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Sources and characteristics of summertime organic aerosol in the Colorado Front Range: perspective from measurements and WRF-Chem modeling

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Supplemental Information

VOC specie	Mean (ppbv)	R coefficient CH_4 regress	R coefficient C_2H_2 regress	R coefficient C_3H_8 regress	Oil/Gas CH_4 emission ratio
CH_4	1975.7	1	0.52	0.678	1
CO	146	0.303	0.854	0.186	0
NOx	5.03	0.369	0.68	0.231	0
C_2H_6	13.8	0.72	0.44	0.987	0.185
C_3H_8	11.1	0.678	0.414	1	0.17
N-Butane	5.76	0.68	0.41	0.994	0.0905
Iso-Butane	2.33	0.676	0.406	0.997	0.0379
N-Pentane	2.27	0.701	0.44	0.985	0.036
Iso-Pentane	1.97	0.702	0.452	0.987	0.0297
2methyl-Pentane	0.215	0.73	0.496	0.966	0.00257
Hexane	0.668	0.731	0.472	0.965	0.00872
Heptane	0.207	0.736	0.497	0.941	0.00236
Octane	0.0583	0.739	0.531	0.894	0.000583
Nonane	0.00668	0.64	0.5	0.726	8.65e-05
Decane	0.0174	0.668	0.732	0.65	6.25e-05
Undecane	0.0115	0.571	0.698	0.513	3.44e-05
Cyclopentane	0.119	0.712	0.452	0.973	0.00186
1m-Cyclopentane	0.741	0.723	0.48	0.963	0.00997
Cyclohexane	0.187	0.724	0.474	0.96	0.00271
1m-Cyclohexane	0.193	0.712	0.464	0.952	0.00267
1e-Cyclohexane	0.0226	0.654	0.483	0.881	0.000325
11dm-Cyclopentane	0.014	0.717	0.463	0.955	0.000196
c13dm-Cyclohexane	0.0232	0.683	0.452	0.927	0.000382
t12dm-Cyclohexane	0.00899	0.704	0.478	0.921	0.000139
t13dm-Cyclohexane	0.00426	0.714	0.521	0.922	5.61e-05
113tm-Cyclohexane	0.00659	0.637	0.47	0.783	7.92e-05
1e1m-Cyclohexane	0.00308	0.708	0.621	0.846	3.45e-05
Benzene	0.166	0.746	0.658	0.904	0.00114
Toluene	0.234	0.722	0.723	0.781	0.00126
m+p Xylenes	0.0882	0.712	0.749	0.722	0.000423
1ethyl-Benzene	0.025	0.639	0.836	0.591	6.7e-05
o Xylene	0.0311	0.677	0.799	0.646	0.000113
ipropyl-Benzene	0.0013	0.681	0.783	0.662	5.43e-06
npropyl-Benzene	0.00321	0.615	0.834	0.548	7.66e-06
1e-3,4m-Benzene	0.0174	0.608	0.798	0.53	3.61e-05
1e-2m-Benzene	0.0023	0.565	0.827	0.468	4.11e-06
123tm-Benzene	0.00504	0.581	0.793	0.471	1.04e-05
124tm-Benzene	0.0201	0.621	0.793	0.546	5.76e-05
135tm-Benzene	0.00841	0.654	0.762	0.606	3.6e-05
C_2H_2	0.177	0.52	1	0.414	0
C_2H_4	0.32	0.594	0.798	0.508	0.000561
C_3H_6	0.079	0.567	0.653	0.502	0.00021
1-Butene	0.00884	0.558	0.741	0.496	1.68e-05
1,3-Butadiene	0.00336	0.443	0.687	0.346	5.55e-06

Table S1. Statistical summary of VOC and NO_x measurements at the BAO tower during the 2012 SONNE study. Shown are means from ~780 samples, r-coefficients from linear regressions relative to CH_4, acetylene and propane, and the derived emission ratios relative to CH_4 specifically from oil/gas activities (ppbv/ppbv).

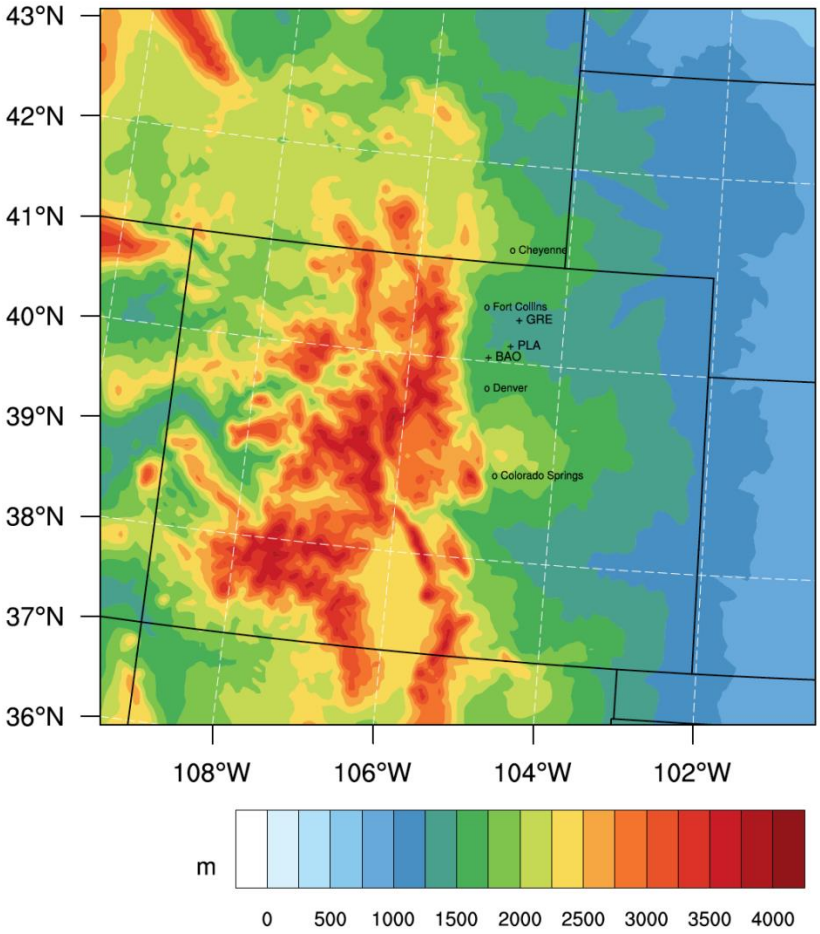

Figure S1. Terrain height (above sea level, in m) in the WRF-Chem model domain, 4 km resolution

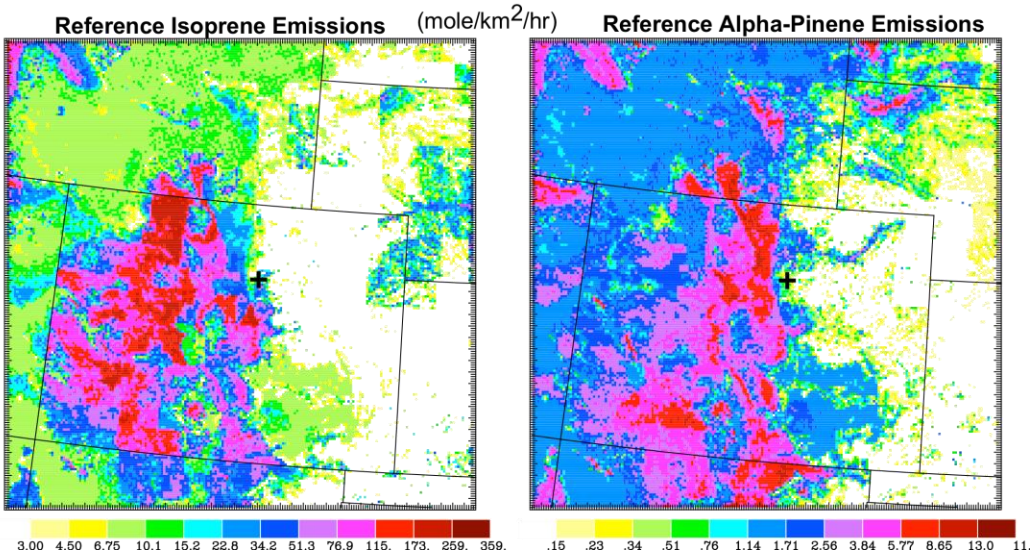

Figure S2. Isoprene and alpha-pinene emissions at reference temperature (30° C) and photosynthetic photon flux density (PPFD = 1000 μmole/m^2/s) from the BEIS inventory over the 4-km model domain. Dark crosses show the location of Denver, CO.

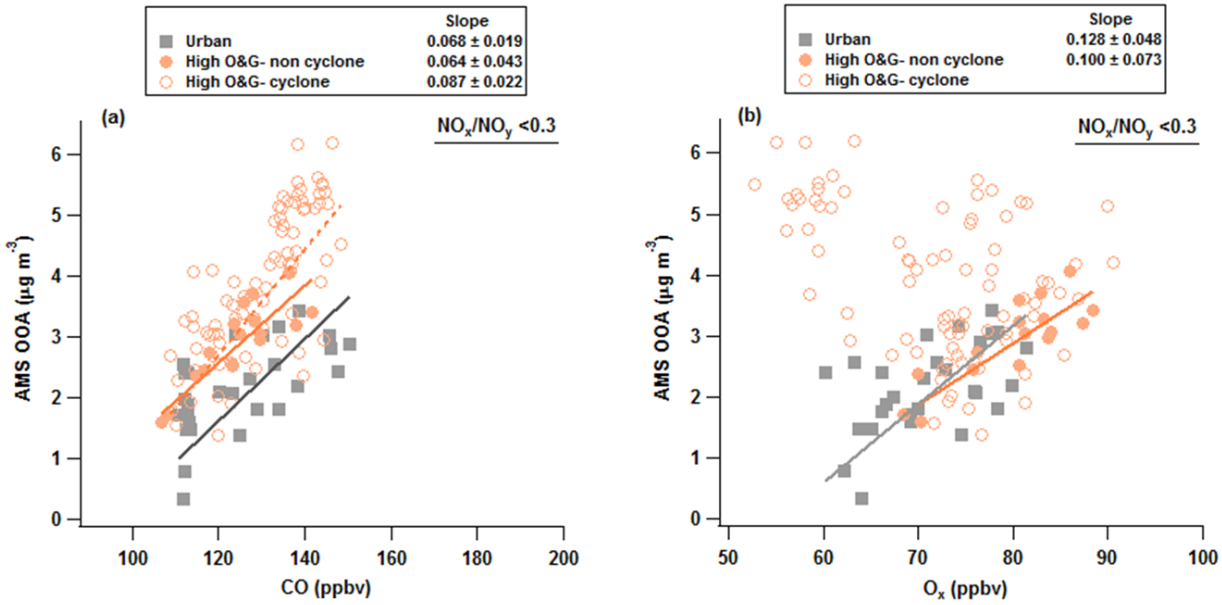

Figure S3. Correlation plots of PMF-derived OOA vs. CO (a) and odd oxygen, O_x defined as O_3 + NO_2 (b) in aged plumes.

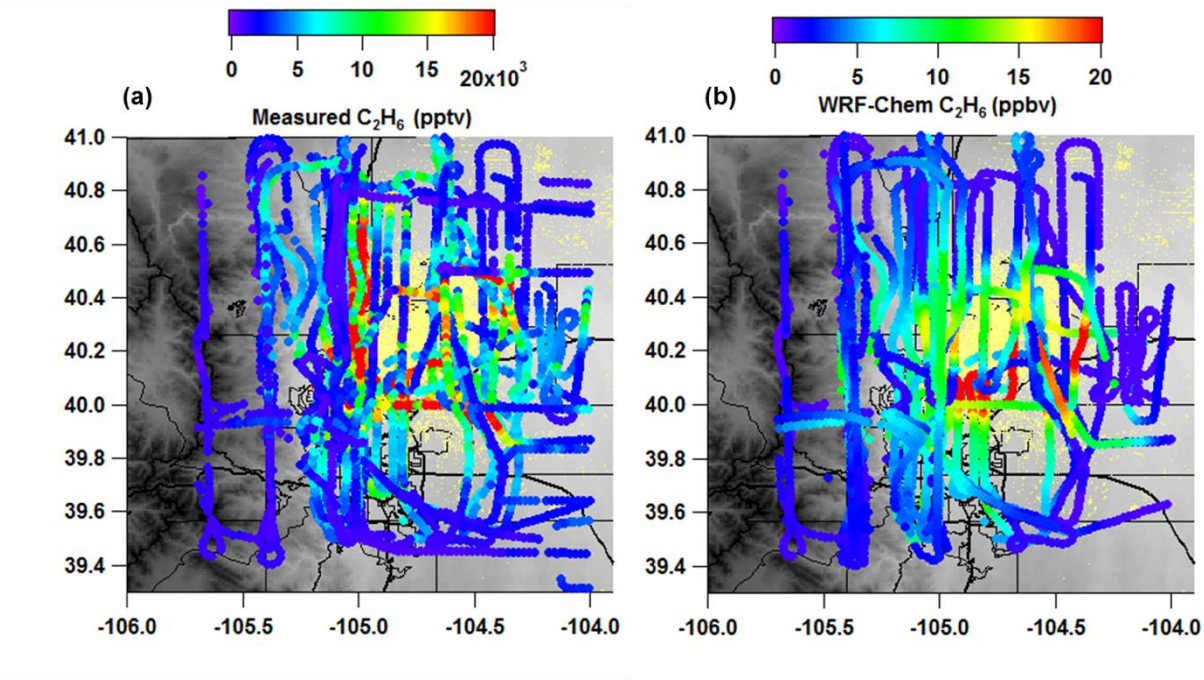

Figure S4. Flight tracks of C130 in the Front Range BL, color coded with ethane values from measurements (a) and BC-tdOG scenario (b). Locations of the O&G wells are shown with yellow dots.