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Supporting Information for

Large-eddy simulation of atmospheric chemistry during the DISCOVER-AQ 2011 campaign

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Introduction

This supporting information provides figures and tables that introduce meteorological (Figure S1, Table S1) and chemical conditions (Table S2) used in the simulations. Vertical cross sections of chemical species and vertical velocity are shown to better understand segregation of isoprene and OH (Figure S2). The bar chart (Figure S3) and the photolysis lifetime table (Table S3) are used as a supplement to show the reactivity of the BVOC species.

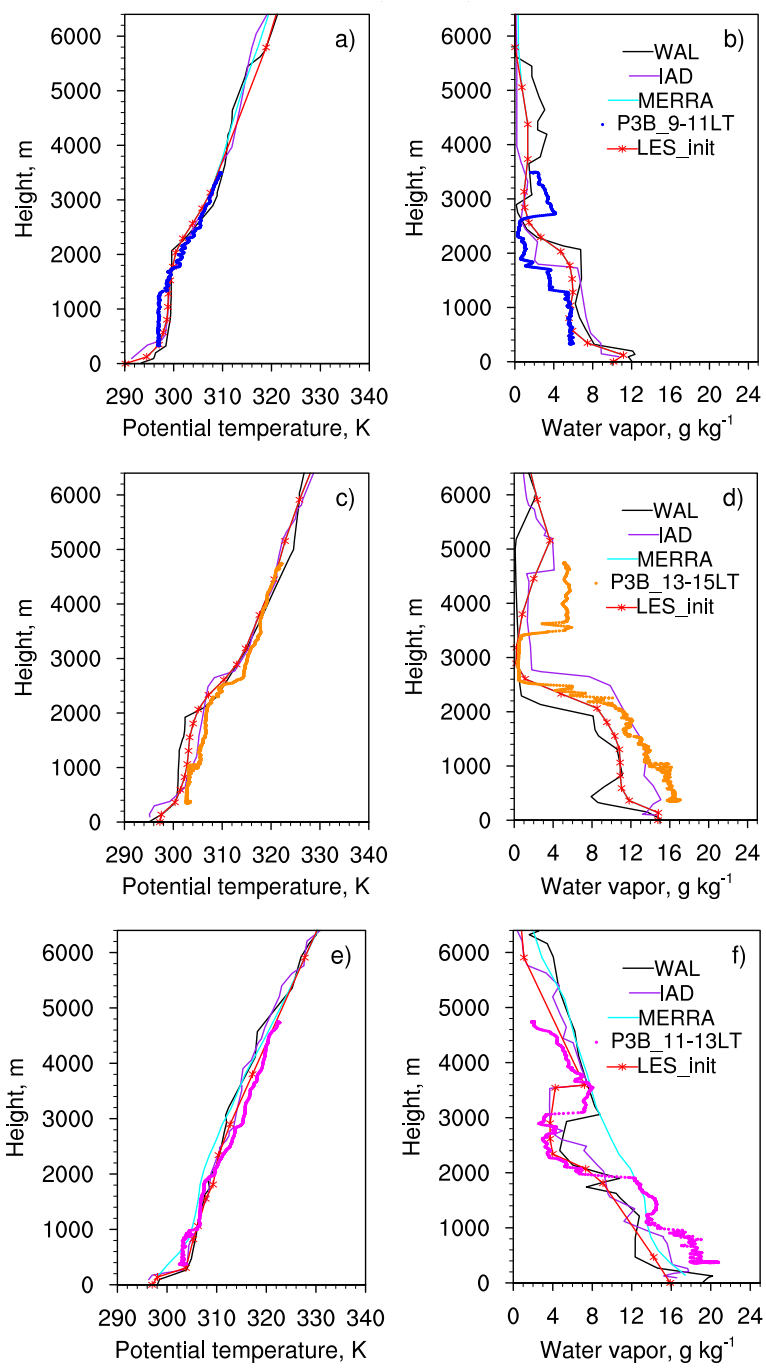

Figure S1. Comparison of potential temperature (K) (a, c, e) and water vapor mixing ratio (g kg^{-1}) (b, d, f) of the initial profiles at 0530 LT used in LES (red), interpolated 0530 LT profiles derived from 6-hourly finer resolution (0.5° × 0.67°) MERRA data (cyan), sounding data at 0800 LT from WAL (black) and IAD (purple) sites, and the earliest P-3B observed profiles (0900-1100 LT for Case 1, 1300-1500 LT for Case 2 and 1100-1300 LT for Case 3) for the three cases (Case 1: a, b; Case 2: c, d; Case 3: e, f).

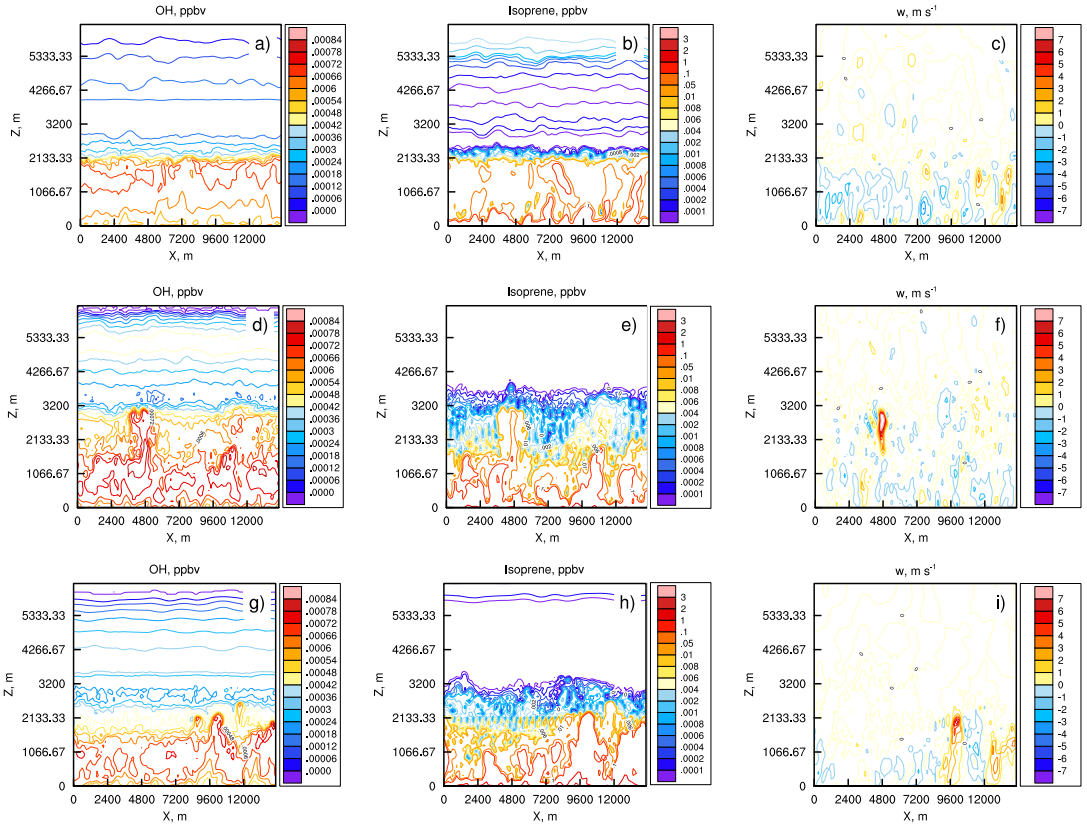

Figure S2. LES simulated instantaneous vertical cross section of OH (a, d, g), isoprene (b, e, h) and vertical velocity w (c, f, i) in the middle of the domain at 1400 LT for the three cases (Case 1: a-c; Case 2: d-f; Case 3: g-i).

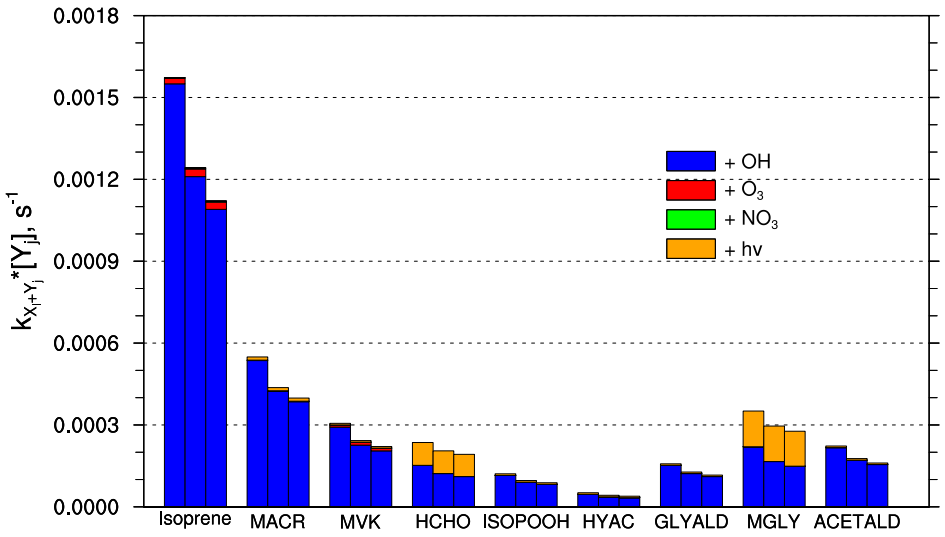

Figure S3. Photochemical box model simulated $k_{Xi+Yj} * [Y_j]$ (s^{-1}) during 1100-1300 LT (with three vertical bars for each BVOC species representing the values for the three cases), where k_{Xi+Yj} is the reaction rate coefficient for each reaction of BVOC species X_i with Y_j and $[Y_j]$ is the ambient concentration of OH, O_3, or NO_3, k_{Xi+Yj} is the photolysis rate and $[Y_j]$ is 1 for the photolysis pathway.

Case 1		Potential temperature tendency (K h^{-1})			Water vapor tendency (g kg^{-1} h^{-1})			Radiative tendency (K h^{-1})		
Time										
LT, hr	UTC, hr	0-1 km	1-2 km	> 2 km	0-1 km	1-2 km	> 2 km	0-1 km	1-2 km	> 2 km
3.5	7.5	-0.190	0.005	-0.143	-0.124	-0.236	-0.129	-0.193	-0.091	-0.078
6.5	10.5	-0.164	-0.016	0.014	-0.362	-0.222	-0.124	-0.112	-0.071	-0.062
9.5	13.5	-0.125	-0.019	0.077	-0.273	-0.325	-0.038	0.051	-0.008	-0.018
12.5	16.5	-0.139	-0.043	0.117	-0.046	-0.233	0.053	0.097	0.030	0.000
15.5	19.5	-0.154	-0.097	0.206	0.066	-0.056	0.044	0.055	0.030	-0.002
18.5	22.5	-0.068	-0.031	0.125	0.086	-0.008	0.034	-0.061	-0.025	-0.032
Case 2		Potential temperature tendency (K h^{-1})			Water vapor tendency (g kg^{-1} h^{-1})			Radiative tendency (K h^{-1})		
Time										
LT, hr	UTC, hr	0-1 km	1-2 km	> 2 km	0-1 km	1-2 km	> 2 km	0-1 km	1-2 km	> 2 km
3.5	7.5	0.142	Interpolated	0.000	0.184	Interpolated	0.000	-0.172	Interpolated	0.000
6.5	10.5	0.125	Interpolated	0.000	0.231	Interpolated	0.000	-0.117	Interpolated	0.000
9.5	13.5	0.005	Interpolated	0.000	0.204	Interpolated	0.000	0.038	Interpolated	0.000
12.5	16.5	-0.003	Interpolated	0.000	0.156	Interpolated	0.000	0.086	Interpolated	0.000
15.5	19.5	-0.051	Interpolated	0.000	0.154	Interpolated	0.000	0.008	Interpolated	0.000
18.5	22.5	0.001	Interpolated	0.000	0.086	Interpolated	0.000	-0.121	Interpolated	0.000
Case 3		Potential temperature tendency (K h^{-1})			Water vapor tendency (g kg^{-1} h^{-1})			Radiative tendency (K h^{-1})		
Time										
LT, hr	UTC, hr	0-1 km	1-2 km	> 2 km	0-1 km	1-2 km	> 2 km	0-1 km	1-2 km	> 2 km
3.5	7.5	0.239	0.065	-0.096	0.310	0.081	-0.079	-0.042	-0.013	-0.088
6.5	10.5	0.156	0.053	0.125	0.239	0.043	-0.166	-0.040	-0.033	-0.077
9.5	13.5	0.120	0.078	0.028	0.060	0.014	-0.102	0.054	-0.018	-0.016
12.5	16.5	0.126	0.088	-0.188	0.039	-0.205	-0.312	0.063	0.010	0.014
15.5	19.5	0.342	0.350	-0.146	-0.111	0.097	-0.172	-0.008	-0.006	0.010
18.5	22.5	0.420	0.339	-0.189	-0.159	0.521	0.240	-0.142	-0.063	-0.036

Table S1. Meteorological boundary conditions for the three LES cases derived from 3-hourly 1.25° × 1.25° MERRA reanalysis data at the Fair Hill site (39.71°N, 75.87°W).

	Case 1		Case 2		Case 3	
Chemical species	Boundary layer (ppbv)	Free atmosphere (ppbv)	Boundary layer (ppbv)	Free atmosphere (ppbv)	Boundary layer (ppbv)	Free atmosphere (ppbv)
O3	59.96	60.44	74.57	73.47	69.48	65.45
NO2_NCAR	1.49	0.02	1.87	0.39	1.14	0.05
NO	0.45	0.02	0.21	0.03	0.20	0.02
HNO3_TD-LIF	0.83	0.08	1.39	0.50	1.69	0.56
CH2O_DFGAS	2.70	0.39	7.29	0.54	6.75	0.51
Isoprene	0.27	0.03	0.93	0.02	0.62	0.01
Monoterpenes	0.06	0.01	0.11	0.01	0.09	0.00
MVK+MAC+ISOPOOH	0.47	0.01	1.79	0.02	1.23	0.01
Acetaldehyde	0.46	0.05	1.23	0.28	1.03	0.22
Methanol	4.65	3.23	6.53	2.45	6.92	1.64
Acetone	2.16	1.91	4.95	2.39	4.37	1.98

Table S2. Initial concentrations (ppbv) for the PBL (below 1 km) and free atmosphere (above 3 km) of P-3B measured chemical species for the three LES cases. Data derived from P-3B measurements from the Fair Hill spiral.

	Photolysis lifetime (τ_{CH}, min)		
	Case 1	Case 2	Case 3
HCHO	201.79 ± 8.91	203.38 ± 9.39	207.92 ± 10.46
MGLY	128.94 ± 4.15	129.67 ± 4.35	131.70 ± 4.85

Table S3. Modeled midday (1100-1300 LT) photolysis lifetimes of HCHO and MGLY for the three cases. Values shown are temporal (1100-1300 LT) averages, with plus and minus one standard deviation.