The Chemistry of Atmosphere-Forest Exchange (CAFE) Model, Part II: Application to BEARPEX-2007 Observations

Supplementary Online Material

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Table S1. BEARPEX-2007 chemical observations. Statistics are calculated from a merged, 30-minute averaged dataset for noontime (11:30 – 12:30 PST) data collected during the hot (28 August – 3 September) and cool (Averages from 13 – 18 September) periods as defined in the main paper. Comma-separated heights denote different measuring heights for hot and cold periods. Mean concentrations ($\overline{C}$) and standard deviations (σ_C) are in ppbv unless otherwise specified. *N* represents the number of points included in the average.

Species	Height m	Hot Period			Cool Period			Ref.[a]
		$\overline{C}$	σ_C	N	$\overline{C}$	σ_C	N	
OH	9.4	6.8	0.5	4	4.0	1.2	7	i
(10^6 molec cm^{-3})	15	8.0	2.7	8	-	-	-	
HO_2	9.4	0.029	0.003	4	0.021	0.004	7	i
	15	0.033	0.005	8	-	-	-	
CO	12.5	97	14	21	116	10	18	ii
O_3	1.2	49.6	11.0	7	44.0	6.6	6	iii
	4.9	51.3	11.4	7	45.5	6.6	6	
	8.75	51.6	11.3	7	45.3	6.0	6	
	12.5	50.8	11.6	7	45.5	5.5	6	
τ_{OH}^{-1} (s^{-1})	9.9	12.4	2.0	17	6.8	1.2	12	iv
$\underline{NO_y}$								
NO_2	4.9	0.273	0.135	3	0.314	0.074	11	v
	9	0.139	0.065	4	0.368	0.115	12	
	12.7	0.050	0.022	3	0.346	0.091	13	
ΣPN[b]	4.9	-	-	-	0.458	0.101	9	v
	9	0.185	0.104	3	0.430	0.099	11	
	12.7	0.295	0.177	3	0.413	0.097	12	
ΣAN[c]	4.9	0.142	0.035	2	0.130	0.072	11	v
	9	0.147	0.146	2	0.119	0.066	11	
	12.7	-	-	-	0.096	0.074	10	
PAN	1.5	0.130	0.078	14	0.458	0.171	12	vi
	5	0.152	0.070	14	0.471	0.154	12	
	17.8	0.159	0.079	7	0.449	0.129	6	

Table S1. Continued.

PPN	1.5	0.006	0.004	14	0.039	0.014	12	vi
	5	0.009	0.005	14	0.041	0.014	12	
	17.8	0.009	0.005	7	0.039	0.011	6	
MPAN	1.5	0.031	0.012	14	0.029	0.009	12	vi
	5	0.031	0.013	14	0.034	0.014	12	
	17.8	0.020	0.011	7	0.030	0.011	6	
HNO_3	16.8	0.555	0.190	16	0.273	0.004	3	vii
HONO	16.8	0.022	0.014	9	0.046	0.007	2	vii
Alkenes								
isoprene	6.4	1.645	0.676	20	0.211	0.071	15	viii
Organic Acids								
CH_3CO_2H	16.8	4.494	2.398	16	2.078	0.149	3	vii
HCOOH	16.8	4.099	2.530	13	2.396	0.028	3	vii
CH_3CO_3H	16.8	0.289	0.087	12	0.138	0.012	3	vii
Alcohols								
MBO	6.4	3.182	1.092	20	0.623	0.261	15	viii
CH_3OH	6.4	5.637	1.683	20	4.644	1.083	15	viii
C_2H_5OH	6.4	1.560	0.519	20	1.400	0.389	15	viii
IPROPOL	6.4	0.080	0.035	20	0.074	0.016	15	viii
Aldehydes								
MACR	6.4	0.404	0.189	20	0.120	0.036	15	viii
CH_3CHO	6.4	0.549	0.185	20	0.426	0.100	15	viii
C_2H_5CHO	6.4	0.066	0.015	20	0.061	0.014	15	viii
GLYOX	3, 12	0.077	0.022	21	0.037	0.002	9	ix
HCHO	11.8	-	-	-	12.5	4.0	9	xi
Ketones								
MVK	6.4	1.448	0.664	20	0.140	0.065	15	viii
CH_3COCH_3	6.4	2.446	0.843	20	1.948	0.371	15	viii
ACETOL	16.8	0.243	0.130	12	0.165	0.025	15	vii
NOPINONE	1.5, 9.2	0.007	0.005	5	0.005	0.004	4	x
Peroxides								
H_2O_2	16.8	0.884	0.191	16	0.634	0.054	3	vii
ISOPOOH+IEPOX	16.8	0.247	0.147	12	0.055	0.010	3	vii

Table S1. Continued.

Terpenoids								
α-pinene	1.5, 9.2	0.079	0.008	5	0.024	0.003	3	x
	6.4	0.047	0.011	20	0.013	0.003	15	viii
β-pinene	1.5, 9.2	0.232	0.005	5	0.074	0.007	4	x
	6.4	0.152	0.042	20	0.044	0.012	15	viii
limonene	1.5, 9.2	0.061	0.006	5	0.012	0.008	4	x
	6.4	0.011	0.003	20	0.003	0.001	15	viii
3-carene	1.5, 9.2	0.148	0.021	5	0.040	0.004	3	x
myrcene	1.5, 9.2	0.009	0.001	5	0.003	0.000	4	x
camphene	1.5, 9.2	0.004	0.002	5	bdl	bdl	4	x
terpinolene	1.5, 9.2	0.004	0.002	5	bdl	bdl	4	x
α-terpinene	1.5, 9.2	bdl[j]	bdl	5	bdl	bdl	4	x
γ-terpinene	1.5, 9.2	0.001	0.001	5	bdl	bdl	4	x
methyl chavicol	1.5, 9.2	0.079	0.013	5	0.037	0.006	4	x
α-bergamotene	1.5, 9.2	0.034	0.002	5	0.003	0.001	4	x
unspeciated SQT	1.5, 9.2	0.022	0.007	5	0.003	0.001	4	x

[a]Measurement technique references: (1) Faloona et al. (2004). (2) Goldstein et al. (2000). (3) Bauer et al. (2000). (4) Mao et al. (2009). (5) Farmer et al. (2010). (6) Wolfe et al. (2009). (7) Crounse et al. (2006). (8) Goldan et al. (2004). (9) Huisman et al. (2008). (10) Bouvier-Brown et al. (2009). (11) Choi et al. (2010).
[b]Sum peroxy nitrates.
[c]Sum alkyl nitrates.
[d]Below detection limit.

Table S2. Model-measurement inter-comparison for selected observations. Comma-separated heights denote different measuring heights for hot and cold periods. Measurements are taken from Table S1. Concentrations are in ppbv unless otherwise specified.

Species	Height	Hot Period			Cool Period		
	m	Model	Meas	% Diff.[a]	Model	Meas	% Diff.
O_3	12.5	50.6	50.8	-0.3	45.6	45.5	0.3
CO	12.5	97	97	0.5	$113	116	-2.9
OH (10^6 molec cm^{-3})	9.4	3.08E-04	3.24E-04	-5.0	1.96E-04	1.87E-04	5.0
HO_2	9.4	0.033	0.029	13.4	0.018	0.021	-14.9
NO_y							
NO_2	9	0.142	0.139	1.9	0.385	0.368	4.6
PAN	17.8	0.207	0.159	29.9	0.438	0.449	-2.5
PPN	17.8	0.009	0.009	-4.2	0.042	0.039	8.5
MPAN	17.8	0.032	0.031	2.8	0.035	0.030	16.5
ΣPN	9	0.290	0.185	56.7	0.533	0.430	24.0
ΣAN	9	0.125	0.142	-12.3	0.093	0.119	-21.8
HNO_3	16.8	0.562	0.555	1.3	0.285	0.273	4.2
HONO	16.8	0.001	0.022	-97.4	0.001	0.046	-92.2
Alkenes							
isoprene	6.4	1.627	1.645	-1.1	0.251	0.211	19.2
Organic Acids							
CH_3CO_2H	16.8	4.582	4.494	2.0	2.055	2.078	-1.1
HCOOH	16.8	4.085	4.099	-0.3	2.417	2.396	0.9
CH_3CO_3H	16.8	0.297	0.289	2.7	0.137	0.138	-0.4
Alcohols							
MBO	6.4	3.237	3.182	1.7	0.659	0.623	5.7
CH_3OH	6.4	5.346	5.637	-5.2	4.297	4.644	-7.5
C_2H_5OH	6.4	1.577	1.56	1.1	1.363	1.400	-2.7
IPROPOL	6.4	0.077	0.08	-3.4	0.071	0.074	-3.4
Aldehydes							
MACR	6.4	0.395	0.404	-2.3	0.112	0.12	-6.9
CH_3CHO	6.4	0.457	0.549	-16.7	0.402	0.426	-5.6
C_2H_5CHO	6.4	0.066	0.066	-0.2	0.057	0.061	-6.0
GLYOX	3, 12	0.071	0.077	-8.4	0.035	0.037	-4.1
HCHO	11.8	4.165	-	-	1.400	12.5	-89

Table S2. Continued.

Ketones							
MVK	6.4	1.432	1.448	-1.1	0.144	0.14	2.5
CH_3COCH_3	6.4	2.545	2.446	4.1	1.892	1.948	-2.9
ACETOL	16.8	0.238	0.243	-2.3	0.164	0.165	-0.7
NOPINONE	1.5, 9.2	0.010	0.007	44.0	0.005	0.005	7.7
Peroxides							
H_2O_2	16.8	0.856	0.884	-3.2	0.531	0.634	-16.3
ISOPOOH+IEPOX	16.8	0.495	0.247	100.4	0.027	0.055	-50.1
Terpenoids							
α-pinene	1.5, 9.2	0.086	0.079	8.6	0.020	0.024	-17.5
β-pinene	1.5, 9.2	0.156	0.232	-32.7	0.030	0.074	-59.7
limonene	1.5, 9.2	0.053	0.061	-13.6	0.015	0.012	21.1
3-carene	1.5, 9.2	0.081	0.148	-45.0	0.020	0.04	-51.0
myrcene	1.5, 9.2	0.037	0.009	311.0	0.009	0.003	185.2
camphene	1.5, 9.2	0.057	0.004	1316.8	0.016	bdl	-
terpinolene	1.5, 9.2	0.008	0.004	110.5	0.002	bdl	-
α-terpinene	1.5, 9.2	0.004	bdl[j]	-	0.001	bdl	-
γ-terpinene	1.5, 9.2	0.009	0.001	777.8	0.002	bdl	-
Methyl chavicol	1.5, 9.2	0.081	0.079	3.0	0.013	0.037	-64.0
α-bergamotene	1.5, 9.2	0.027	0.034	-19.6	0.008	0.003	173.0
unspeciated SQT	1.5, 9.2	0.008	0.022	-64.7	0.004	0.003	31.4

[a]Calculated as 100*(Model - Meas)/Meas.
[b]Below detection limit.

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