A Steady State Continuous Flow Chamber for the Study of Daytime and Nighttime Chemistry under Atmospherically Relevant NO levels

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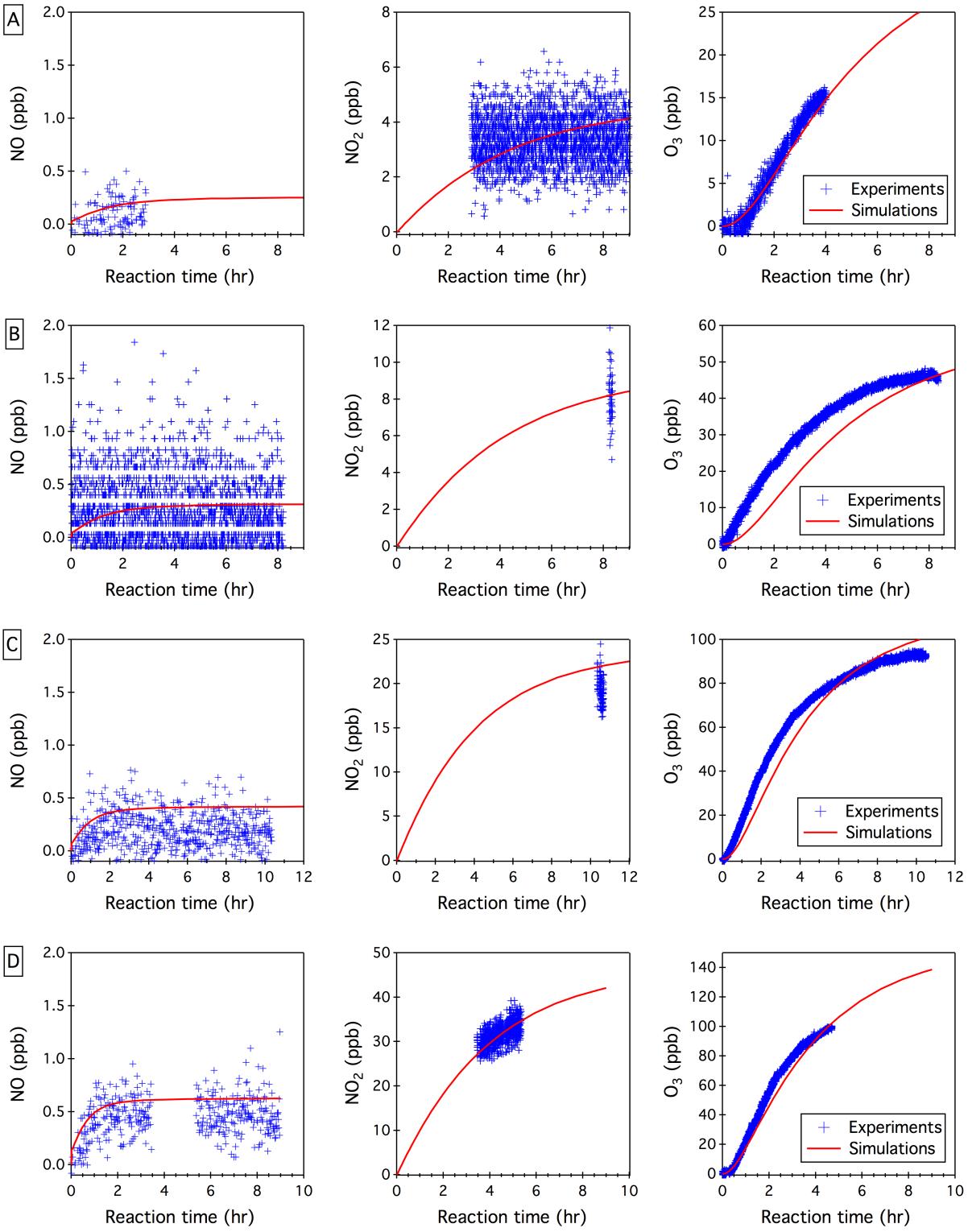

A
B
C
D
NO (ppb)
NO2 (ppb)
O3 (ppb)
Reaction time (hr)
Experiments
Simulations

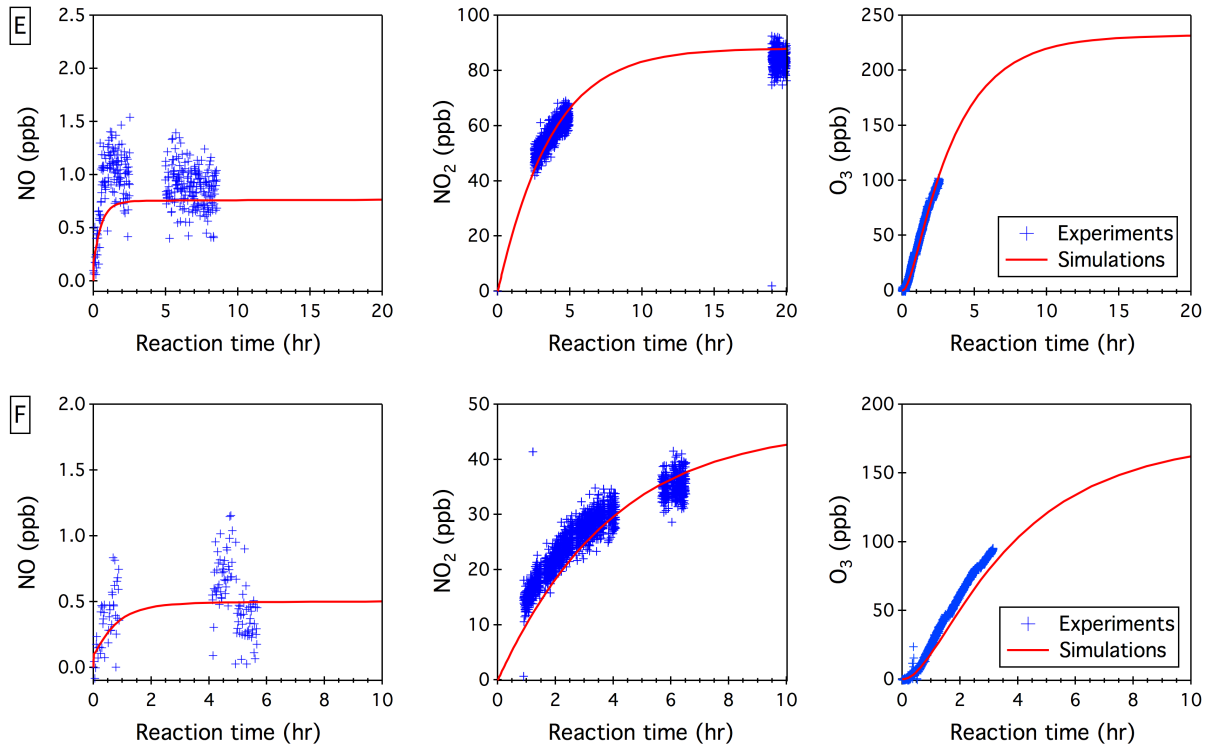


Figure S1. Simulated vs. measured temporal profiles of O_3 and NO_x in six continuous-flow photochemical blank experiments. It takes in general 16 hours to reach steady state, although the duration of most experiments was in the range of 8 to 10 hours for the preservation of injection sources. One experiment lasted for 20 hours to ensure the establishment of predicted steady state NO_x concentrations. Inflow H_2O_2 and NO concentrations used for these experiments are (A) 658 ppb and 5 ppb, (B) 1316 ppb and 10 ppb, (C) 3290 ppb and 25 ppb, (D) 3290 ppb and 50 ppb, (E) 6580 ppb and 100 ppb, and (F) 6580 ppb and 50 ppb, respectively.

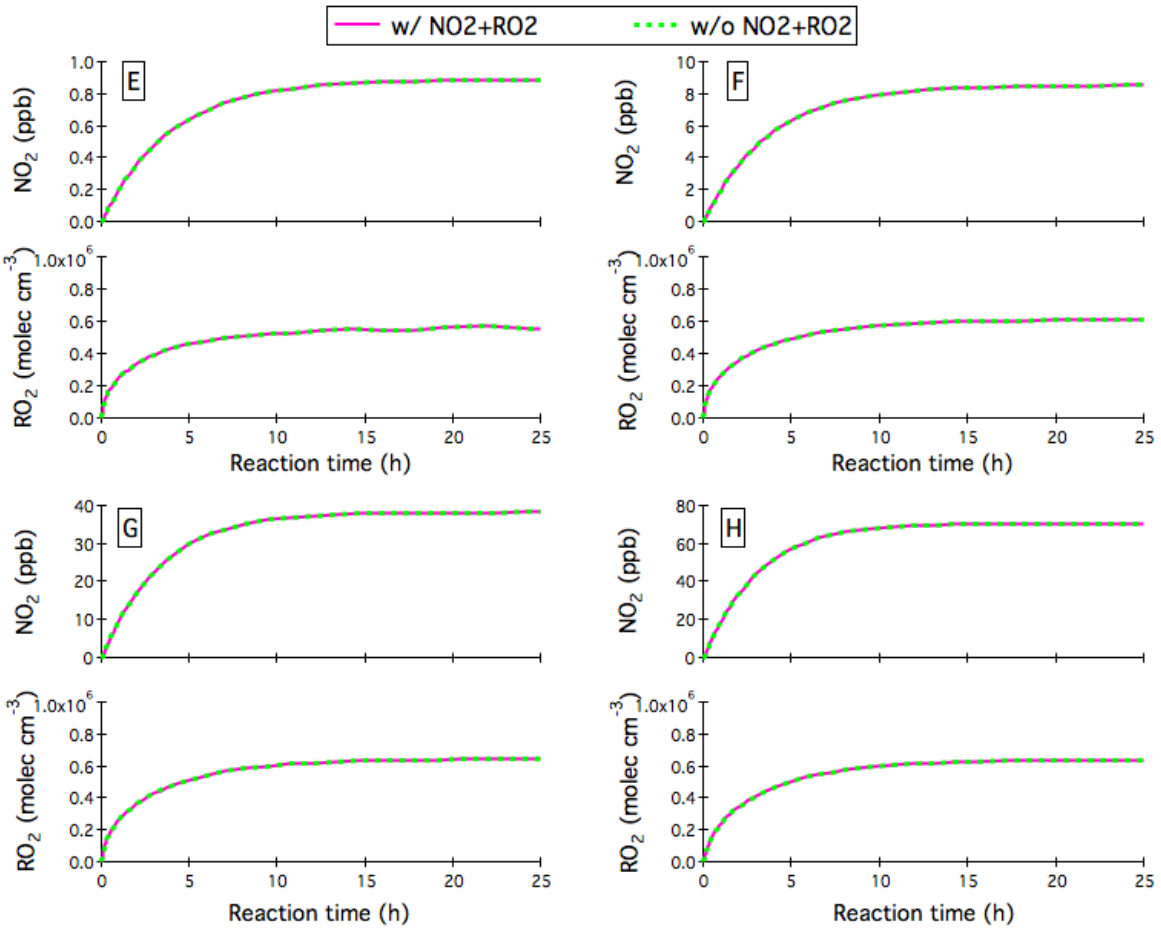
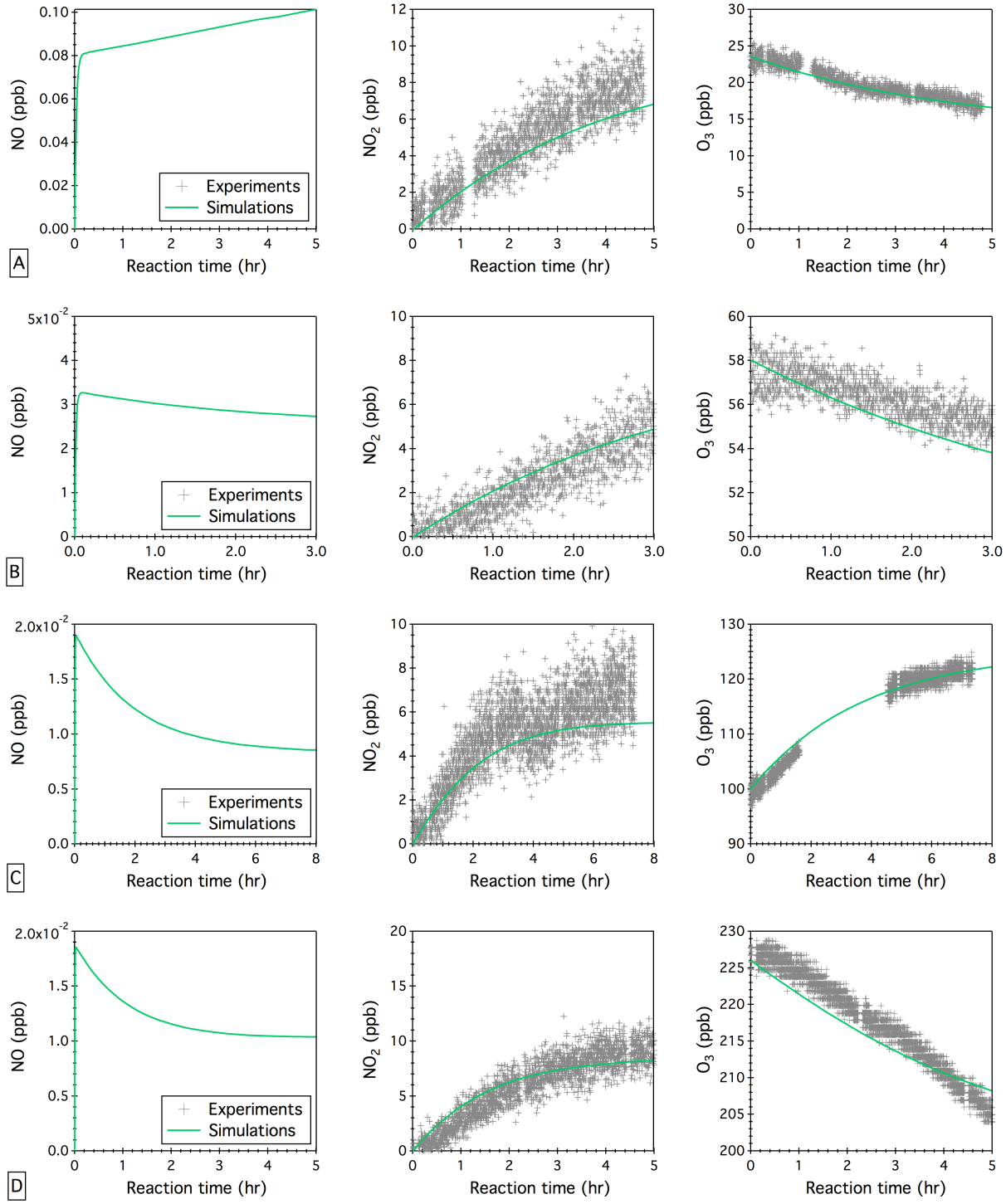


Figure S2. Simulated temporal profiles of ethylperoxy radicals ($C_2H_5O_2$) generated from OH oxidation of ethane in the presence (red) and absence (green) of the $C_2H_5O_2+NO_2+M \leftrightarrow C_2H_5O_2NO_2+M$ reaction under ~1–80 ppb steady state NO_2 levels in the chamber.


A
B
C
D
NO (ppb)
NO2 (ppb)
O3 (ppb)
Reaction time (hr)
Experiments
Simulations
5x10-2
2.0x10-2

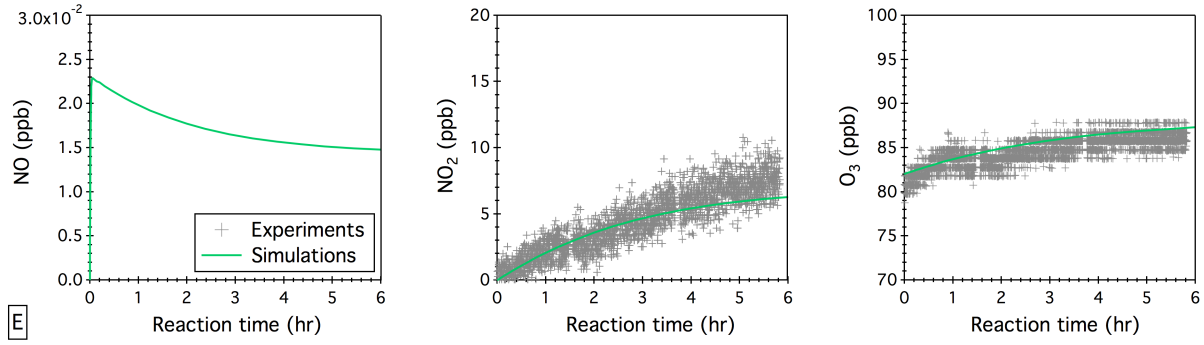


Figure S3. Simulated vs. measured temporal profiles of O_3 and NO_x in five continuous-flow dark blank experiments. Inflow O_3 and NO concentrations used for these experiments are (A) 22 ppb and 10 ppb, (B) 57 ppb and 10 ppb, (C) 110 ppb and 10 ppb, (D) 225 ppb and 20 ppb, and (E) 85 ppb and 10 ppb, respectively. Rises in the O_3 concentrations in panel (C) and (E) result from the higher O_3 concentrations in the continuous injection flow compared with the initial O_3 concentrations in the chamber.

Table S1. Initial conditions used for modeling and experiments comparison.

No.	T (K)	RH (%)	UV lights	H_2O_2 (ppb)	NO (ppb)	O_3 (ppb)	HCHO (ppb)	C_5H_8 (ppb)
1	305-306	4-5	√	658	5	0	0	0
2	305-306	4-5	√	1316	10	0	0	0
3	305-306	4-5	√	3290	25	0	0	0
4	305-306	4-5	√	3290	50	0	0	0
5	305-306	4-5	√	6580	100	0	0	0
6	305-306	4-5	√	6580	50	0	0	0
7	294-295	8-9	×	0	0	22	0	0
8	294-295	8-9	×	0	0	57	0	0
9	294-295	8-9	×	0	0	100	0	0
10	294-295	8-9	×	0	0	85	0	0
11	294-295	8-9	×	0	0	225	0	0
12	305-306	4-5	√	600	19	0	0	19.9
13	294-295	8-9	×	0	59	0	0	10.2

Table S2. A spreadsheet for calculating the H_2O_2 mixing ratio in the injection flow from the infused concentration of H_2O_2 aqueous solution.

Row 1	Column A	Column B
Row 2	Constants	
Row 3	P (Pa)	8.60E+04
Row 4	T (K)	298.15
Row 5	R (J K^{-1} mol^{-1})	8.31
Row 6	Avogadro constant (molecules mol^{-1})	6.02E23
Row 7	Density (g cm^{-3})	1.11*B9+1.00*(1-B9)
Row 8	Molecular weight (g mol^{-1})	34.01*B9+18.02*(1-B9)
Row 9	H_2O_2 percent in aqueous solution	0.01
Row 10	Chamber parameters	
Row 11	Volume of chamber (m^3)	10.00
Row 12	Desired steady state H_2O_2 concentration in chamber (ppm)	1.31
Row 13	In/Out flow rate (L/min)	40.00
Row 14	Calculation intermediates	
Row 15	Residence time (s)	B11*1000*60/B13
Row 16	Incoming number concentration of H_2O_2 in chamber (molecules cm^{-3})	B6*B3*B12*1E-12/B5/B4
Row 17	Incoming molar concentration of H_2O_2 to chamber (mol L^{-1})	1000*B16/B6
Row 18	Target	
Row 19	Injection rate (uL/hr)	60*B17*B13*B8/B7/B9/0.001