

Supplementary Information

for

Secondary Organic Aerosol Production from Diesel Vehicle Exhaust: Impact of Aftertreatment, Fuel Chemistry and Driving Cycle

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Fuel Analyses

The fuels were analyzed with nitric oxide ionization spectrometry evaluation (NOISE) at a commercial lab specializing in this analysis (Triton Analytics, Houston, TX). NOISE quantifies hydrocarbons by carbon number and hydrogen deficiency [42]. In addition to measuring the mono-, di-, tri-, and tetra-aromatic content, this GC-MS based technique provides weight percentages of 10 other classes of compounds. Basic chemical characteristics of the three ULSD used with D1, D2 and D3 are provided in Table S.1, and a more detailed analysis is given in Figure S.1. NOISE analysis was not performed with the diesel and biodiesel fuels used in experiments with D4 or D5.

Table S.1 Selected characteristics of the three ULSD fuels used in the HDDV smog chamber experiments. A more detailed chemical analysis is provided in Figure S.1 of the SI.

	low aromatic ULSD	mid-aromatic ULSD	high aromatic ULSD
alkanes (%)	19.9	26.4	29.3
cycloalkanes (%)	70.9	61.2	42.7
mono-aromatics (%)	8.8	11.7	23.7
di-aromatics (%)	0.4	0.7	4.2
tri-aromatics (%)	0.0	0.0	0.2
tetra-aromatics (%)	0.0	0.0	0.0
avg # carbons	15.0	14.1	14.7
avg # hydrogens	28.5	27.0	27.2
avg mol wt	208.5	196.7	203.7

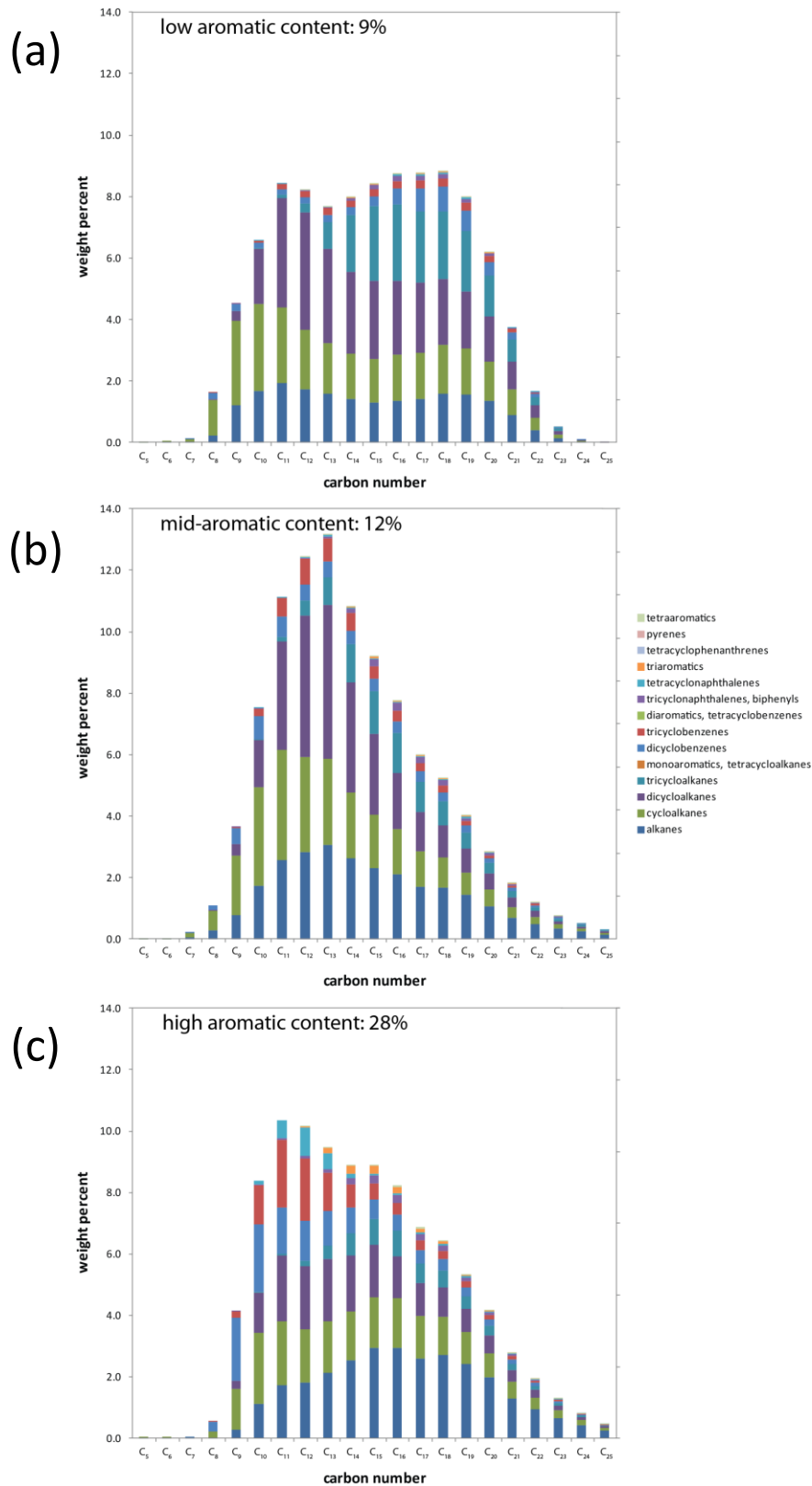


Figure S.1 The weight percent of 14 different classes of compounds in the (a) low-aromatic, (b) mid-aromatic and (c) high aromatic content fuels used in the heavy-duty diesel vehicle experiments as a function of carbon number.

Quantifying SOA Production

To quantify SOA production in the smog chamber we corrected the measured concentrations of suspended particles for (a) the loss of organic particles and vapors to the chamber walls, (b) the increase in the particle loss rate for experiments in which nucleation occurs, and (c) the lower particle detection efficiency by the aerosol mass spectrometer (AMS) for particles smaller than about 60 nm. Wall-loss corrections (a) are important in every experiment, whereas corrections for (b) and (c) are significant only in a few experiments (e.g., as a result of particle nucleation during DPF regeneration when chamber concentrations were dominated by smaller particles). Correction (a) is described below; corrections (b) and (c) are described in the SI.

Organic particles and vapors are lost to the chamber walls as a function of time, and total OA is the sum of the measured (via the AMS) suspended mass plus the mass of organics on the chamber walls

$$OA_{total,t} = OA_{sus,t} + OA_{wall,t} \quad (1)$$

Organics may be lost to the chamber walls as particles or vapors. Loss of organic particles is treated as a first-order process [48] with a rate constant determined from the decay of BC measured by the aethalometer

$$C(t) = C_0 e^{-kt}$$

where C is the BC concentration at time t , C_0 is the initial BC concentration and k is the wall-loss rate constant. The wall-loss rate constant depends on the size and composition of the particles, turbulence in the chamber, the size and shape of the chamber, and particle charge [49]. Therefore, it was determined for each experiment by fitting each time series of BC data. Aethalometer measurements can be influenced by particle coating [50]; therefore, a single particle soot photometer (SP2, DMT, Inc.) was used in parallel with the aethalometer to quantify BC, and the two instruments showed excellent agreement: average difference between the wall-loss rates calculated from the aethalometer and the SP2 was 4% ($n=8$). The particle wall-loss rate for MDDV experiments ranged from 0.57 to 0.66 hr^{-1} (i.e., after approximately 1.5 hr the BC concentration decreased to 37% of its initial value). Wall-loss rates for

the HDDV without AT varied between 0.46 to 0.53 hr⁻¹ for different experiments. For experiments without enough BC to calculate a rate constant the decay of sulfate seed particles was used. In two experiments (D2.12 and D2.8) there was not enough BC or sulfate, and an average rate constant from the other experiments was used instead.

Using BC as a tracer for wall-loss assumes that it is internally mixed with the OA. This assumption was valid for most experiments because the size resolved data (SMPS and AMS) only showed growth of the primary mode aerosol. However, the majority of particle mass in the two regeneration experiments was formed from nucleation. Therefore, in these experiments it was necessary to adjust the wall-loss rate to account for the more rapid loss of smaller nucleation mode particles. This correction is discussed in the SI.

The loss of condensable organic vapors to wall-bound particles is constrained by considering two limiting cases: the first (Method #1) assumes that no organic vapors condense to wall-bound particles, and the second (Method #2) assumes that organic vapors remain in equilibrium with both wall-bound and suspended particles. The loss of organic vapors directly to the chamber walls (in distinction to their loss to wall-bound particles) is highly uncertain, and in keeping with virtually every other chamber study in the literature, we do not account for it here. If it were included, it would *increase* our estimate of SOA production.

Method #1 provides a lower bound estimate of the SOA mass production; it is equivalent to the “ $\omega = 0$ ” correction utilized in previous studies [22, 51]. Method #1 assumes that mass transfer resistance to the walls is much greater than to the suspended particles. This is a reasonable assumption since condensable vapors are in continuous, intimate contact with suspended particles, whereas their interaction with wall-bound particles is likely to be far less frequent. A consequence of this wall-loss assumption is that suspended and wall-bound particles may have different compositions.

Assuming no loss of vapors to the walls in Method #1, the rate at which OA mass is lost to the chamber walls is

$$\frac{d}{dt}(OA_{wall}) = OA_{sus}(-k) \quad (2)$$

where OA_{sus} is the AMS-measured (i.e., suspended) OA mass at time t and k is the negative wall-loss rate constant of black carbon [22]. The total OA in the chamber is calculated by numerically integrating equation (2) and adding the calculated OA lost to the wall to the measured OA concentration (equation (1)).

Method #2 assumes that particles lost to the walls during an experiment remain in equilibrium with the vapor phase. This case corresponds to the “ $\omega = 1$ ” correction [22]. The total OA mass at time t is equal to the suspended particle mass scaled by the ratio of the initial black carbon concentration to the black carbon concentration at time t

$$OA_{total,t} = OA_{sus,t} \cdot \frac{C_0}{C_t} \quad (3)$$

where C_0 is the initial black carbon concentration and C_t is the measured black carbon concentration at time t . As only *suspended* OA is referenced in equation (3), the PM on the wall and in suspension has the same composition.

In experiments with low BC concentrations, the total OA estimates from Method #2 can be noisy due to their inverse dependence on BC in (3). For such experiments, we implemented Method #2 using the previously described exponential fit to the BC data rather than the actual BC data themselves,

$$OA_{total,t} = \frac{OA_{sus,t}}{e^{-kt}} \quad (4)$$

where k is the wall-loss rate constant of black carbon.

Experiments of Weitkamp et al. [22] indicate that the rate of vapor uptake to particles on the walls is the same as the rate for suspended particles (Method #2), suggesting that the mass transfer resistance of organic vapors to wall-bound particles is comparable with that to suspended particles. Equations (3) and (4) indicate that in Method #2 the loss of organic vapors to particles on the walls scales with the mass fraction of particles on the walls to particles in suspension. Initially (before any particle loss) there is no loss of vapors to wall but it increases as an experiment progresses. Therefore, estimates based on Method #1 and #2 diverge as more particles are lost to the wall, and the uncertainty in the observed SOA production increases as an experiment progress [52]. Given this increasing uncertainty, we imposed a 5:1 upper bound on the ratio of OA on the wall to suspended OA. This condition was binding

in roughly half the experiments, and when it was binding, it was typically only later in the experiment after 1.5-2.5 hours of photo-oxidation. The average and range of OA from Methods #1 and #2 is reported in the results.

Chamber blank experiments performed after filling the chamber with CVS dilution air, HONO, and ammonium sulfate seed particles produced 1-3 $\mu\text{g}/\text{m}^3$ of SOA over a 3 hour photo-oxidation period. This SOA is likely formed from the residual vapors that desorb from the CVS, transfer line and chamber wall. Therefore, for every chamber experiment we assume an SOA blank of 0 $\mu\text{g}/\text{m}^3$ at $t=0$ that increases linearly to 2 $\mu\text{g}/\text{m}^3$ of SOA at $t=3$ h and subtract this artifact from the reported SOA production.

Wall-loss Rate Correction for Nucleation

Particle loss to chamber walls is a size-dependent process (smaller particles are lost faster); therefore, in regeneration experiments where a major fraction of the particle mass is created during a nucleation event, we must modify the wall-loss rate to account for the more rapid loss of nucleation mode particles compared to BC (which is in the accumulation mode). In these cases a large fraction of the OA mass is not internally mixed with BC. We corrected the wall-loss rate, k , in these experiments by assuming that wall-loss of nucleation mode particles is governed by Brownian diffusion. Crump and Seinfeld derived an expression for the size-dependent wall-loss rate for particles in a spherical chamber of radius R

$$k_w(D_p) = \frac{6\sqrt{k_e D}}{\pi R} D_1\left(\frac{\pi v_s}{2\sqrt{k_e D}}\right) + \frac{v_s}{4R/3} \quad (5)$$

where D is the Brownian diffusivity for particles of diameter D_p , k_e (units of time^{-1}) is a function of the turbulent kinetic energy in the chamber, v_s is the gravitational settling velocity of the particle (negligible for nucleation mode particles) and $D_1(\dots)$ is the Debye function [79].

Equation (5) indicates that the wall-loss rate scales with the square root of diffusivity, which in turn, is inversely proportional to particle diameter [39]. We therefore scale the wall-loss rate of the nucleation mode, k_{nuc} , using the wall-loss rate of the primary mode, k , and the diameters of the nucleation mode, d_{nuc} , and the primary mode, d

$$k_{nuc} = k \cdot \sqrt{\frac{d}{d_{nuc}}} \quad (6)$$

AMS Corrections: Comparison with SMPS Measurements

Theoretically, the sum of the PM mass from the non-refractory components (measured by the AMS) and BC (measured by the aethalometer) should be equal to the mass calculated from the SMPS size distributions. These three sets of data provide two independent methods of calculating PM, but each method has limitations, complicating the comparison.

First, the SMPS measures particle mobility diameter, while the AMS measures mass. To convert SMPS measurements to mass one must assume a particle shape and density. We assume that particles are spherical with average density of 1 g/cm³. However, fractal-like particles will cause the SMPS to overestimate the spherical equivalent diameter and therefore overestimate particle mass. While commonly made, the unit density [80] and sphericity [81-82] assumptions have both been shown to not always be valid for aerosol with high EC (e.g., diesel emissions). After SOA production begins the sphericity assumption improves as the organics coat the primary particles, making them more spherical [62].

Second, the mass measured by the AMS will be less than the true PM mass due to three artifacts whose product is referred to as the AMS collection efficiency, C_e :

$$C_e(d_{va}) = E_L(d_{va}) \times E_S(d_{va}) \times E_B(d_{va}) \quad (7)$$

where d_{va} is the particle vacuum aerodynamic diameter. The transmission efficiency, E_L , of the AMS's aerodynamic lens is size-dependent with a detection window that falls off above 600 nm and below 120 nm [83]. E_S is the striking efficiency, which refers to the tendency of non-spherical particles to miss the AMS's vaporizer as they are conveyed from the time-of-flight chamber. E_B quantifies the fraction of particles that bounce off of the AMS's vaporizer before they are measured. Bounce is a function of particle phase (solid/liquid), particle acidity and ambient RH, among other factors. For an internally mixed aerosol (which is likely in these experiments once SOA forms), the same collection efficiency should be used for all chemical species [84]. Losses due to striking efficiency appear to be less than 20% for ambient particles [85].

In several of the MDDV experiments (e.g., Figure S.2) the sum of the non-refractory components and BC were significantly lower than the mass calculated from the SMPS size distributions (assuming spherical particles and density of 1 g cm^{-3}). Such deviations are likely due differences in collection efficiency (e.g., E_S and E_B), and we assume that the difference in mass has the same chemical composition as the speciated components. We then calculate a scaling factor, $AMS_{s.f.}$, that increases the sizes of the four colored wedges in **Error! Reference source not found.** proportionally such that their sum closes the gap with the SMPS measurement (dashed line). The scaling factor is

$$AMS_{s.f.} = \frac{C_{SMPS} - C_{BC}}{C_{org} + C_{SO_4} + C_{NO_3} + C_{NH_4}} \quad (8)$$

where C_{SMPS} is the total particle concentration measured by the SMPS, C_{BC} is the black carbon concentration measured by the aethalometer, C_{org} , C_{SO_4} , C_{NO_3} , and C_{NH_4} are the concentrations of organics, sulfate, nitrate and ammonium measured by the AMS. The values for $AMS_{s.f.}$ were calculated for each time step after nucleation, excluding the times when the aerosol passed through the thermodenuder and then used to scale the AMS data for the MDDV. We set a maximum value of 2.0 for the $AMS_{s.f.}$.

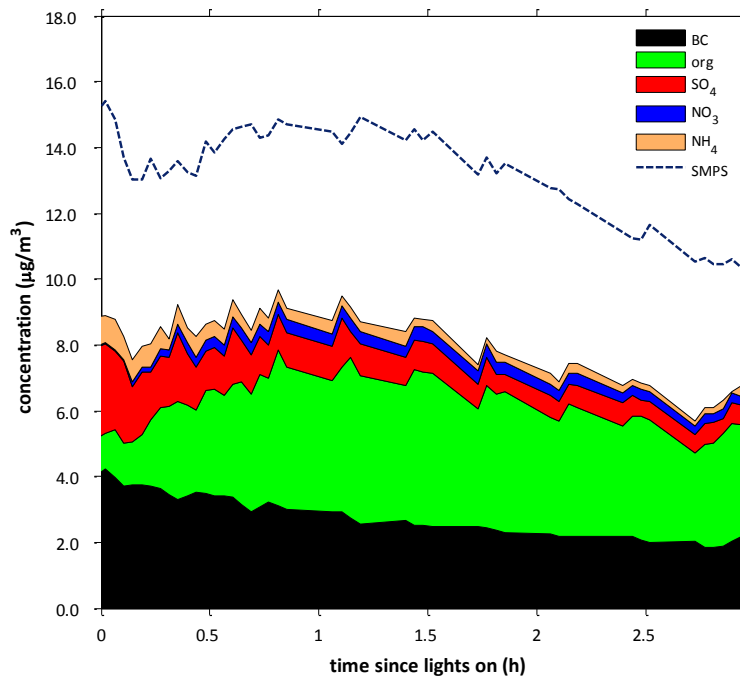


Figure S.2 Comparison of the sum of BC (measured by the aethalometer), organics, sulfate, nitrate and ammonium (measured by the AMS) against the total particle mass measured by the SMPS. Data are not wall-loss corrected.

Table S.2 Dynamometer driving test cycles. The UC was used with the MDDV, and the 2xUDDS and 3xcreep+idle were used with the HDDV. The older FTP-75 cycle was not used in these tests, but we include it for reference since it was more commonly used in the past.

driving cycle	duration (s)	distance (mi)	avg speed (mph)	max speed (mph)	max accel (mph/s)	stops/mile	% idle	notes
UC	2035	9.8	24.6	67.0	6.2	1.52	16.4	600 s hot soak w/o emissions sampling is not included in avg speed or % idle values
2xUDDS	2125	11.1	18.8	58.0	4.4	2.52	33.4	UDDS cycle is run 2 times consecutively
3xcreep + idle	2553	0.377	1.8	8.2	2.3	24.17	42.3	creep phase of the 4-phase HHDDT (251 s each) run 3 times + 1800 s idle (not included in avg speed or % idle values)
FTP-75	1377	7.5	19.6	56.7	3.3	2.41	19	for comparison only; not used in this study

Sources:

- <http://www.dieselnet.com/standards/cycles/hhddt.php>
- <http://www.arb.ca.gov/msei/onroad/briefs/Publication3.pdf>

Table S.3 Initial conditions in the chamber (except for NMOG, which is measured in the CVS) for all experiments with HDDV, MDDV and a dynamic blank (blank used air from the CVS, but no vehicle exhaust).

test date	expt ID	model year	vehicle class	eng. size (l)	mileage	emissions controls	fuel	driving cycle	VOC/NOx	seeded?	mpg	POA ($\mu\text{g}/\text{m}^3$)	BC ($\mu\text{g}/\text{m}^3$)	ΔCO_2 (ppm)	NO (ppb)	NO ₂ (ppb)	propene (ppm)	NMOG (ppmC)
7/11/2011	D1.1	2010	HHDD, Class 8 Tractor	14.9	11,000	*DOC, DPF, SCR	28% arom. ULSD	2xUDDS	3.1	Y	4.4	0.3	0.6	354	170	376	0.60	0.41
7/12/2011	D1.4							2xUDDS	3.0	Y	4.5	0.6	0.6	258	200	389	0.60	0.00
7/13/2011	D1.7							2xUDDS	3.8	Y	4.6	0.8	0.2	252	249	443	0.87	0.00
7/14/2011	D1.10							2xUDDS	3.3	Y	4.6	1.2	0.1	287	143	384	0.60	0.00
7/15/2011	D1.11							2xUDDS	3.1	Y	4.6	1.5	0.2	280	186	440	0.67	0.00
7/19/2011	D1.14							2xUDDS	3.1	Y	4.5	0.9	0.2	247	140	373	0.60	0.00
7/20/2011	D1.15							2xUDDS	3.1	N	n/a	1.9	4.4	243	299	335	0.73	2.13
6/9/2011	D2.2	2007	HHDD, Class 8 Tractor	12.8	22,000	*DOC, DPF	EPA hybrid ULSD	2xUDDS	3.1	N	4.9	0.0	1.1	107	0.4	0	0.13	0.00
6/16/2011	D2.13						2xUDDS	3.3	Y	4.9	n/a	0.3	248	250	727	1.10	0.00	
6/10/2011	D2.3						2xUDDS	3.0	Y	4.9	0.0	1.0	284	650	842	1.73	0.00	
6/13/2011	D2.8						2xUDDS	3.4	Y	4.8	1.0	-0.3	143	99	201	0.53	0.00	
6/14/2011	D2.7						2xUDDS	3.1	Y	5.0	1.3	-0.1	224	142	599	0.80	0.00	
6/15/2011	D2.12						2xUDDS	3.1	Y	4.9	0.5	0.2	303	180	727	0.93	0.00	
6/17/2011	D2.18						2xUDDS	3.1	Y	n/a	7.5	3.2	240	468	360	0.93	24.87	
6/22/2011	D3.1	2006	HHDD, Class 8 Tractor	10.8	94,000	*none	28% arom. ULSD	2xUDDS	3.5	Y	5.0	38.2	80.8	301	1057	436	1.73	244.69
6/23/2011	D3.4						2xUDDS	3.0	N	5.0	6.7	86.6	235	860	475	1.20	330.12	
6/24/2011	D3.5						3xcreep+idle	3.3	N	0.9	1.3	7.2	48	551	409	0.93	257.02	
6/28/2011	D3.9						2xUDDS	2.9	N	0.0	0.0	0.0	0	1059	434	1.33	319.49	
6/29/2011	D3.10						2xUDDS	3.0	N	5.0	7.6	91.7	275	1074	195	1.73	318.78	
6/30/2011	D3.13						2xUDDS	3.1	N	5.1	6.8	87.8	256	933	485	1.47	285.20	
7/1/2011	D3.14						2xUDDS	3.0	N	5.1	6.5	93.8	261	932	445	1.33	271.46	
6/11/10	D4.1	2005	MDV	6.6	65,934	DOC	ULSD	Cold UC	4.1	N	11.9	3.0	87.9	181	840	96	1.30	198.37
6/14/10	D4.2						ULSD	Cold UC	1.2	N	11.7	8.4	130.2	229	1326	154	0.50	124.42
6/18/10	D5.3						ULSD	Cold UC	3.2	N	14.4	14.4	94.9	147	1570	0	2.20	81.77
6/17/10	D5.2	2001	MDV	5.9	158,850	none	B100	Cold UC	3.8	N	13.0	9.3	33.3	181	1570	0	3.00	54.95
6/16/10	D5.1						B100	Cold UC	0.7	N	13.7	7.4	34.0	166	1570	0	0.50	50.16
Blank	7/18/2011	dyn blank	n/a	n/a	n/a	n/a	n/a	n/a	3.2	Y	n/a	0.5	1.2	1	397	274	0.73	0.00

* Additional emission controls listed in CARB executive order include: direct diesel injection, turbo charger, charge air cooler, powertrain or engine control module and exhaust gas recirculation.

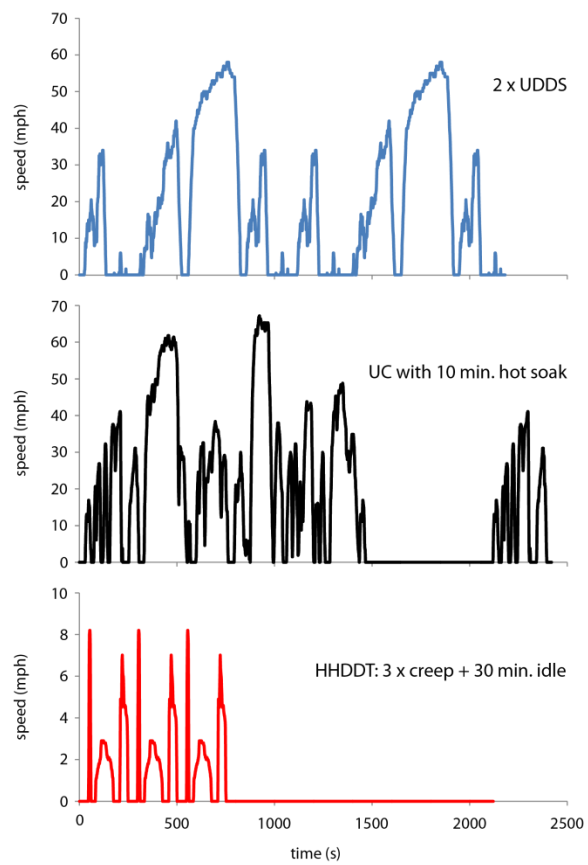


Figure S.3 The speed vs. time profiles of the three different driving cycles used in the smog chamber experiments.

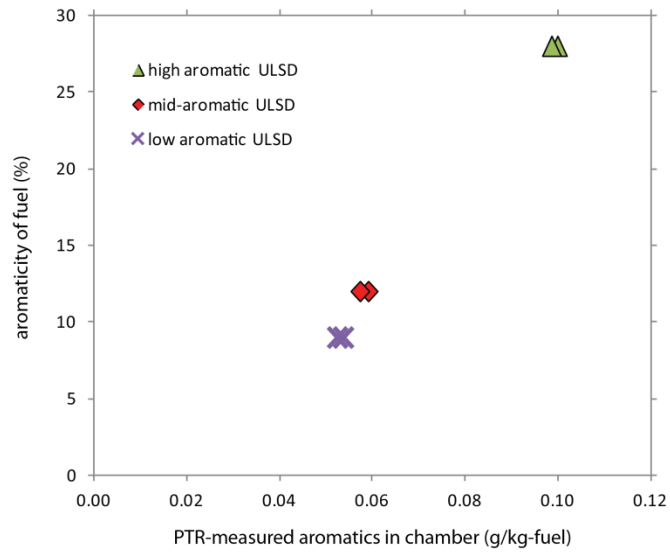


Figure S.4 Aromaticity of the three fuels used in the HDDV experiments is positively correlated with the aromaticity of their combustion emissions. Two duplicate experiments with each fuel are shown; in all six experiments driving cycle is 2xUDDS and vehicle is D3.

Table S.4 NMOGs as discussed in Figure 4, their OH reaction rates and the SOA yield cases in which they are included (Figure 6).

Hydrocarbons	Compound	measured in which expts?	SOA precursor (Fig. 4b)?	included only in lower SOA yield estimate (Fig. 6)?	OH rxn rate (cm³- molec⁻¹ sec⁻¹)
	ethane	both	no	no	2.48E-13
	ethene	both	no	no	8.52E-12
	propane	both	no	no	1.09E-12
	propene	both	no	no	2.63E-11
	methylpropane	both	no	no	2.12E-12
	ethyne	both	no	no	8.15E-13
	n-butane	both	no	no	2.36E-12
	1,2-propadiene	both	no	no	9.82E-12
	trans-2-butene	both	no	no	6.40E-11
	1-butene	both	no	no	3.14E-11
	2-methyl-2-butene	both	no	no	8.69E-11
	cis-2-butene	both	no	no	5.64E-11
	2,2-dimethylpropane	both	no	no	6.69E-13
	2-methylbutane	both	no	no	3.60E-12
	1-propyne	both	no	no	7.14E-12
	1,2-butadiene	both	no	no	2.60E-11
	1,3-butadiene	both	no	no	6.66E-11
	trans-2-pentene	both	no	no	6.70E-11
	2-methylpropene	both	no	no	5.14E-11
	1-pentene	both	no	no	3.14E-11
	2-methyl-1-butene	both	no	no	6.10E-11
	cis-2-pentene	both	no	no	6.50E-11
	1-buten-3-yne	both	no	no	4.01E-11
	2-butyne	both	no	no	2.73E-11
	1-butyne	both	no	no	8.10E-12
	1,3-butadiyne	MDDV	no	no	1.82E-11
	3-methyl-1-butene	MDDV	no	no	2.86E-11
	n-pentane	MDDV	no	no	3.80E-12
	2-methyl-1,3-butadiene	MDDV	no	no	1.00E-10
	3,3-dimethyl-1-butene	MDDV	no	no	2.80E-11
	trans-1,3-pentadiene	MDDV	no	no	1.60E-12
	2,2-dimethylbutane	MDDV	no	no	2.23E-12
	cyclopentene	MDDV	no	no	6.70E-11
	4-methyl-1-pentene	MDDV	no	no	3.02E-11
	3-methyl-1-pentene	MDDV	no	no	3.02E-11
	cyclopentane	MDDV	no	no	4.97E-12
	2,3-dimethylbutane	MDDV	no	no	5.78E-12
	2,3-dimethyl-1-butene	MDDV	no	no	5.38E-11
	methyl-tert-butyl-ether	MDDV	no	no	2.26E-12
	4-methyl-cis-2-pentene	MDDV	no	no	5.88E-11
	2-methylpentane	MDDV	no	no	5.45E-12
	4-methyl-trans-2-pentene	MDDV	no	no	6.64E-11
	3-methylpentane	MDDV	no	no	5.73E-12
	1-hexene	MDDV	no	no	3.70E-11
	2-methyl-1-pentene	MDDV	no	no	5.40E-11
	n-hexane	MDDV	no	no	6.97E+12
	trans-3-hexene	MDDV	no	no	6.62E-11

	Compound	measured in which expts?	SOA precursor (Fig. 4b)?	included only in lower SOA yield estimate (Fig. 6)?	OH rxn rate (cm ³ - molec ⁻¹ sec ⁻¹)
Hydrocarbons	cis-3-hexene	MDDV	no	no	5.86E-11
	trans-2-hexene	MDDV	no	no	6.66E-11
	2-methyl-2-pentene	MDDV	no	no	8.90E-11
	3-methyl-trans-2-pentene	MDDV	no	no	8.83E-11
	3-methylcyclopentene	MDDV	no	no	5.97E-11
	cis-2-hexene	MDDV	no	no	5.90E-11
	3-methyl-cis-2-pentene	MDDV	no	no	8.83E-11
	1-ethyl-tert-butyl-ether	MDDV	no	no	7.60E-12
	2,2-dimethylpentane	MDDV	no	no	3.23E-12
	methylcyclopentane	MDDV	no	no	5.66E-12
	2,4-dimethylpentane	MDDV	no	no	4.77E-12
	2,2,3-trimethylbutane	MDDV	no	no	3.81E-12
	3,4-dimethyl-1-pentene	MDDV	no	no	3.16E-11
	2,4-dimethyl-1-pentene	MDDV	no	no	5.54E-11
	1-methylcyclopentene	MDDV	no	no	8.94E-11
	benzene	both	yes	no	1.22E-12
	3-methyl-1-hexene	MDDV	no	no	3.16E-11
	3,3-dimethylpentane	MDDV	no	no	2.97E-12
	2,4-dimethyl-2-pentene	MDDV	no	no	8.94E-11
	cyclohexane	MDDV	no	no	6.97E-12
	2-methyl-trans-3-hexene	MDDV	no	no	6.74E-11
	4-methyl-trans-2-hexene	MDDV	no	no	6.80E-11
	2-methylhexane	MDDV	no	no	6.86E-12
	2,3-dimethylpentane	MDDV	no	no	7.14E-12
	cyclohexene	MDDV	no	no	6.77E-11
	3-methylhexane	MDDV	no	no	7.15E-12
	trans-1,3-dimethylcyclopentane	MDDV	no	no	6.80E-12
	cis-1,3-dimethylcyclopentane	MDDV	no	no	6.80E-12
	3-ethylpentane	MDDV	no	no	7.56E-12
	trans-1,2-dimethylcyclopentane	MDDV	no	no	6.80E-12
	2,2,4-trimethylpentane	MDDV	no	no	3.34E-12
	1-heptene	MDDV	no	no	4.00E-11
	3-methyl-trans-3-hexene	MDDV	no	no	8.92E-11
	trans-3-heptene	MDDV	no	no	6.76E-11
	n-heptane	MDDV	no	no	6.76E-12
	2,4,4-trimethyl-1-pentene	MDDV	no	no	5.32E-11
	2-methyl-2-hexene	MDDV	no	no	8.96E-11
	trans-2-heptene	MDDV	no	no	6.80E-11
	3-ethyl-2-pentene	MDDV	no	no	8.92E-11
	3-methyl-cis-2-hexene	MDDV	no	no	8.96E-11
	2,3-dimethyl-2-pentene	MDDV	no	no	1.03E-10
	cis-2-heptene	MDDV	no	no	6.04E-11
	methylcyclohexane	MDDV	no	no	9.64E-12
	2,2-dimethylhexane	MDDV	no	no	4.64E-12
	2,4,4-trimethyl-2-pentene	MDDV	no	no	8.77E-11
	ethylcyclopentane	MDDV	no	no	7.24E-12
	2,5-dimethylhexane	MDDV	no	no	8.27E-12
	2,4-dimethylhexane	MDDV	no	no	8.55E-12
	1,2,4-trimethylcyclopentane	MDDV	no	no	7.95E-12
	3,3-dimethylhexane	MDDV	no	no	4.38E-12
	1a,2a,3b-trimethylcyclopentane	MDDV	no	no	7.95E-12
	2,3,4-trimethylpentane	MDDV	no	no	6.60E-12
	toluene	both	yes	no	5.63E-12
	2,3,3-trimethylpentane	MDDV	no	no	4.37E-12
2,3-dimethylhexane	MDDV	no	no	8.55E-12	
2-methylheptane	MDDV	no	no	4.77E-12	
4-methylheptane	MDDV	no	no	8.56E-12	
3,4-dimethylhexane	MDDV	no	no	8.84E-12	
3-methylheptane	MDDV	no	no	8.56E-12	
cis-1,2-dimethylcyclohexane	MDDV	no	no	1.19E-11	

	Compound	measured in which expts?	SOA precursor (Fig. 4b)?	included only in lower SOA yield estimate (Fig. 6)?	OH rxn rate (cm ³ - molec ⁻¹ sec ⁻¹)
Hydrocarbons	trans-1,4-dimethylcyclohexane	MDDV	no	no	1.19E-11
	2,2,5-trimethylhexane	MDDV	yes	no	6.05E-12
	trans-1-methyl-3-ethylcyclopentane	MDDV	no	no	8.39E-12
	cis-1-methyl-3-ethylcyclopentane	MDDV	no	no	8.39E-12
	1-octene	MDDV	no	no	3.30E-11
	2,2,4-trimethylhexane	MDDV	yes	no	6.33E-12
	trans-4-octene	MDDV	no	no	6.90E-11
	n-octane	both	no	no	8.11E-12
	trans-2-octene	MDDV	no	no	6.94E-11
	trans-1,3-dimethylcyclohexane	MDDV	no	no	1.19E-11
	2,4,4-trimethylhexane	MDDV	yes	no	5.78E-12
	cis-2-octene	MDDV	no	no	6.18E-11
	2,3,5-trimethylhexane	MDDV	yes	no	9.96E-12
	2,4-dimethylheptane	MDDV	yes	no	9.97E-12
	cis-1,3-dimethylcyclohexane	MDDV	no	no	1.19E-11
	2,6-dimethylheptane	MDDV	yes	no	9.68E-12
	ethylcyclohexane	MDDV	no	no	1.20E-11
	3,5-dimethylheptane	MDDV	yes	no	1.02E-11
	ethylbenzene	both	yes	no	7.00E-12
	1,3,5-trimethylcyclohexane	MDDV	yes	no	1.35E-11
	2,3-dimethylheptane	MDDV	yes	no	9.97E-12
	m-xylene	both	yes	no	2.31E-11
	p-xylene	MDDV	yes	no	1.43E-11
	4-methyloctane	MDDV	yes	no	9.97E-12
	2-methyloctane	MDDV	yes	no	9.69E-12
	3-methyloctane	MDDV	yes	no	9.97E-12
	styrene	both	yes	no	5.80E-11
	o-xylene	both	yes	no	1.36E-11
	2,2,4-trimethylheptane	MDDV	yes	no	7.75E-12
	1-methyl-4-ethylcyclohexane	MDDV	yes	no	1.37E-11
	2,2,5-trimethylheptane	MDDV	yes	no	7.75E-12
	1-nonene	MDDV	yes	no	3.44E-11
	n-nonane	both	yes	no	9.70E-12
	3,3-dimethyloctane	MDDV	yes	no	7.21E-12
	(1-methylethyl)benzene	MDDV	yes	no	6.90E-12
	2,3-dimethyloctane	MDDV	yes	no	1.14E-11
	2,2-dimethyloctane	MDDV	yes	no	7.47E-12
	2,5-dimethyloctane	MDDV	yes	no	1.14E-11
	2,4-dimethyloctane	MDDV	yes	no	1.14E-12
	2,6-dimethyloctane	MDDV	yes	no	1.14E-13
	n-propylbenzene	MDDV	yes	no	5.80E-12
	1-methyl-3-ethylbenzene	MDDV	yes	no	1.39E-11
	1-methyl-4-ethylbenzene	MDDV	yes	no	7.44E-12
	1,3,5-trimethylbenzene	MDDV	yes	no	5.67E-11
	2-methylnonane	MDDV	yes	no	1.11E-11
	1-methyl-2-ethylbenzene	MDDV	yes	no	7.44E-12
	1,2,4-trimethylbenzene	MDDV	yes	no	3.25E-11
	(2-methylpropyl)benzene	MDDV	yes	no	8.71E-12
	(1-methylpropyl)benzene	MDDV	yes	no	8.50E-12
	n-decane	both	yes	no	1.10E-11
	1-methyl-3-(1-methylethyl)benzene	MDDV	yes	no	1.45E-11
	1,2,3-trimethylbenzene	MDDV	yes	no	3.27E-11
	1-methyl-4-(1-methylethyl)benzene	MDDV	yes	no	8.54E-12
	indan	MDDV	yes	no	8.28E-12
	1-methyl-2-(1-methylethyl)benzene	MDDV	yes	no	8.54E-12
	1,3-diethylbenzene	MDDV	yes	no	3.25E-11
	1-methyl-3-n-propylbenzene	MDDV	yes	no	1.52E-11
	1,4-diethylbenzene	MDDV	yes	no	3.25E-11
	1-methyl-4-n-propylbenzene	MDDV	yes	no	8.80E-12
	1,3-dimethyl-5-ethylbenzene	MDDV	yes	no	3.44E-11

	Compound	measured in which expts?	SOA precursor (Fig. 4b)?	included only in lower SOA yield estimate (Fig. 6)?	OH rxn rate (cm ³ - molec ⁻¹ sec ⁻¹)
Hydrocarbons	1,2-diethylbenzene	MDDV	yes	no	5.80E-12
	1-methyl-2-n-propylbenzene	MDDV	yes	no	8.80E-12
	1,4-dimethyl-2-ethylbenzene	MDDV	yes	no	1.69E-11
	1,3-dimethyl-4-ethylbenzene	MDDV	yes	no	1.76E-11
	1,2-dimethyl-4-ethylbenzene	MDDV	yes	no	1.69E-11
	1,3-dimethyl-2-ethylbenzene	MDDV	yes	no	1.76E-11
	n-undecane	both	yes	no	1.25E-11
	1,2-dimethyl-3-ethylbenzene	MDDV	yes	no	1.69E-11
	1,2,4,5-tetramethylbenzene	MDDV	yes	no	3.25E-11
	1,2,3,5-tetramethylbenzene	MDDV	yes	no	4.31E-11
	1-(dimethylethyl)-2-methylbenzene	MDDV	yes	no	6.74E-12
	5-methylindan	MDDV	yes	no	1.79E-11
	4-methylindan	MDDV	yes	no	1.79E-11
	1-ethyl-2-n-propylbenzene	MDDV	yes	no	9.47E-12
	2-methylindan	MDDV	yes	no	9.42E-12
	1,2,3,4-tetramethylbenzene	MDDV	yes	no	2.05E-11
	n-pentylbenzene	MDDV	yes	no	1.01E-11
	1-methyl-2-n-butylbenzene	MDDV	yes	no	1.02E-11
	naphthalene	MDDV	yes	no	2.30E-11
	1-(dimethylethyl)-3,5-dimethylbenzene	MDDV	yes	no	3.01E-11
	1,3-di-n-propylbenzene	MDDV	yes	no	1.08E-11
	n-dodecane	both	yes	no	1.32E-11
	Carbonyls	formaldehyde	MDDV	no	no
acetaldehyde		MDDV	no	no	1.50E-11
acrolein		MDDV	no	no	2.58E-11
acetone		MDDV	no	no	1.70E-13
propionaldehyde		MDDV	no	no	2.20E-11
crotonaldehyde		MDDV	no	no	3.62E-11
methacrolein		MDDV	no	no	2.90E-11
MEK		MDDV	no	no	1.33E-12
butyraldehyde		MDDV	no	no	2.40E-11
benzaldehyde		MDDV	yes	no	1.20E-11
valeraldehyde		MDDV	no	no	2.74E-11
m-tolualdehyde		MDDV	yes	no	1.70E-11
hexanal		MDDV	no	no	3.00E-11
Other	unidentified Kovats < 800	HDDV	no	no	2.79E-11
	unidentified Kovats ≥ 800	HDDV	yes	no	1.67E-11
	unspeciated NMOG	both	yes	yes	2.00E-11
	SVOC/IVOC	both	yes	yes	3.00E-11