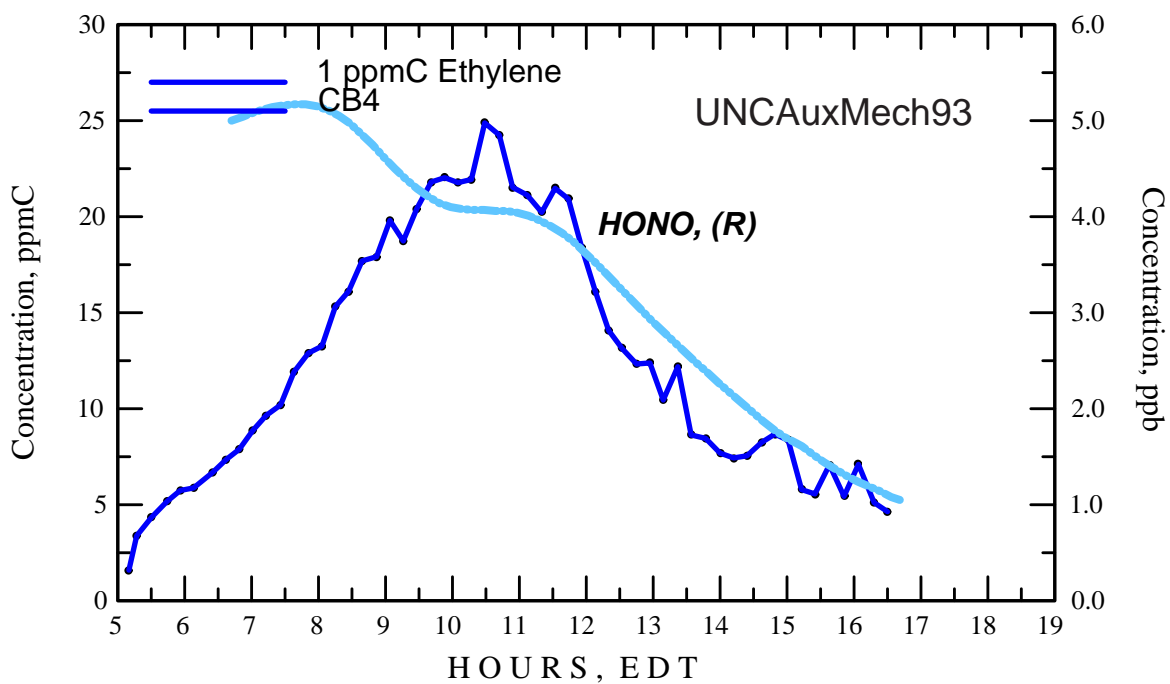
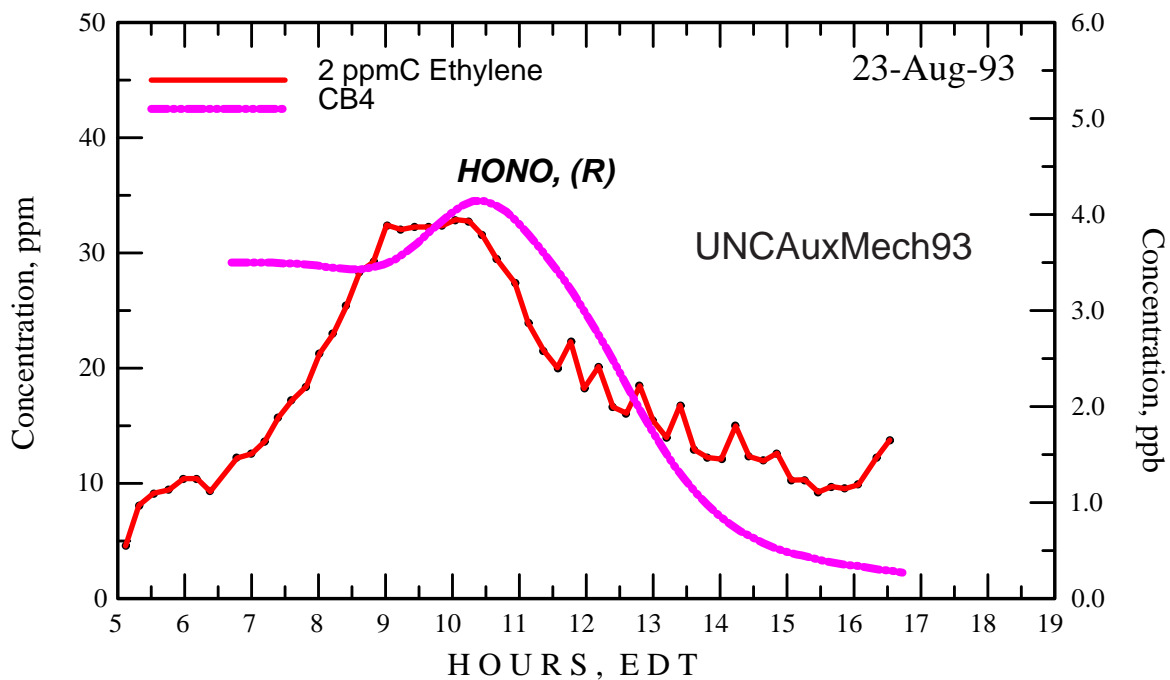
```
}
```

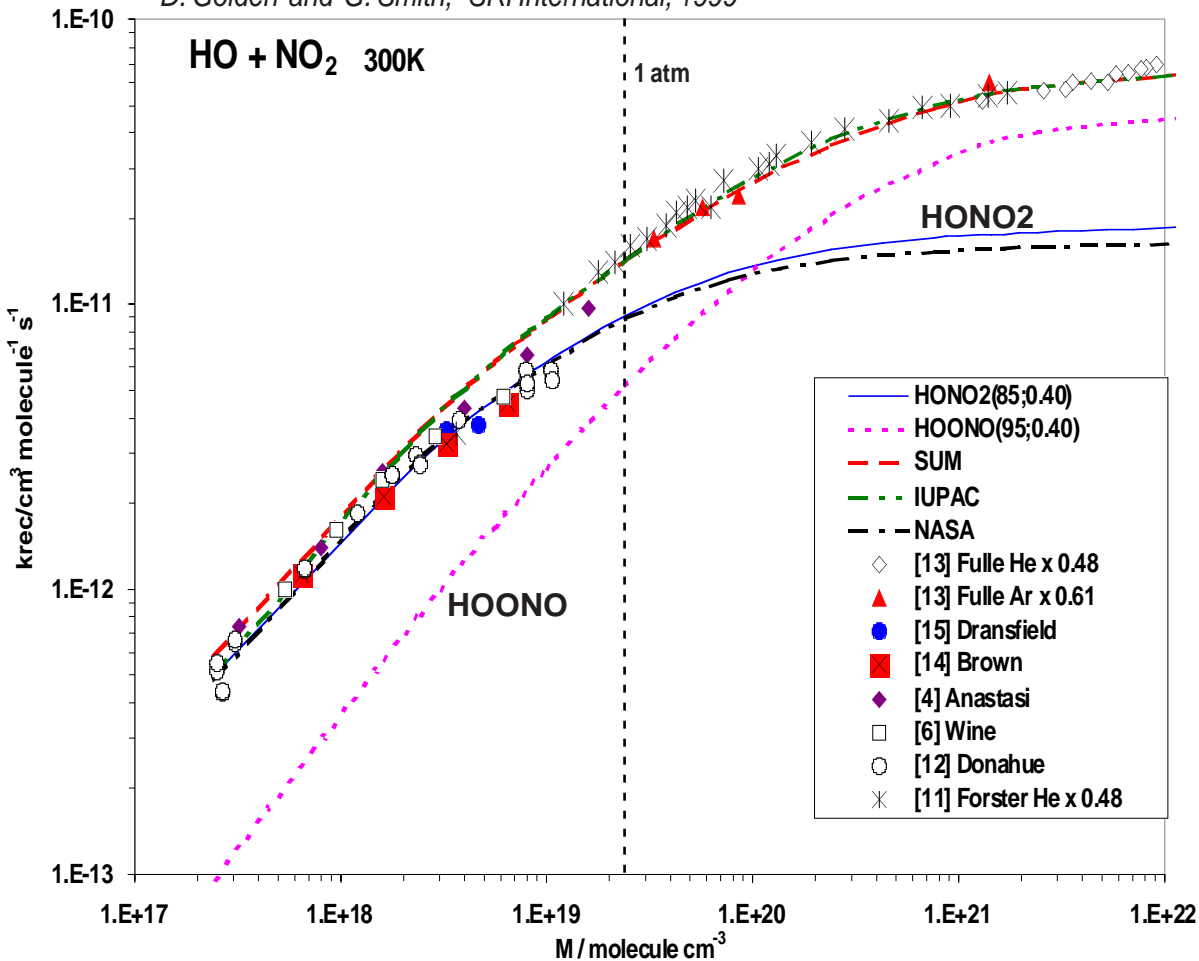












UNCAux99_03.react

```
// Ambient Air background (all runs)
```

```
INJECT
```

```
{  
  1790 PPB CH4  
  580 PPB H2  
}
```

```
// Seasonally variable Biogenic VOCs
```

```
INJECT
```

```
{  
  0.140 PPM BVOC  
}
```

```
// Initialize wall related species
```

```
INJECT
```

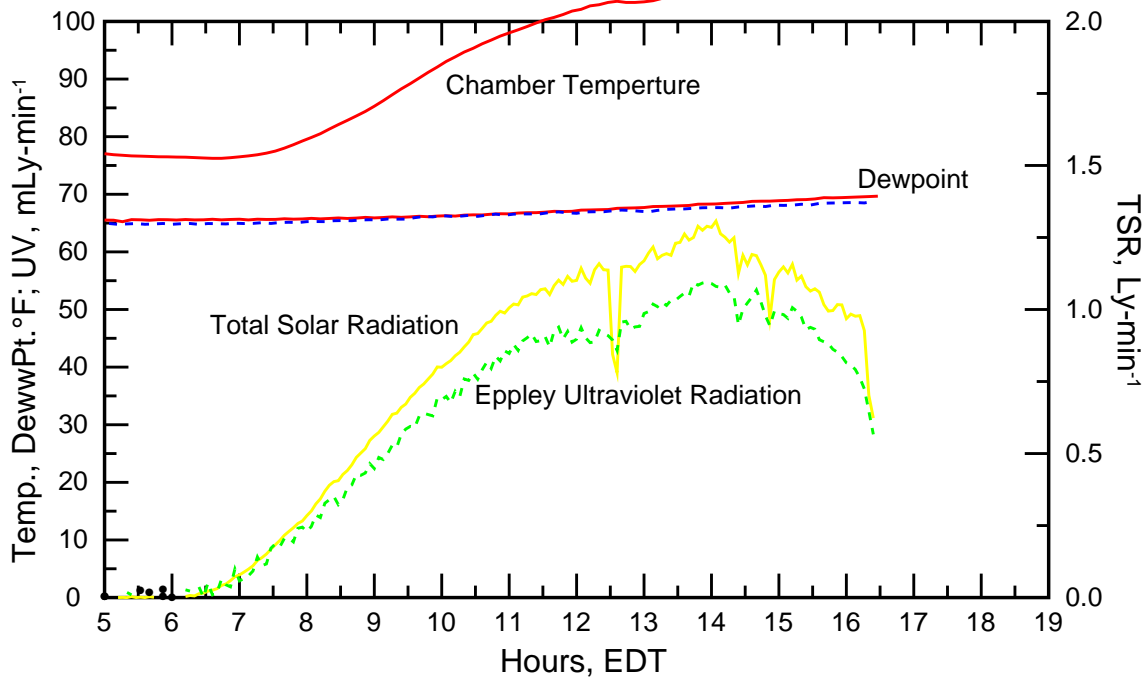
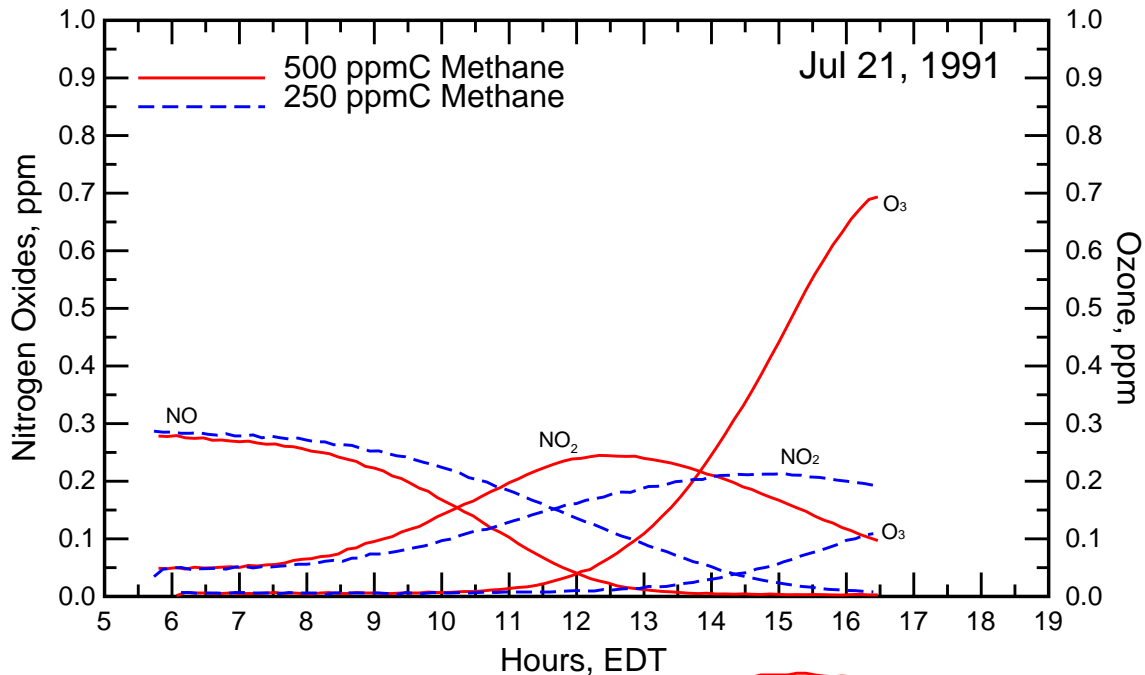
```
{  
  0.5 PPB HONO  
  4.0 PPB WHNO3  
}
```

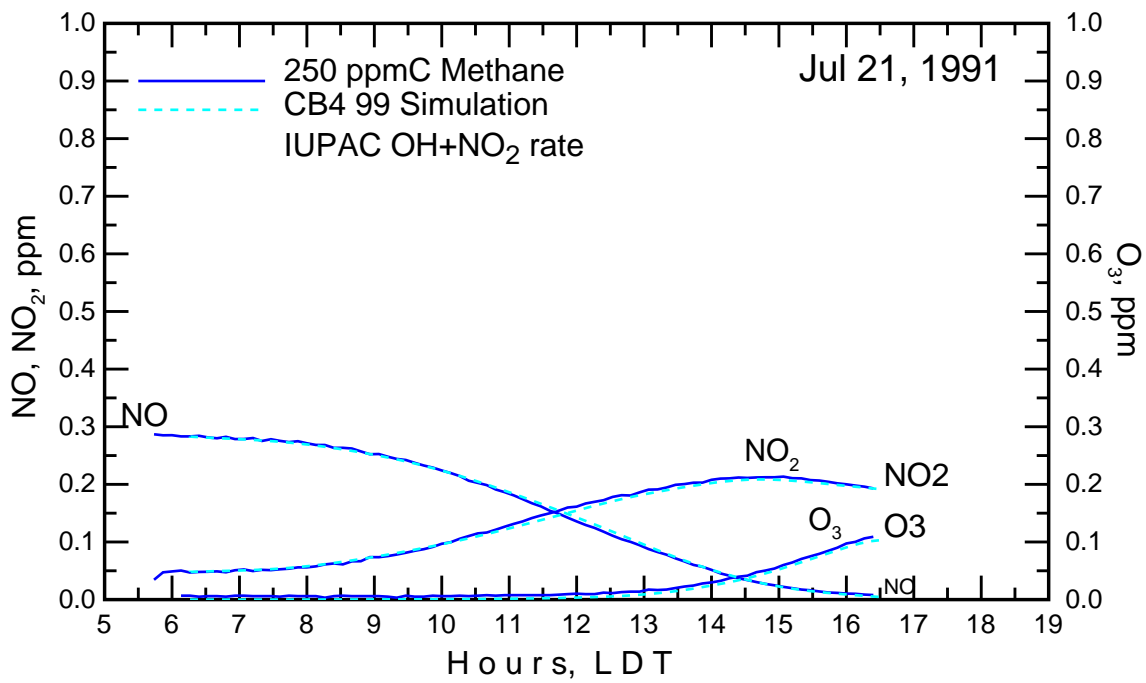
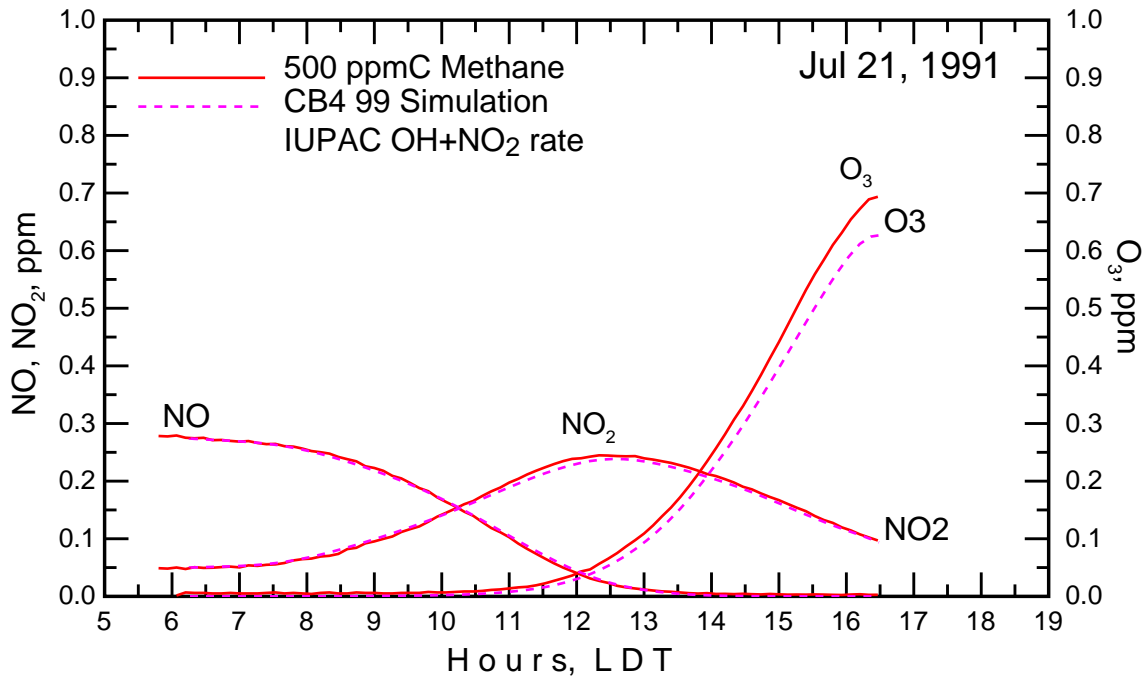
```
// set the wall conditions
```

```
// NO2 -hv--> HONO @ j[N02_to_03P] * sf_HONO_wall_src
```

```
VARIABLES
```

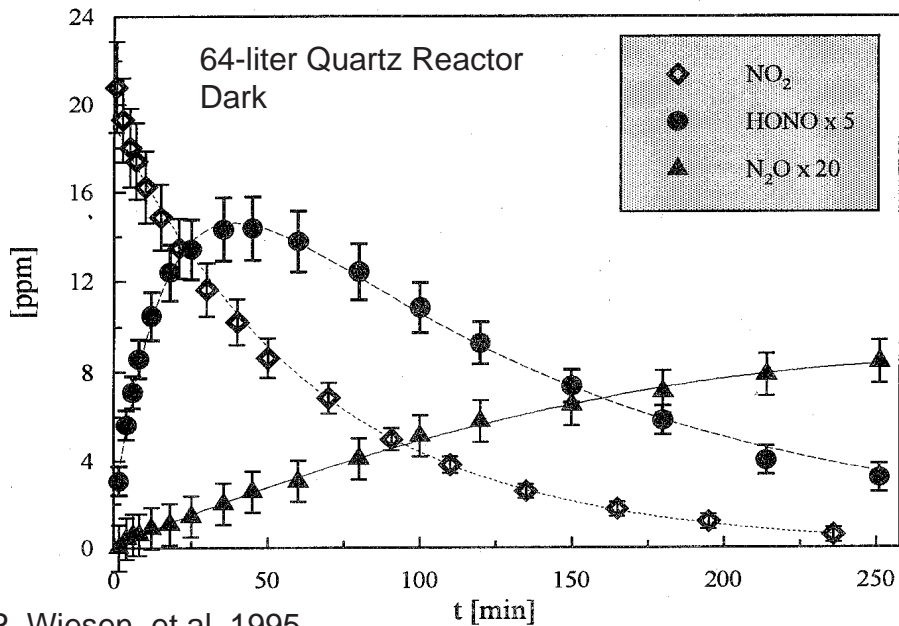
```
{  
  sf_HONO_wall_src = 0.8E-3  
}
```

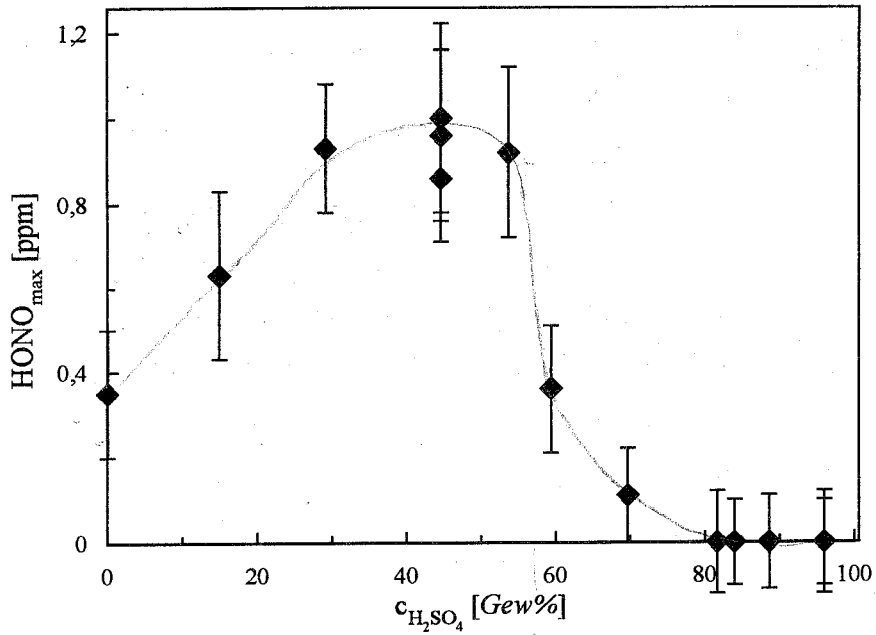


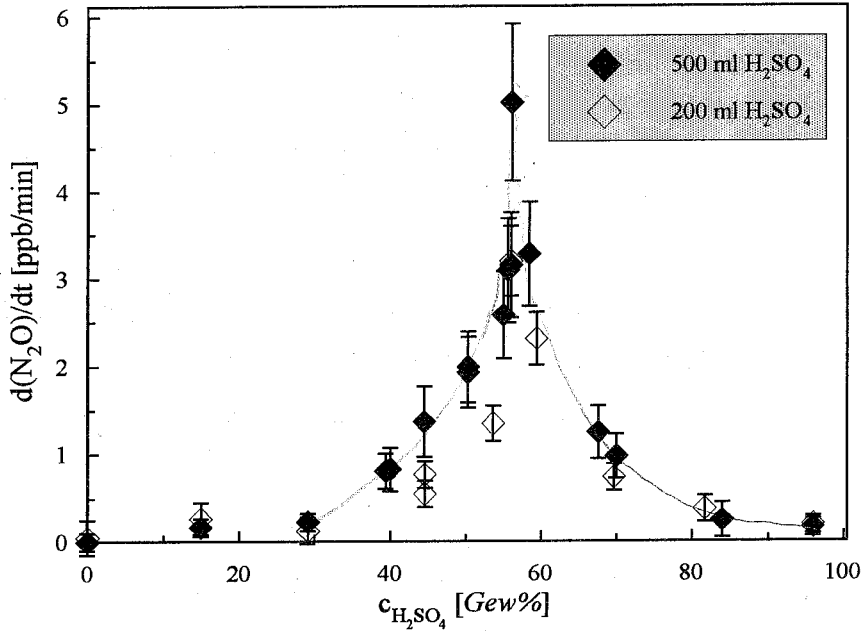


IUPAC OH+NO2 Rate

Initial	CH4	500 ppm	250 ppm	CH4	Reaction	613 MINS
Reaction	ppb	ppb	ppb	in		
I b7	2.96	0.14	0.14		N2O5+H2O----->	2.0*HN03
I c4	16.17	3.02	3.02		O1D+H2O----->	2.0*OH
I d3	41.22	67.75	67.75		OH+NO----->	HONO
I d4	137.82	170.32	170.32		HONO----->	OH+NO
I f1	216.69	154.08	154.08		OH+NO2----->	HN03
I g2	417.51	158.39	158.39		OH+CH4----->	XO2+HCHO+HO2
C1_4	108.67	35.16	35.16		OH+HCHO----->	HO2+CO
BVOC	37.36	29.48	29.48		OH+BVOC----->	0.667*(XO2+HCHO+HO2)+...
XO_1	443.78	182.71	182.71		XO2+NO----->	NO2
I e1	648.00	271.48	271.48		HO2+NO----->	OH+NO2
C1_1	54.31	26.11	26.11		HCHO-hv->	2.0*HO2+CO
DepoH2O2	2.67	0.00	0.00		H2O2----->	
DepoO3	11.57	2.24	2.24		O3-->	
DepoN2O5a	0.15	0.01	0.01		N2O5----->	2.0*WHNO3
DepoN2O5b	11.77	0.53	0.53		N2O5+WH2O----->	2.0*WHNO3
DepoHN03	154.46	106.04	106.04		HN03----->	WHNO3
WH2OpNO	2.19	2.50	2.50		NO+WH2O----->	WHNO3
WH2OpNO2	1.51	1.26	1.26		NO2+WH2O----->	WHNO3
WHNO3pNO	31.92	48.53	48.53		NO+WHNO3----->	1.5*HONO+0.5*NO2
WHNO3pNO2	12.75	6.64	6.64		NO2+WHNO3----->	1.5*HONO+0.5*NO2
WNO2hvHONO	32.67	25.77	25.77		NO2-hv->	HONO

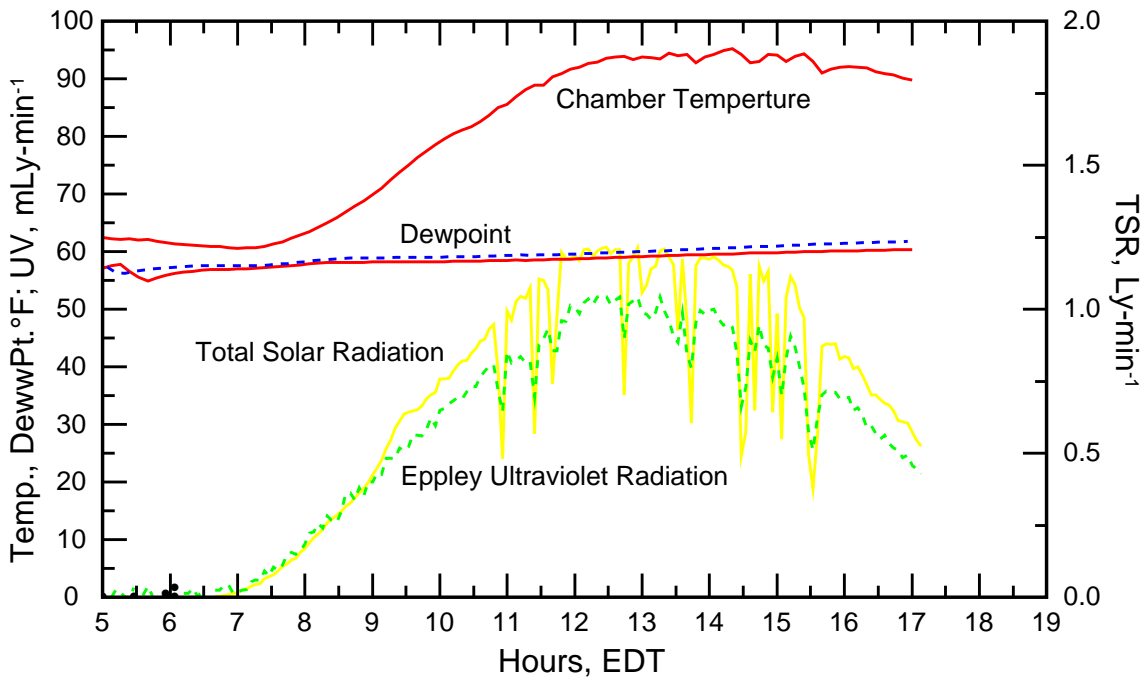
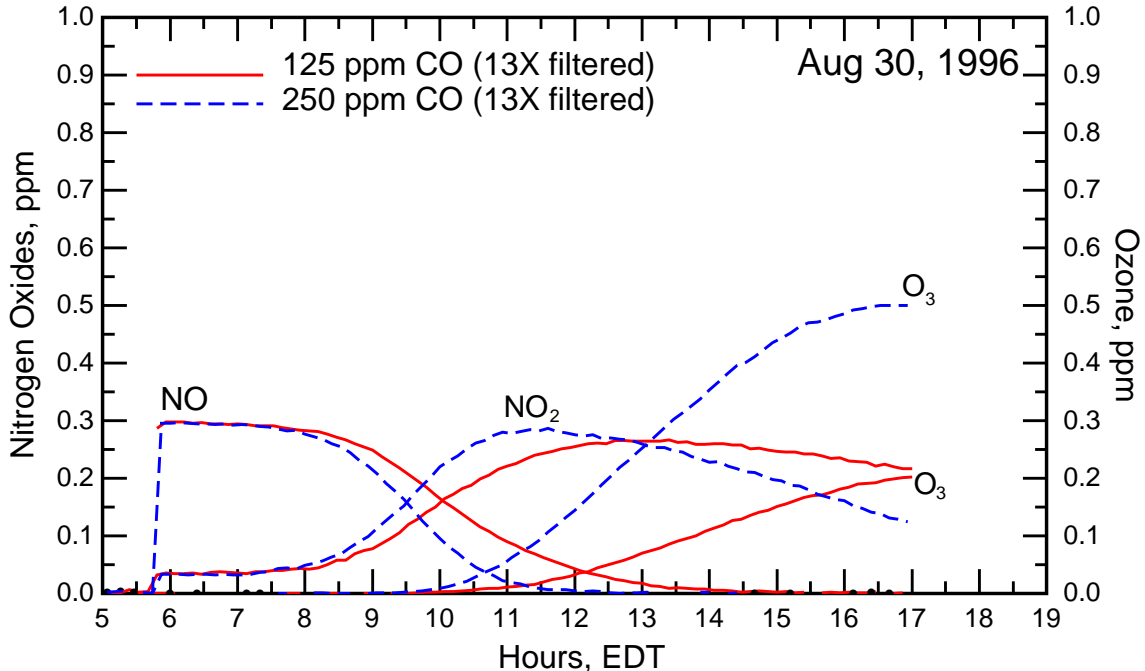


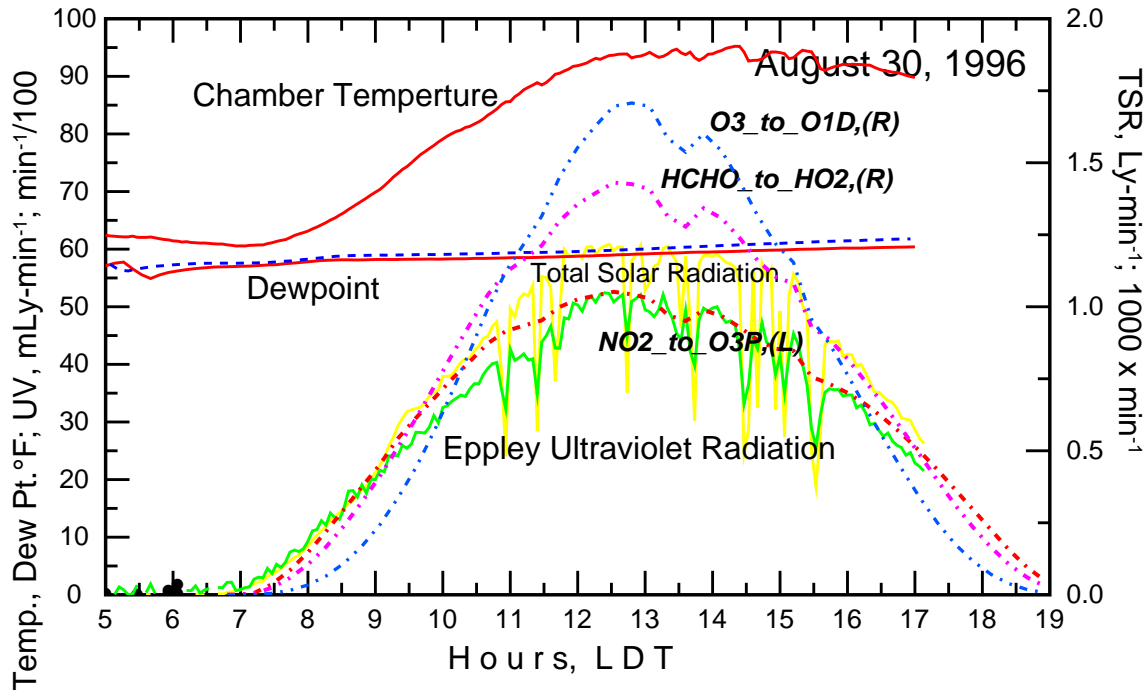


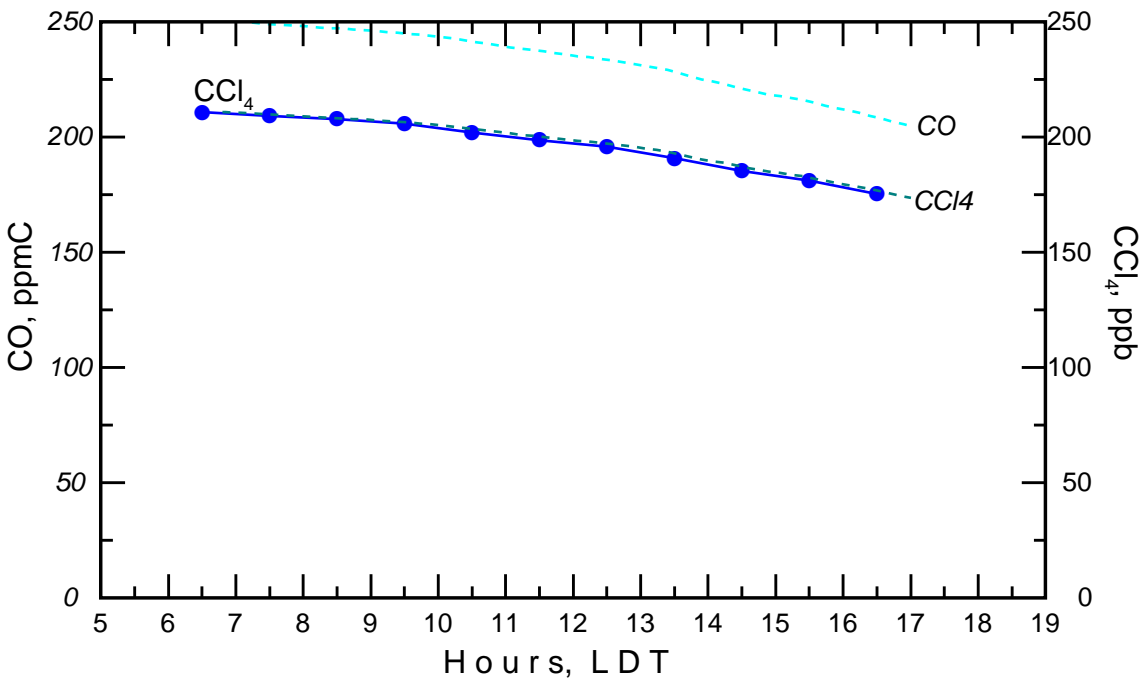
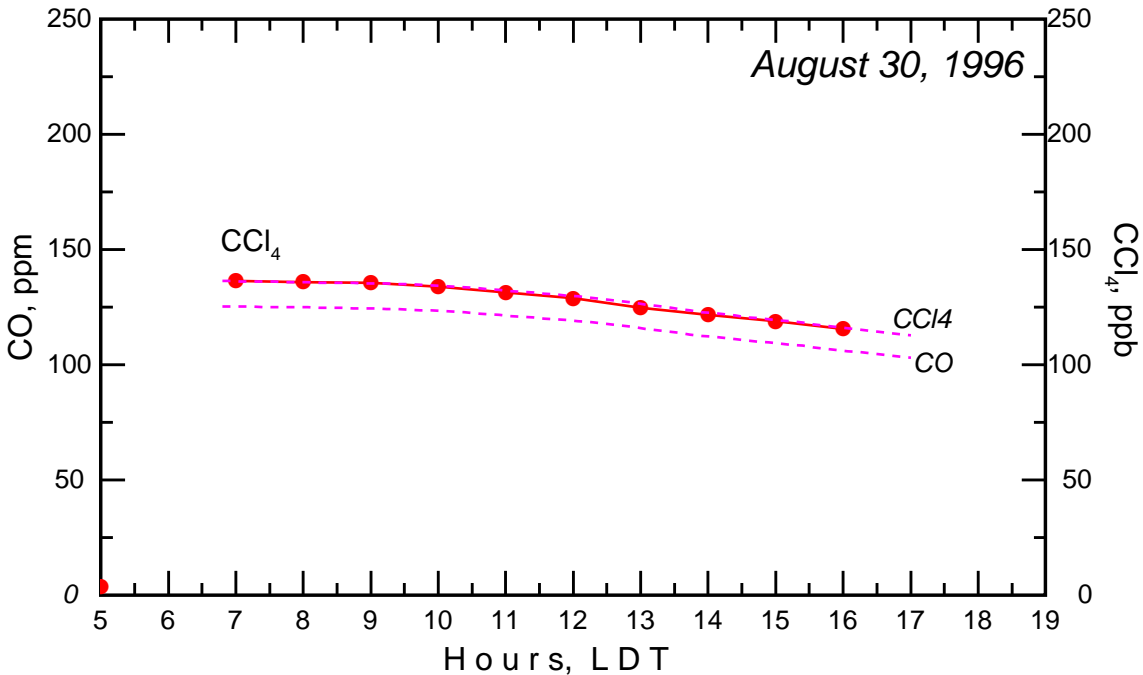


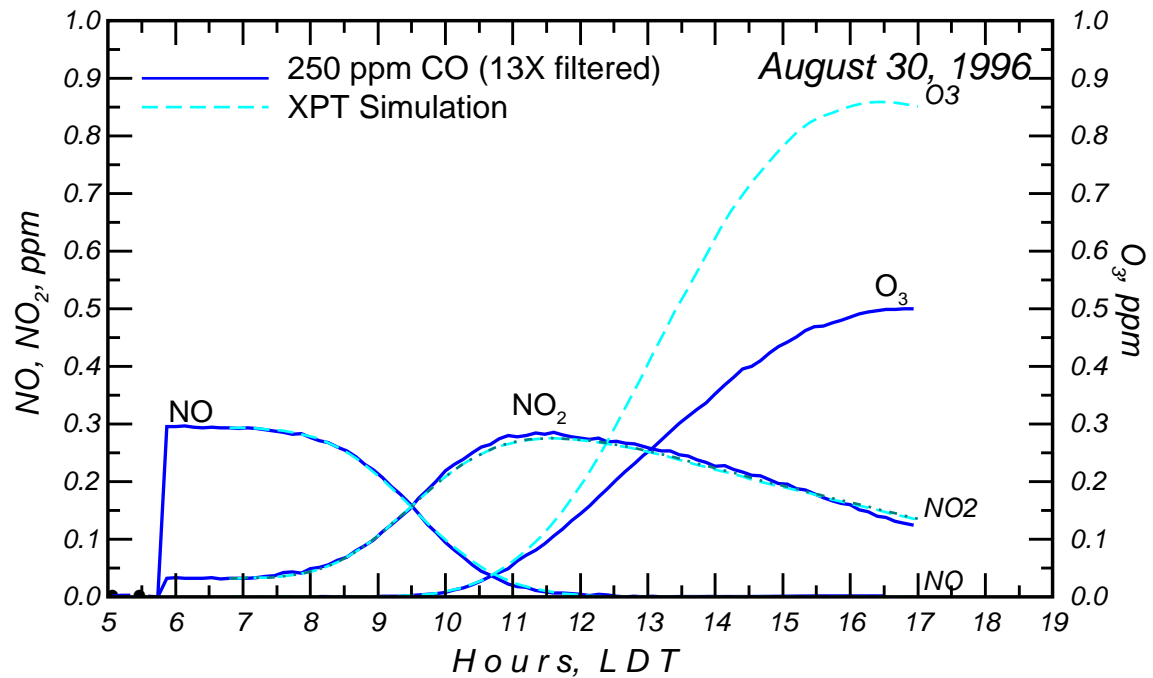
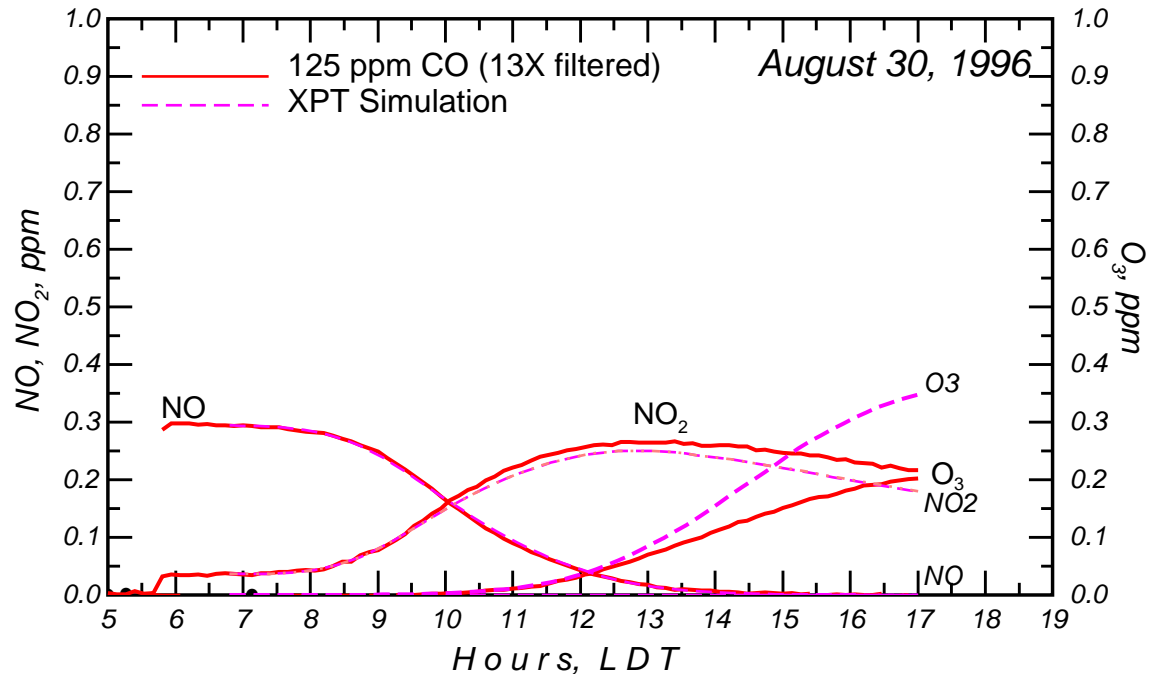
UNCAuxMech99_09.rxn

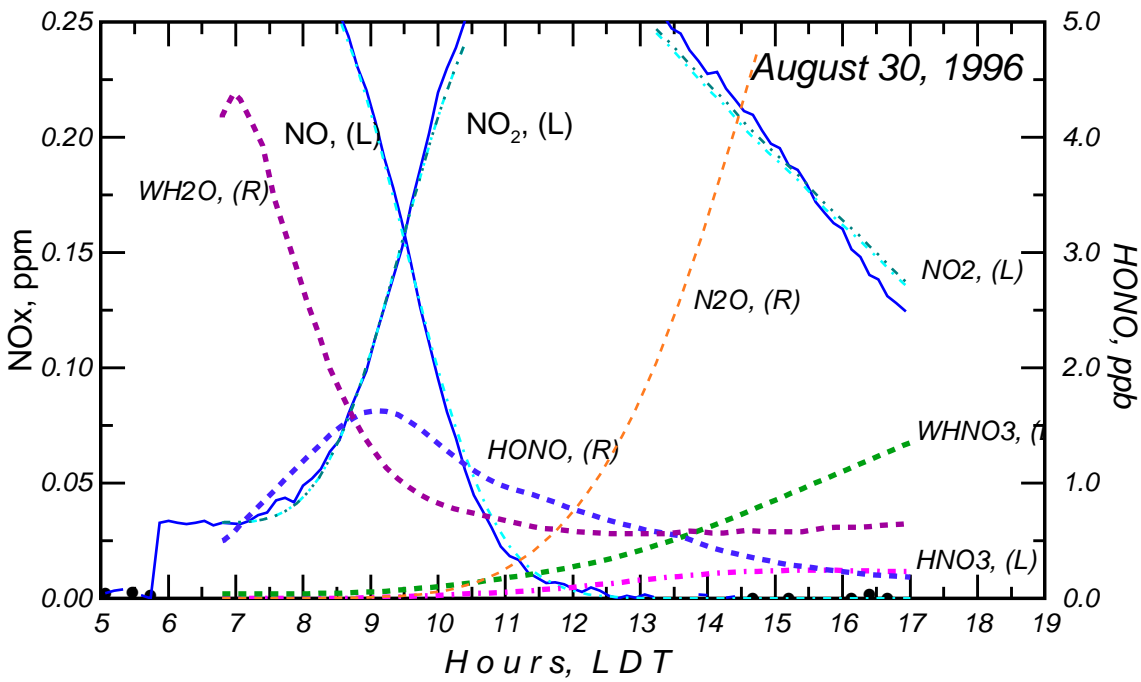
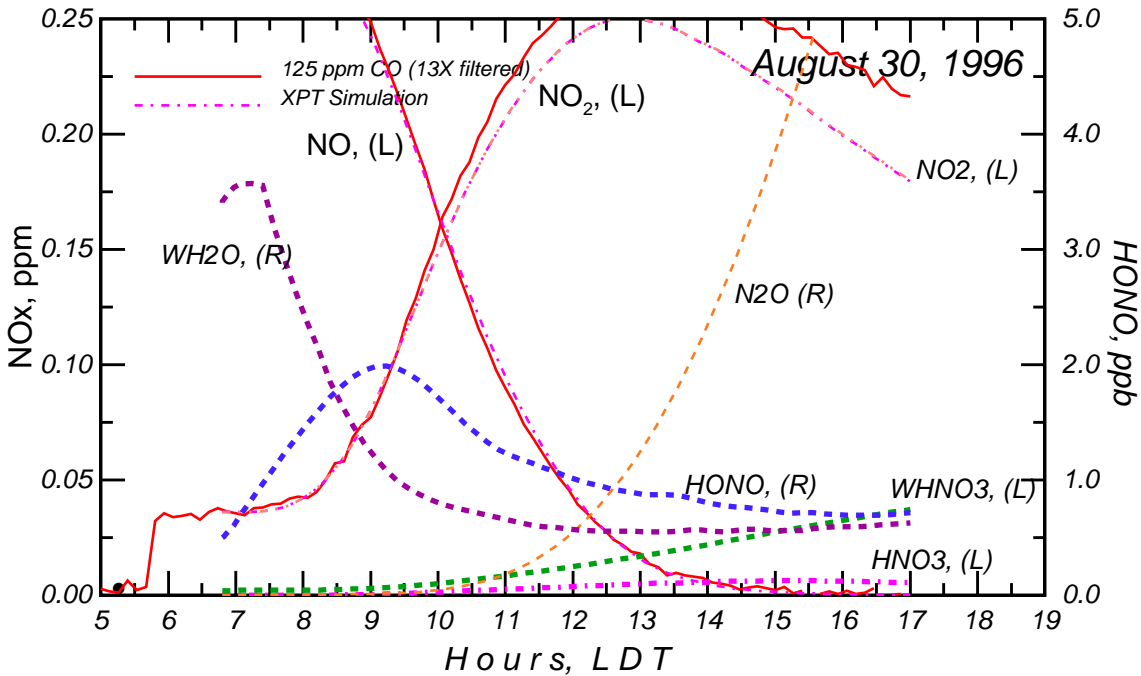
```
// =====  
//                                     H2O2 and O3 wall deposition  
//  
SCALAR  
k_depo_H2O2 = 6.7E-4, // measured loss rate, 1/sec  
k_depo_O3   = 2.3E-6; // measured loss rate, 1/sec (EUPHORE 3.0E-6 /sec)  
  
R[DepoH2O2] = H2O2 -----> @ k_depo_H2O2 ;  
R[DepoO3 ]  = O3 -----> @ k_depo_O3 ;  
  
// =====  
//                                     N2O5 wall deposition and hydrolysis  
// rate is based on Julich Chamber; here 5E-5 /s * WH2O  
  
R[DepoN2O5] = N2O5 + WH2O -----> 2.0 * WHNO3 @ 3.05E-21 ;  
  
// =====  
//                                     HNO3 wall deposition and emission  
// EUPHORE first order dry rate was 8.2E-5 /sec  
  
R[DepoHNO3f] = HNO3 + WH2O -----> WHNO3 @ 2.6E-18 ;  
R[DepoHNO3r] = WHNO3 -----> HNO3 @ 6.6E-7 ;  
R[DepoHNO3l] = WHNO3 -----> @ 3.0E-7 ;  
  
// =====  
//                                     HONO wall deposition and emission  
//  
R[DepoHONOf] = HONO + WH2O -----> WHONO @ 8.9E-21 ;  
R[DepoHONOr] = WHONO -----> HONO @ 6.6E-4 ;  
  
// =====  
//                                     NO2 wall water reactions  
//  
R[DepoNO2f ] = NO2 + H2O -----> WN02 @ 2.5E-23 ;  
R[DepoNO2r ] = WN02 -----> NO2 @ 6.6E-7 ;  
  
R[WN02pWN02] = WN02 + WN02 -----> WN2O4 @ 1.0E-10 ;  
R[WH2OpWN2O4] = WN2O4 + WH2O -----> WHONO + WHNO3 @ 1.0E-14 ;  
  
// =====  
//                                     WN02 acid reactions  
//  
R[WN02pWHNO3 ] = WN02 + WHNO3 -----> 'W(NO2)NO3' + WH2O @ 1.0E-12 ;  
R[WN02pWHNO2P] = WN02 + 'W(NO2)NO3' -----> WHONO + WHNO3 @ 1.0E-9 ;  
R[WHNO2PpWHNO2P] = 'W(NO2)NO3' + 'W(NO2)NO3' -----> 2.0*(WHONO + WHNO3) @ 1.0E-14 ;  
  
// =====  
//                                     WHONO acid reactions  
//  
R[WHONOpWHNO3a] = WHONO + WHNO3 + WHNO3 -----> N2O + WHNO3 @ 1.0E-26 ;
```

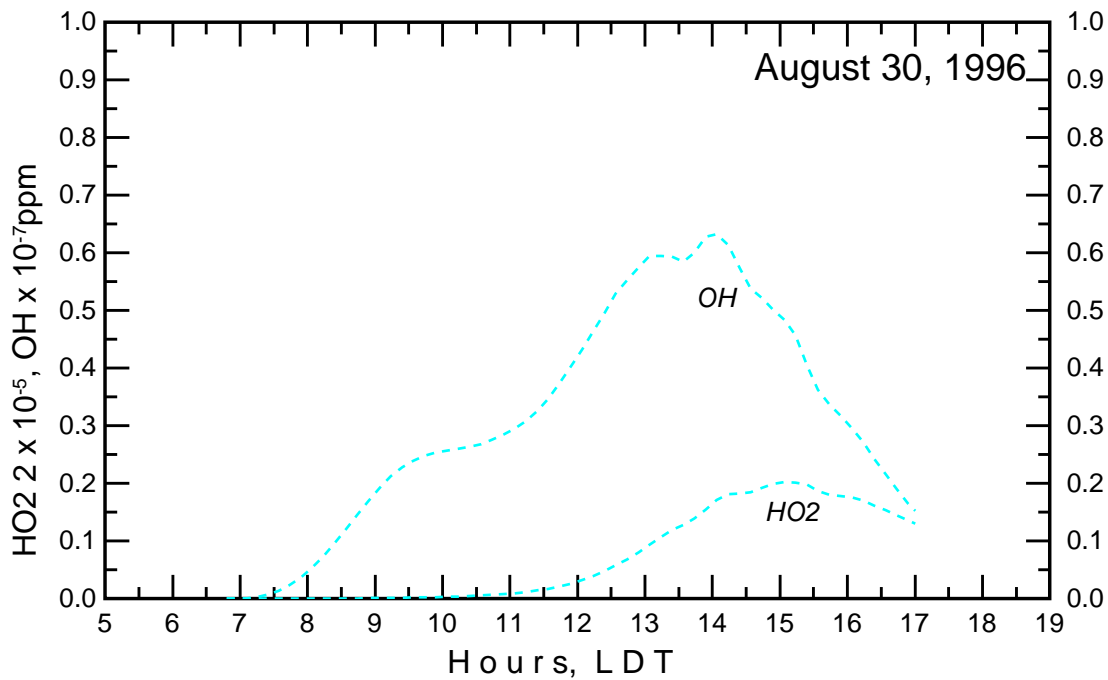
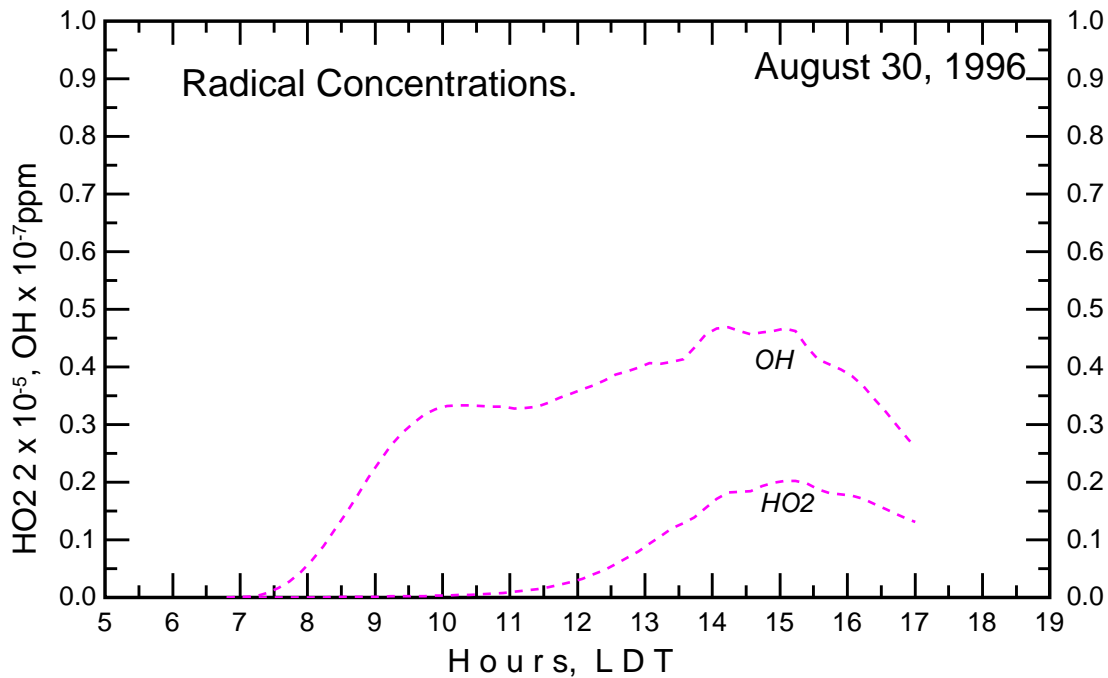






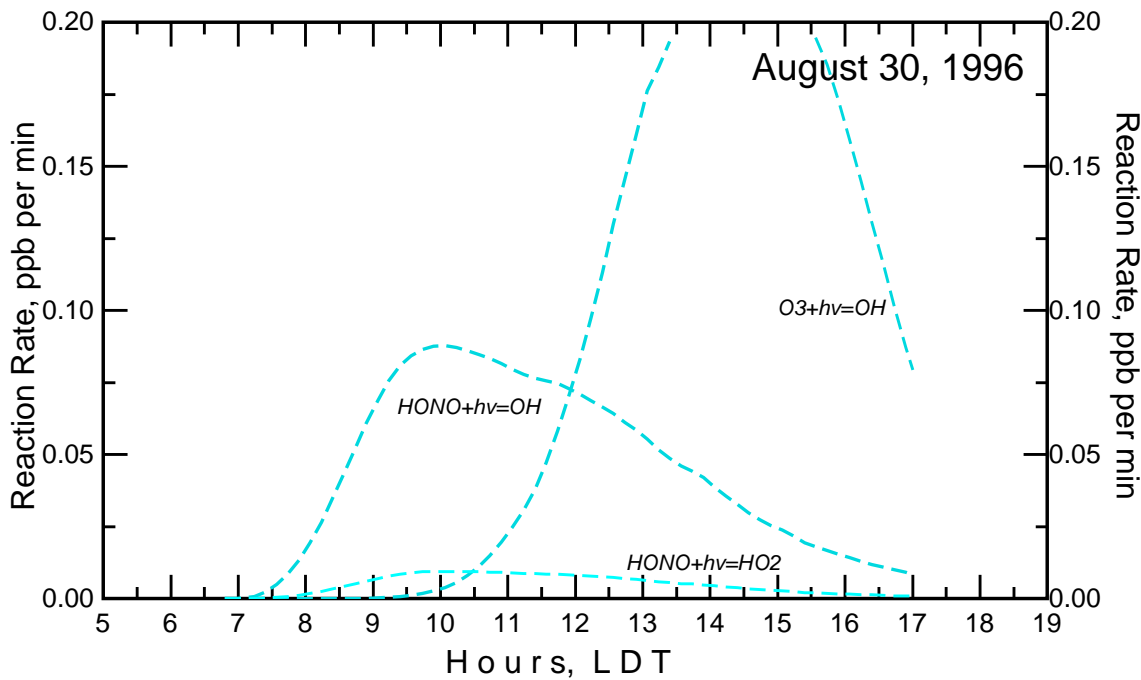
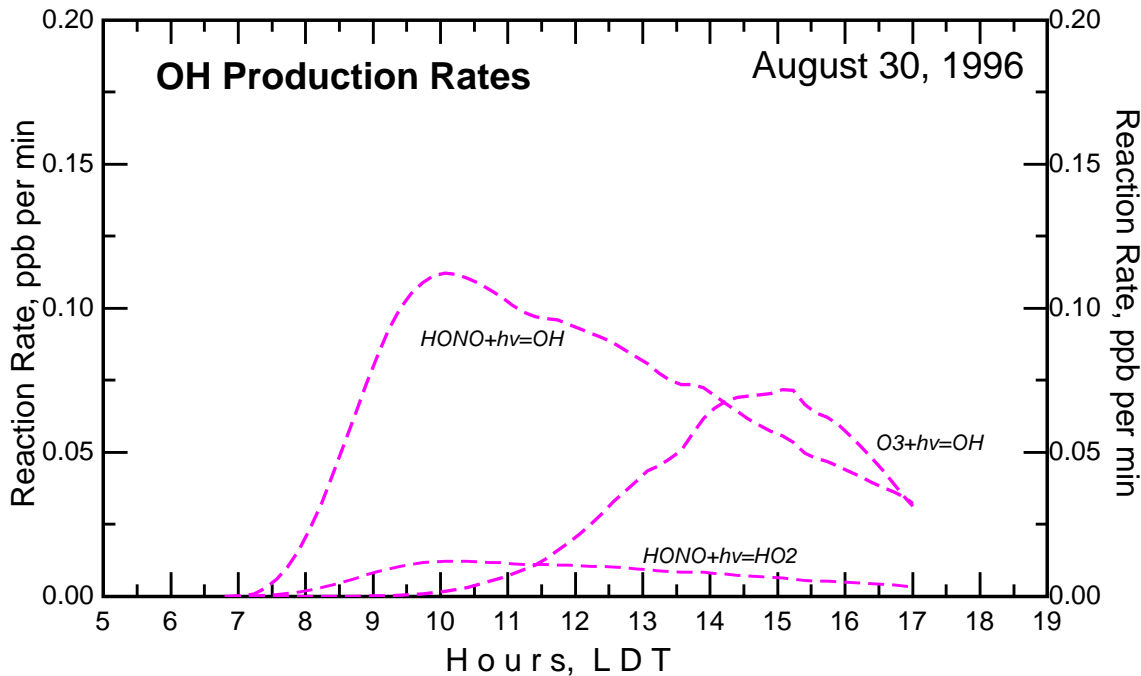


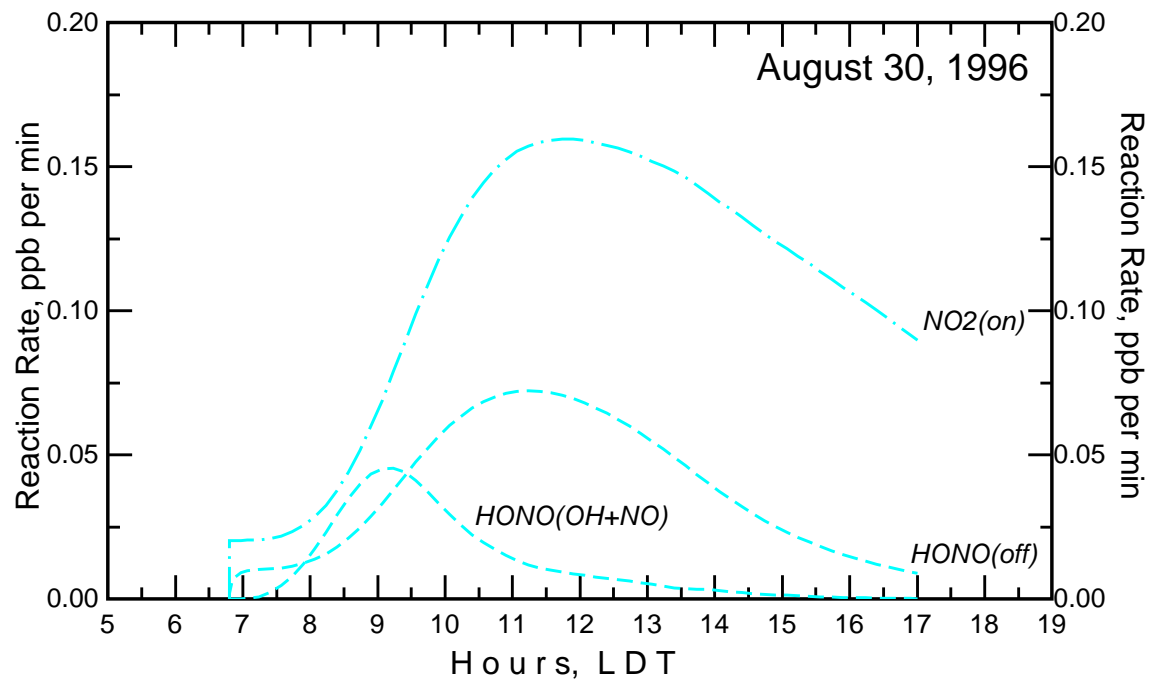
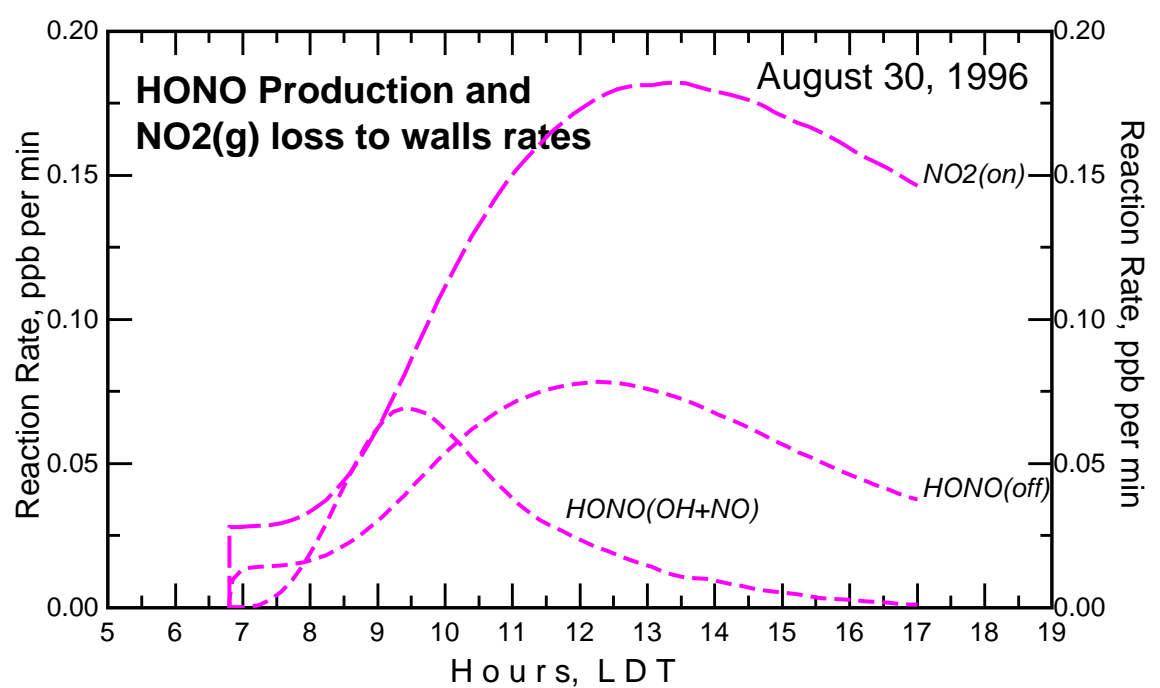


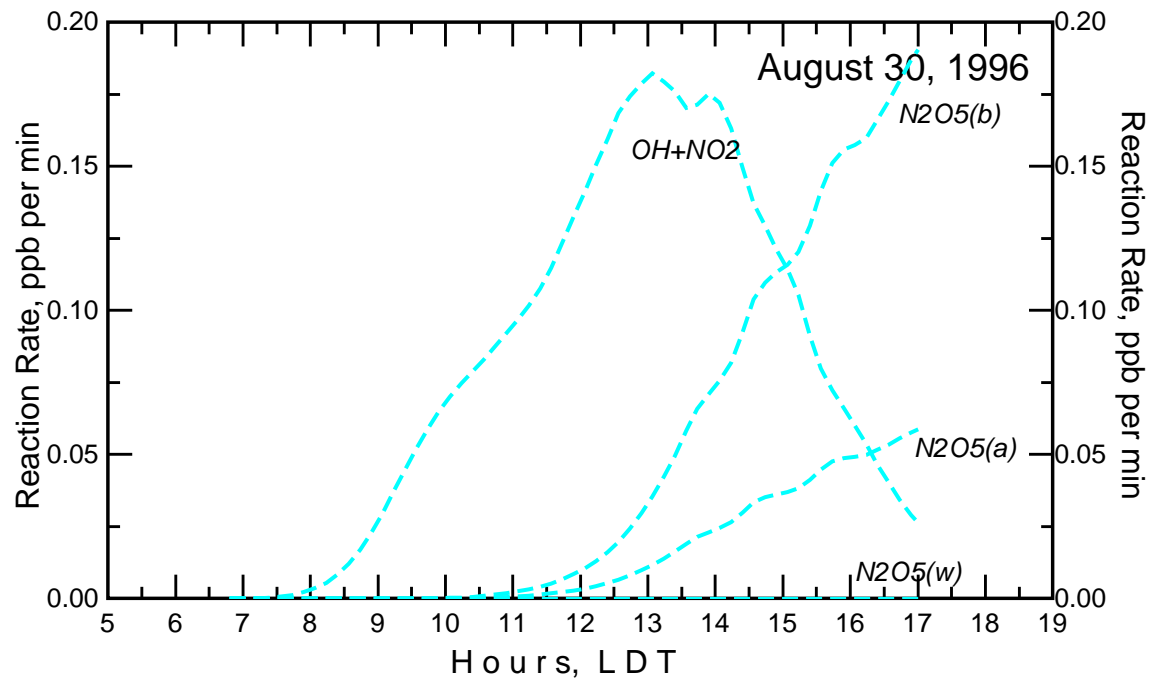
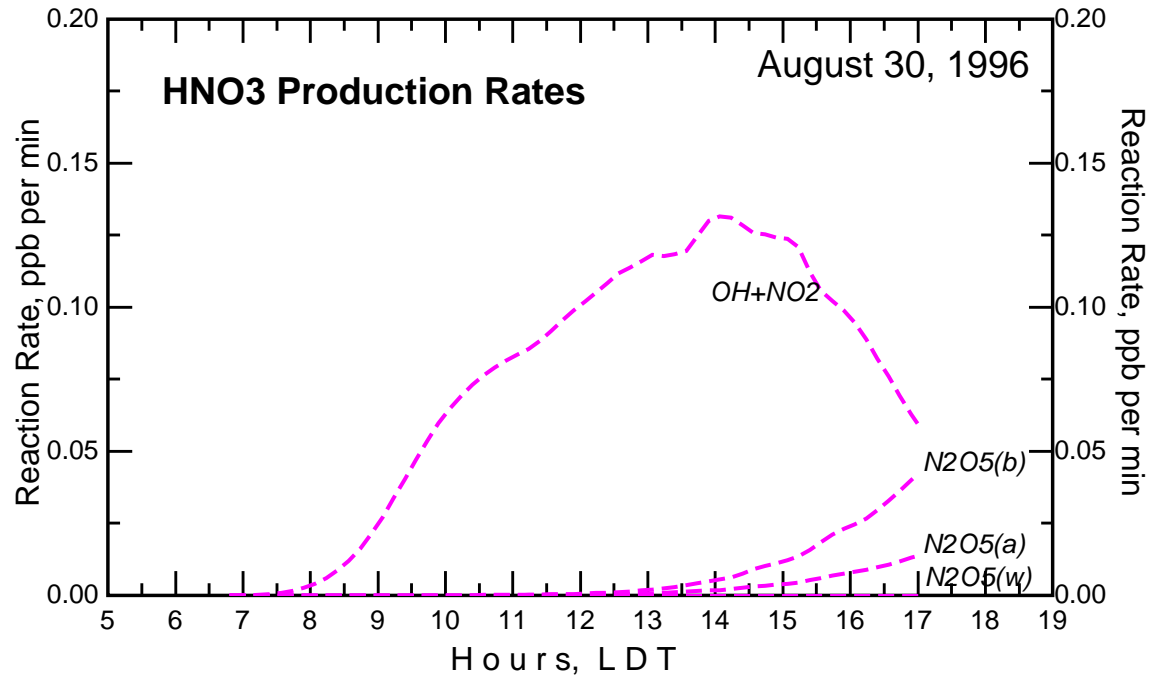


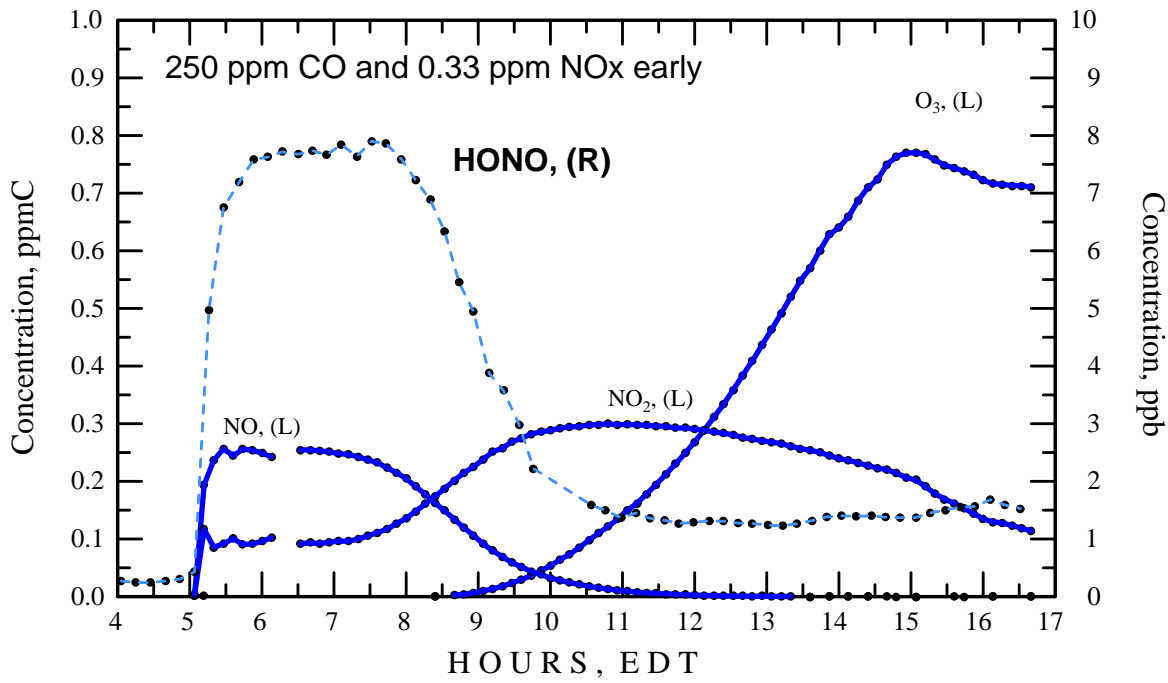
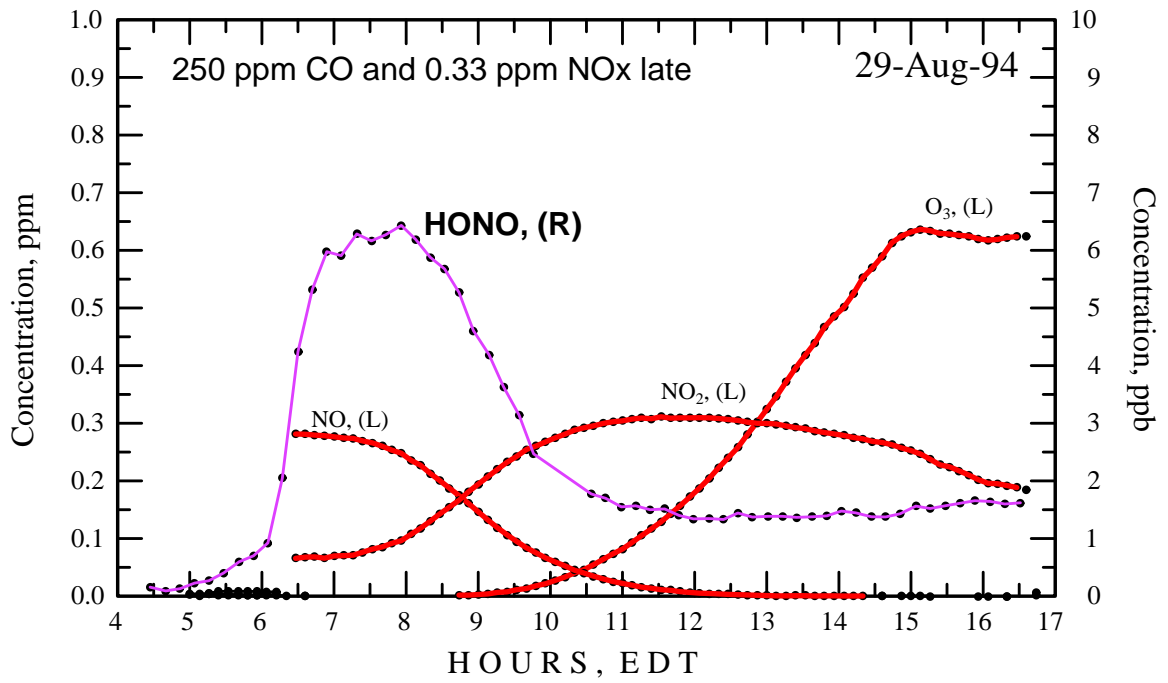
OH Production Rates

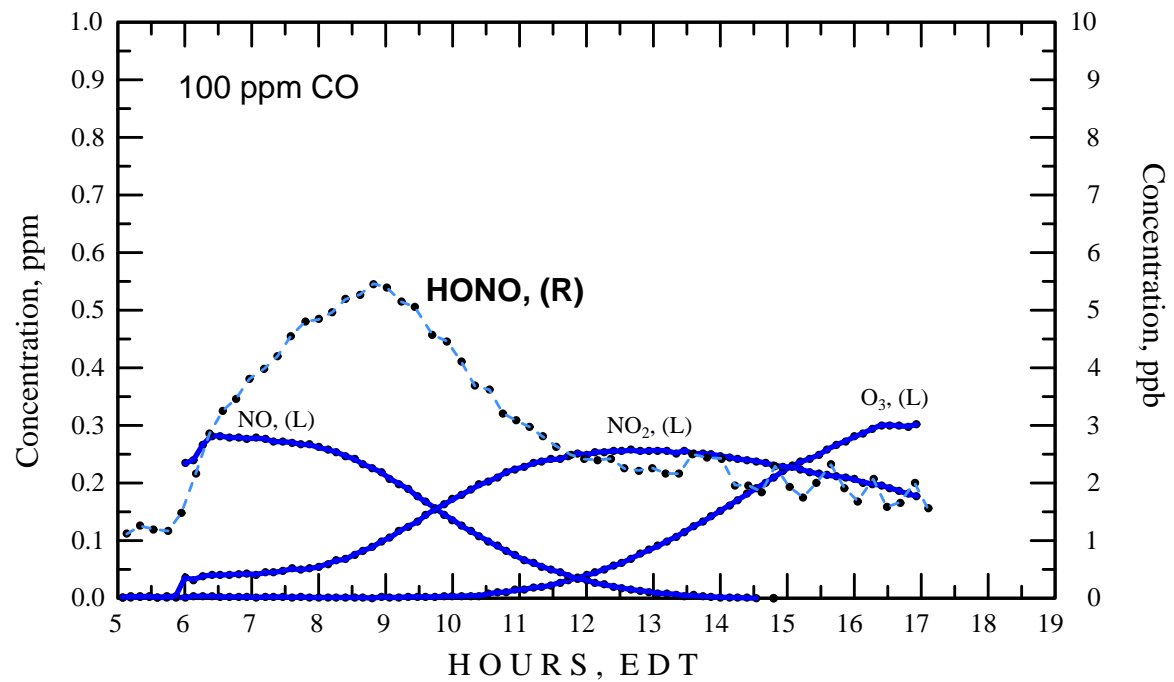
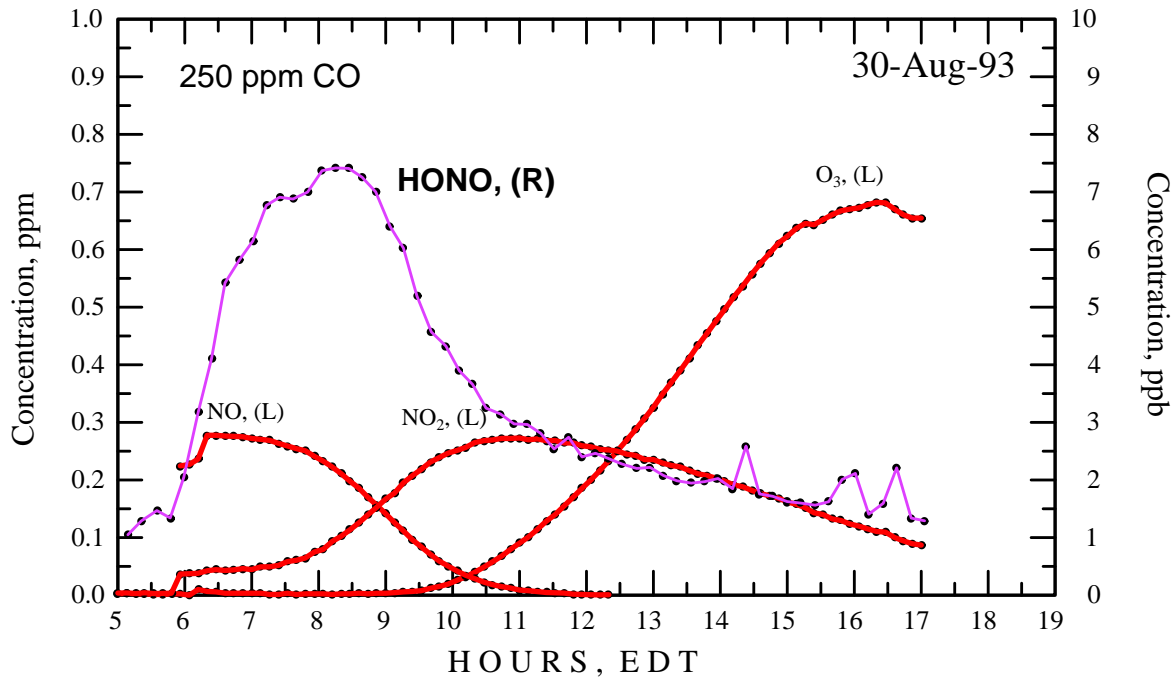
August 30, 1996











Explicit Mechanism with UNCAuxMech99_09 AU3096

NASA97* OH + NO2 Rate

Initial CO	RED	BLUE	
	125 ppm	250 ppm	
	ppb	ppb	in 612 MINS
lc6a	0.62	4.57	N2O5+H2O---->2.0*HNO3
lc6b	1.87	14.41	N2O5+H2O+H2O---->2.0*HNO3+H2O
lb4	8.32	28.49	O1D+H2O---->2.0*OH
ld3	14.49	7.62	OH+NO---->HONO
ld5a	40.86	28.00	HONO---->OH+NO
ld5b	4.52	3.09	HONO---->HO2+NO2
lf1a	46.12	52.11	OH+NO2---->HNO3
lf1b	27.68	31.25	OH+NO2---->HOONO
lf1c	27.67	31.25	HOONO---->OH+NO2
lf2	0.00	0.00	OH+HOONO- ->NO+H2O+O2
lh1	754.29	1552.75	OH+CO---->HO2+CO2
le1	756.38	1486.59	HO2+NO---->OH+NO2
DepoN2O5	0.00	0.02	N2O5+WH2O---->2.0*WHNO3
DepoHNO3f	45.07	79.10	HNO3+WH2O---->WHNO3
DepoHONO r	31.54	23.46	WHONO---->HONO
DepoNO2f	79.10	66.87	NO2+H2O---->WN02
WN02pWN02	1.72	1.49	WN02+WN02---->WN2O4
WH2OpWN2O4	1.72	1.49	WN2O4+WH2O---->WHONO+WHNO3
WN02pWHNO3	37.86	31.98	WN02+WHNO3---->W(NO2)NO3+WH2O
WN02pWHNO2P	37.82	31.90	WN02+W(NO2)NO3---->WHONO+WHNO3
WHNO2PpWHNO2P	0.00	0.01	W(NO2)NO3+W(NO2)NO3---->2.0*(WHONO+WHNO3)
WHONOpWHNO3a	7.85	9.89	WHONO+WHNO3+WHNO3---->N2O+WHNO3