

1 **Chemical data quantify Deepwater Horizon hydrocarbon flow rate and**
2 **environmental distribution**

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21 Abbreviations: DWH, Deepwater Horizon; ROV, remotely operated vehicle; GOR, gas to oil ratio; GC-
22 FID, gas chromatography-flame ionization detection; LMRP, lower marine riser package; BTEX, benzene,
23 toluene, ethylbenzene, and total xylenes; PAHs, polycyclic aromatic hydrocarbons; DOSS, dioctyl sodium
24 sulfosuccinate (di-(2-ethylhexyl) sodium sulfosuccinate); FWHM, full width at half maximum; pptv, parts
per trillion by volume.

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28 **Classification:**

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27 **Major Category:** PHYSICAL SCIENCES

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29 **Minor Category:** Environmental Sciences

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31 **Abstract.**

32 Detailed airborne, surface, and subsurface chemical measurements, primarily
33 obtained in May and June 2010, are used to quantify initial hydrocarbon compositions
34 along different transport pathways – in deep subsurface plumes, in the initial surface
35 slick, and in the atmosphere – during the *Deepwater Horizon (DWH)* oil spill.

36 Atmospheric measurements are consistent with a limited area of surfacing oil, with
37 implications for leaked hydrocarbon mass transport and oil drop size distributions. The
38 chemical data further suggest relatively little variation in leaking hydrocarbon
39 composition over time. While readily soluble hydrocarbons made up ~25% of the
40 leaking mixture by mass, subsurface chemical data show these compounds made up
41 ~69% of the deep plume mass; only ~31% of deep plume mass was initially transported
42 in the form of trapped oil droplets. Mass flows along individual transport pathways are
43 also derived from atmospheric and subsurface chemical data. Subsurface hydrocarbon
44 composition, dissolved oxygen, and dispersant data are used to provide a new assessment
45 of release of hydrocarbons from the leaking well. We use the chemical measurements to
46 estimate that $(7.8 \pm 1.9) \times 10^6$ kg of hydrocarbons leaked on June 10, 2010, directly
47 accounting for roughly three-quarters of the total leaked mass on that day. The average
48 environmental release rate of $(10.1 \pm 2.0) \times 10^6$ kg/day derived using atmospheric and
49 subsurface chemical data agrees within uncertainties with the official average leak rate of
50 $(10.2 \pm 1.0) \times 10^6$ kg/day derived using physical and optical methods.

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53 **Introduction.**

54 Knowledge of the composition, distribution, and total mass of the hydrocarbon
55 mixture (gas plus oil) emitted following loss of the *Deepwater Horizon (DWH)* drilling
56 unit is essential to plan mitigation approaches and to assess environmental impacts of the
57 resulting spill. Estimates of *DWH* hydrocarbon flow rate were originally derived using
58 physical and optical methods applied during the spill; values were subsequently refined
59 and an official government estimate of oil flow rate was published (1). Analysis of
60 airborne atmospheric chemical data provided information on hydrocarbon evaporation
61 into the air and a lower limit to the flow rate (2); however, a more detailed description of
62 environmental distribution has not been available. Here we present combined
63 atmospheric, surface, and subsurface chemical data to better constrain physical transport
64 pathways, and the resulting composition and mass flow rate of *DWH* hydrocarbon
65 mixtures along each pathway, following subsurface release from the leaking well in
66 early- to mid-June 2010.

67 Our analysis primarily focuses on the period following installation of Top Hat #4
68 on June 3 (3), which includes flights by a chemically-instrumented P-3 aircraft (2, 4) and
69 ROV sampling of leaking fluid at the well (5), and ends roughly in late June at the
70 conclusion of the R/V *Endeavor* cruise (Fig. S1). The suite of deployed subsurface,
71 surface, and airborne measurements offers spatial, temporal, and chemical detail that is
72 unique to this period and to this spill. We use atmospheric, surface, and subsurface
73 measurements of hydrocarbons, dissolved oxygen, and dispersant from throughout this
74 period, and consider additional chemical data following closure of the well, to define the

75 initial compositions, distributions, and mass flow rates of the hydrocarbon mixtures
76 evolving along different pathways following release into the marine environment.

77

78 **Results.**

79 **1. Composition data constrain physical transport pathways**

80 *DWH* hydrocarbons were released at ~1500 m depth in a high-pressure jet,
81 resulting in gas bubbles and liquid oil droplets with an initial number and volume
82 distribution that is not yet well quantified (1). Size and chemical composition of the
83 hydrocarbon bubbles and droplets evolved extremely rapidly following release from the
84 well (6). A complex interplay of physical processes determined hydrocarbon-water
85 plume mixing dynamics (7, 8) and affected the composition and three-dimensional
86 distribution of the hydrocarbon mixtures within the water column, at the surface in the
87 resulting oil slick, and in the overlying atmosphere (2).

88 Prediction of mass fluxes along environmental transport pathways following a
89 deepwater blowout requires accurate understanding of time-dependent dynamical
90 behavior and evolving chemical composition along various transport pathways, on time
91 scales of seconds to weeks following release. Three observed features of the *DWH* spill
92 offer key insights into marine transport pathways:

93

94 **a. Short surfacing time constrains oil droplet size.** Visual observations from
95 response vessels suggested a ~3-hour lag time between deliberate intervention at
96 the well and the onset of change in the fresh surface slick. This time corresponds
97 to a mean buoyant velocity of 0.14 m/sec from 1500 m depth and is generally

98 consistent with the 70-minute surfacing time observed during the DeepSpill
99 experiment following an intentional release of gas and oil from 844 m depth in the
100 North Sea (9). Further, narrow atmospheric plumes observed under nearly
101 orthogonal wind directions on June 8 and June 10, 2010 by the NOAA P-3
102 aircraft (2) indicate that the surface expression was limited to a small area
103 laterally offset 1.0 ± 0.5 km from the well, a finding also consistent with
104 observations from the DeepSpill experiment (9). Acoustic Doppler current
105 profiler data recorded at the well site
106 (www.ndbc.noaa.gov/download_data.php?filename=42916b2010.txt.gz&dir=data/historical/adcp2/) indicate a net horizontal velocity (integrating from depths of
107 1200 m to the surface) of ~0.03 m/sec on June 8 and 10, 2010. Combined with
108 the lateral offset at the surface, this would imply a mean vertical transport time of
109 no more than ~10 hours, corresponding to a mean buoyant velocity of no less than
110 ~0.05 m/sec. The 3-10 hour lag time indicates that droplets with ~millimeter-
111 scale diameters transported the majority of the surfacing hydrocarbon mass (Figs.
112 S3a and b) (10, 11). This average diameter is consistent with visual observations
113 of droplet size distributions within the near-field plume source regions, both prior
114 to and after shearing of the well riser pipe (5, 12), and approaches the maximum
115 stable droplet diameter of ~10 mm (13).

117 **b. Small surfacing area implies a narrow droplet mass distribution.** Gaussian
118 fits to data in the narrow atmospheric plume of hydrocarbons, with no detectable
119 volatile hydrocarbon mass outside of the narrow plume (Fig. 1b) ~10 km
120 downwind of *DWH* (2) imply that essentially all of the buoyant mass surfaced

121 within a ~2 km² area (Fig. 1a and b). This is a robust result, as the airborne
122 instruments were sufficiently sensitive to have detected and quantified a similar
123 mass of oil surfacing over an area of ~2000 km² with a plume signal-to-noise ratio
124 of ~60 for alkanes and ~25 for aromatics (Fig. S2). However, the airborne
125 measurements provide strong evidence that negligible mass surfaced outside of
126 the ~2 km² area immediately adjacent to the spill site (Figs. 1c and d).

127 **c. Atmospheric hydrocarbon relationships imply minimal variability in**
128 **surfacing times.** Within the atmospheric plume, the tight correlations and single
129 molar enhancement ratios, defined as $\Delta[X_A]/\Delta[X_B]$ between pairs of alkanes A
130 and B with different solubility and volatility, and aromatic-alkane pairs of
131 different solubility (Fig. 1c and d), provide further direct evidence for a narrow
132 distribution of surfacing times. Surfacing times appreciably shorter or longer than
133 3-10 hours would have resulted in lesser or greater removal of partially soluble
134 hydrocarbons and thus variable atmospheric enhancement ratios for a given
135 hydrocarbon pair. The tight correlation between each hydrocarbon pair (Fig. 1)
136 provides further evidence for a narrow mass distribution of large droplets (11).

137
138 The available atmospheric observations thus argue for a single pathway transporting
139 the majority of surfacing hydrocarbon mass directly and promptly to the surface. We
140 conclude that the surface oil slick was fed primarily by this single pathway, with
141 negligible mass transported to the surface via smaller droplets surfacing after longer
142 transport times and thus at greater distances from the well (Fig. 1a).

143 The available subsurface observations have been described in detail elsewhere (5,
144 14-22). These reports conclude that the majority of subsurface mass was detected
145 generally between 1000 and 1300 m depth in concentrated deep hydrocarbon plumes.
146 This finding is consistent with a physical mechanism that predicts formation of horizontal
147 intrusions, or plumes, of dissolved species and small undissolved droplets of liquid oil
148 formed in the turbulent *DWH* jet (8). Although concentration enhancements outside of
149 these plume depths have been reported (*e.g.*, (17, 21)) no significant *DWH* hydrocarbon
150 mass enhancement above or below these discrete layers is evident in the subsurface
151 chemical data to date (5, 14-22). Numerical simulations of this mechanism predict the
152 observed depth of the deep plumes (8) and further predict additional discrete plumes at
153 shallower depths with negligible mass compared to the deep plumes.

154 In the following sections we interpret the available chemical data in terms of a
155 simplified model in which leaked *DWH* hydrocarbon mass was transported primarily
156 along two initial pathways, either directly into the deep plume or directly to the surface;
157 after surfacing, further evaporation into the air occurred (Fig. 1a).

158

159 **2. Composition data quantify partitioning into dissolved, evaporated, and**
160 **undissolved hydrocarbon mixtures**

161 Here we compare the measured hydrocarbon compositions of atmospheric and
162 subsurface *DWH* plume samples to the composition leaking from the Macondo well;
163 observed differences define the extent and nature of alteration due to dissolution and
164 evaporation over time along different transport pathways (2). The hydrocarbon
165 composition of subsurface samples can further be altered on multi-day time scales by

166 differential biodegradation during transport from the well (14, 16, 17, 19, 21). To
167 minimize this confounding effect, the analysis here considers hydrocarbon composition
168 data from the closest and most concentrated subsurface samples, *i.e.*, those taken within 5
169 km of the well and characterized by very large concentration enhancements ($\text{CH}_4 >$
170 $45,000 \text{ ng}/\mu\text{L}$ seawater or toluene $> 1,000 \text{ ng}/\mu\text{L}$ seawater).

171

172 **Leaking fluid composition data defines transported mixtures.**

173 The *DWH* drilling unit was destroyed due to uncontrolled high-pressure release of
174 natural gas and liquid oil (3). The hydrocarbon composition leaking into the Gulf of
175 Mexico may have differed from the composition measured in the pre-spill reservoir, due
176 to potentially abrupt reservoir composition changes associated with the blowout, phase
177 separation, fractionation, or gas washing (23) within the flowing reservoir during the
178 ensuing 83-day spill. A previous report (2) calculated the distribution of gas and oil
179 compounds between the atmosphere and the water column, and a lower limit to the
180 leaking mass flow rate, by assuming the composition of leaking fluid was unchanged
181 from the pre-spill reservoir composition. This assumption resulted in a large uncertainty
182 in the lower limit flow rate calculated from airborne atmospheric hydrocarbon data alone
183 (2). This uncertainty is minimized, and partitioning and mass flow estimates improved,
184 by use of composition data from a sample of leaking fluid taken during the spill (5).

185 The hydrocarbon composition of a sample taken directly within the leaking
186 LMRP (5) is qualitatively similar (Fig. 2a) to that inferred from pre-spill analysis of
187 reservoir fluid (2). Different values of the derived gas-to-oil ratio (GOR) result primarily
188 from the different abundances of compounds in the gas fraction (*i.e.*, CH_4 through

189 isomers of C₅; Fig. 2a and Fig. S4a). Additional differences are noted but have a
190 proportionally smaller effect on the conclusions presented here. Analytical uncertainties
191 of $\pm 5\%$, with no additional uncertainty due to unspecified treatment of chromatographic
192 unresolved complex material (UCM) (2) in the analysis of the leaking fluid (see Fig. S2
193 in (5)), significantly improve the utility of atmospheric data to determine hydrocarbon
194 distributions between the air and the water column and to quantify hydrocarbon mass
195 flow rates, as described separately below.

196 Use of the leaking fluid composition (5) leads to a calculated distribution of *DWH*
197 hydrocarbons between air and water similar to that previously derived using the inferred
198 pre-spill composition (2). The mass fraction of each compound *X* in air is

199
200 The numerator is the slope of a linear regression to X and 2-methylheptane measured in
201 the atmosphere, and the denominator is the mass abundance of X relative to 2-
202 methylheptane in the leaking fluid (5). Here we normalize to 2-methylheptane, but the
203 results are insensitive to the choice of undissolved and volatile hydrocarbon for the
204 denominator. The present analysis utilizes atmospheric hydrocarbon data obtained from
205 ships and the P-3 aircraft between mid-May and end of June 2010, sampling a much
206 longer time period than the two days previously reported (2). The overall picture
207 developed from this larger atmospheric data set and the leaking fluid composition is
208 qualitatively similar to that reported in (2), and is shown graphically in Fig. 2b. The air-
209 water distribution of individual hydrocarbon species reported below is highly constrained

210 by the chemical data; uncertainties of $\pm 10\%$ in the calculated distributions are determined
211 by propagation of GC-FID calibration uncertainties of $\pm 5\%$ (5, 24). The general
212 similarity of the atmospheric composition, illustrated by data taken over the period of a
213 month, suggests little change in the average composition of the surfacing *DWH*
214 hydrocarbon mixture during this period.

215

216 *Hydrocarbon mixture remaining subsurface.* *DWH* hydrocarbon transport into
217 the subsurface resulted from two separate processes operating simultaneously during the
218 spill (8). The first process involved dissolution of hydrocarbons from large, mm-scale
219 diameter buoyant droplets during ascent to the surface. Continued buoyant ascent
220 physically transported the resulting droplets out of the trapped intrusion (8), leaving
221 behind dissolved hydrocarbons in the subsurface. The dissolved hydrocarbon
222 composition is determined from observed differences between atmospheric *DWH* plume
223 composition measured from surface ships and aircraft (2) and the leaking composition
224 measured directly in the well (5). Dissolved mass fractions are given by (1 – fraction of
225 X in air) for compounds more soluble than 2-methylheptane, and are set to zero for less
226 soluble species (filled red squares, upper panel in Fig. 2b). Multiplying these mass
227 fractions by leaking fluid mass abundances gives the dissolved mixture composition,
228 which accounted for ~25% of the mass of the leaking mixture. Methane (CH_4), ethane
229 (C_2H_6), propane (C_3H_8), and isomers of butane (C_4H_{10}) accounted for 89% of the
230 dissolved hydrocarbon mass.

231 The second process transporting hydrocarbons into the persistent subsurface
232 plumes involved physical trapping of small droplets of leaking hydrocarbon fluid (8).

233 Trapped small droplets are expected to remain suspended following loss of dissolved
234 hydrocarbons into the surrounding seawater (8). We focus on the deep plume data
235 because subsurface samples (5, 14, 16-22) show little evidence for substantial
236 hydrocarbon mass initially deposited at depths above 1000 m or below 1300 m. The
237 relative contribution from *a*) dissolved hydrocarbon mass and *b*) suspended droplet mass
238 in the deep plume is estimated by comparing subsurface plume chemical composition
239 data to the composition of the unmodified leaking fluid and to its dissolved fraction,
240 below.

241 The deep plume composition is identical to that of the leaking fluid for the highly
242 soluble species, but begins to differ for less soluble species., Published subsurface data
243 on alkanes larger than propane, and aromatics larger than toluene (14-17), were examined
244 for samples within 5 km of the well and for which measured methane >45,000 ng/ μ L of
245 seawater or toluene > 1,000 ng/ μ L of seawater. These concentrated near-field plume
246 measurements (blue squares in Figs. 3a, b, and c) are normalized to the most soluble
247 measured compound and compared to the compositions of dissolved (red circles) and
248 leaking (black bars) mixtures defined above. In each published data set, the observed
249 pattern of subsurface hydrocarbons relative to measured methane reported in Joye *et al.*
250 (2010) (Fig. 3a), benzene in Camilli *et al.* (2010) (Fig. 3b), or toluene in Hazen *et al.*
251 (2010) (Fig. 3c), respectively, approximates the composition of just the dissolved fraction
252 of the leaking mixture. The deep persistent subsurface plumes were primarily composed
253 of dissolved species and were relatively depleted in the more sparingly soluble species.
254 This finding, based on subsurface chemical measurements, is qualitatively consistent with
255 a standard oil drop size parameterization (11) in which droplet number decreases

256 exponentially with increasing diameter, suggesting proportionally little mass can be
257 transported in the form of suspended droplets of liquid oil (Fig. S3b).

258 However, the actual drop size distributions of the DWH leaks are not known, and
259 may not be well described by this standard parameterization. Since transport in the
260 subsurface is highly dependent on the actual drop size distribution (8), the mass initially
261 suspended in the deep plumes as small droplets of oil remains one of the largest
262 uncertainties in the *DWH* hydrocarbon budget to date. Initially suspended droplets are
263 predicted (8), were positively identified by ROV cameras (14), and are qualitatively
264 confirmed by published subsurface enhancements of sparingly soluble polycyclic
265 aromatic hydrocarbons (PAHs) (15, 16). These latter composition measurements, all
266 taken very close to (within 1 km radius of) the leaking well, are not sufficient to quantify
267 hydrocarbon mass transported in the form of suspended droplets. No direct
268 measurements have been presented to quantify this suspended mass to date.

269 To begin to address this uncertainty, here we use chemical data to define the
270 fractional contribution of sparingly soluble compounds relative to dissolved compounds
271 for samples taken in the deep persistent plume. An approximate estimate is afforded by
272 further analysis of published data (16) on C₁₀ to C₃₂ *n*-alkanes from samples taken within
273 the concentrated deep plume at varying distances from the well (Fig. 3d). These data
274 show a large systematic depletion (by ~85%) of heavier *n*-alkanes relative to the highly
275 soluble aromatic compound toluene (C₇H₈), further demonstrating that proportionally
276 little mass was transported into the deep plume in the form of suspended small droplets.
277 Minimal biodegradation in these samples is indicated by (*n*-C₁₇/pristane) and (*n*-
278 C₁₈/phytane) ratios (Fig. 3d) similar to those in the leaking fluid. Sparingly soluble *n*-

279 alkane mass abundances of ~15% (range 5 to 25%; Fig. 3d) in the deep plume relative to
280 the leaking fluid suggests that 31% (range 13 to 43%) of the subsurface plume mass can
281 be accounted for by transport of hydrocarbons in the form of initially suspended droplets.
282 We note this conclusion is qualitatively consistent with *DWH* simulations showing that
283 only small droplets were trapped (8), and extrapolations from standard dispersed oil
284 droplet size parameterizations (Fig. S3b) suggesting that small droplets do not transport
285 the bulk of the mass (11). However, a different drop size distribution could also be
286 consistent with these observations. More accurate size information through the full range
287 of potential drop size diameters is needed to further constrain these extrapolations.

288

289 *Volatile mixture evaporating to the atmosphere.* Undissolved volatile and semi-
290 volatile hydrocarbons evaporate on characteristic time scales of hours to days after
291 reaching the surface (2, 4, 25). The undissolved and volatile hydrocarbon mixture
292 evaporating within 2-3 hours of surfacing (2) was determined directly with uncertainties
293 of $\pm 10\%$ (24) using shipborne and airborne measurements of CH₄ through *n*-C₁₁. The
294 evaporated fraction of unmeasured semi-volatile hydrocarbons greater than *n*-C₁₁ is
295 calculated (Fig. S5a) using the volatility distribution of the oil mixture determined from
296 the chemical composition and the net evaporation measured in the laboratory (4). The
297 sum of volatile and semi-volatile masses (Fig. 2b) shows that 14% of the surfacing
298 mixture was both sufficiently insoluble to reach the surface and sufficiently volatile to
299 evaporate from the slick within 1-2 days of surfacing. As not all the leaked mass reached
300 the surface, a smaller percent actually evaporated; this amount is quantified below.

301 Summing the amounts dissolved and evaporated shows that these processes
302 together reduced the mass of hydrocarbons in the surface slick by $(1 - (0.75 * 0.86)) =$
303 0.36, or approximately one-third, relative to the slick mass that would have occurred in
304 the absence of these processes. Further evaporation of less-volatile compounds likely
305 removed little additional mass from the slick after the second day (26). The evaporating
306 mixture chemical composition is shown graphically in Fig. 4a; *n*-heptane, *n*-octane, *n*-
307 nonane, and methylcyclohexane were the four most abundant hydrocarbons by mass in
308 the evaporating mixture.

309 The atmospheric composition data taken aboard surface vessels and the research
310 aircraft, together with the subsurface composition data, demonstrate relatively little
311 variation in evaporating hydrocarbon composition from late May through the end of June
312 2010 (Fig. 2b). The F/V *Eugenie* cruise data were taken prior to shearing the broken riser
313 pipe on June 2 and installation of the LMRP cap on June 3. The atmospheric data taken
314 subsequently showed no significant change following this event (Fig. 2b), suggesting
315 little change in the composition of the surfacing hydrocarbon mixture as a result of this
316 intervention. The absence of atmospheric CH₄ enhancements associated with any *DWH*
317 hydrocarbons in these data (Fig. 2b) confirms earlier reports of complete CH₄ dissolution
318 in the subsurface (2, 18, 19, 21, 22, 27), and demonstrates that no emissions of CH₄ to the
319 atmosphere were detected through at least the first two months of the spill. These
320 atmospheric measurements further demonstrate that leaked benzene (C₆H₆) was nearly
321 completely removed in the water column, minimizing its impact at the surface.

322

323 *Hydrocarbon mixture remaining in the surface oil slick.* Leaked and surfacing
324 hydrocarbons that neither dissolved nor evaporated within the first 1-2 days of surfacing
325 determined the initial composition of the persistent surface oil slick. Slick chemical
326 composition ~2 days after surfacing is shown graphically in Fig. 4b; *n*-C₁₇, *n*- C₁₆, *n*-C₁₈,
327 and *n*-C₁₅ were the four most abundant hydrocarbons by mass in the initial surface slick.
328 Slick composition inferred from the airborne and shipborne atmospheric data is
329 qualitatively confirmed by GC-FID analysis of oil samples taken from R/V *Endeavor*
330 directly in the surface slick 1.5 km horizontally from the well on June 20, 2010 (Fig. S5b,
331 lower trace).

332

333 **3. Composition data constrain mass flow along different transport pathways**

334 The combined data sets are used to estimate the mass flow rates of leaked
335 hydrocarbons along each of the identified transport pathways (Fig. 4d) in early June 2010
336 that can be accounted for by the available chemical composition measurements. These
337 are compared to the consensus government estimate of total mass flow from the well,
338 calculated from the official volume flow rate estimate (1) in barrels of liquid oil (Fig. S1,
339 black circles). Total hydrocarbon mass flow rate, including the gas fraction, is calculated
340 by multiplying the government estimate of leaked oil volume flow by 132.2 kg per stock
341 tank barrel of liquid oil and by a mass ratio of ((gas + oil)/oil) = 1.31±0.08 measured at 1
342 atmosphere and 15.6 °C from the WHOI sample of leaking fluid (5) (Fig. S1, red circles),

343

344 *i). DWH hydrocarbon mass recovered to the surface ship*

345 *Discoverer Enterprise* was the only surface ship recovering hydrocarbons in early
346 June 2010 via the installed LMRP cap (Top Hat #4); liquid oil was collected after
347 separation from recovered gas, which was combusted continuously in a flare. Airborne
348 data in the atmospheric CO₂ plume downwind of the flare on June 10 verify, within error
349 limits, gas and oil recovery rates reported for *Discoverer Enterprise* (2). We use the
350 reported value of 15402 barrels of liquid oil recovered on June 10, 2010 (13), a gas-to-oil
351 ratio (GOR) of 1600 standard cubic feet per stock tank barrel consistent with the leaking
352 fluid composition (5), and estimate a ±10% uncertainty to derive a mass flow of (2.7 ±
353 0.3) x10⁶ kg/day of hydrocarbons recovered via the cap on June 10, with the gas fraction
354 flared and the liquid fraction collected in a tanker. Flared gas and recovered oil amounts
355 are shown schematically in Fig. 4d.

356

357 ***ii). Hydrocarbon evaporation to the atmosphere.***

358 The airborne data on June 10, 2010 show a steady-state atmospheric hydrocarbon
359 mass flux of (0.46±0.23) x10⁶ kg/day (Fig. 4d), which is the sum of directly measured
360 hydrocarbon mass evaporating within ~2-3 hours of surfacing (2) plus the lesser-volatile
361 hydrocarbon mass evaporating within 1-2 days of surfacing as inferred from atmospheric
362 aerosol data (4). The uncertainty of ±50% is primarily due to uncertainties in the
363 integration of atmospheric plume hydrocarbon data. These values are indicated in Fig.
364 4d.

365

366 ***iii). Hydrocarbon flow into the surface oil slick.***

367 An estimate of mass flow into the surface slick is obtained by summing the
368 dissolved and evaporated masses, and subtracting this sum from the initially buoyant
369 plume mass (after (2), from the slope of the linear fit (red line) in Fig. S4b) of (2.0 ± 1.0)
370 $\times 10^6$ kg/day. This estimate suggests that $(1.0 \pm 0.5) \times 10^6$ kg/day of leaked hydrocarbons
371 were producing the surface slick in early June.

372 Analysis of airborne remote sensing data from the AVIRIS instrument overflights
373 suggested a lower limit to the average daily flow into the surface slick of (0.68 to 1.30)
374 $\times 10^6$ kg/day (129,000 to 246,000 barrels of detectable liquid oil remaining on the surface
375 25 days after the spill began) (28). This value is consistent with the estimate from P-3 *in*
376 *situ* measurements, although different amounts of hydrocarbons were being recovered to
377 the surface on these two dates. The flow rate into the slick derived from *in situ*
378 measurements on June 10, 2010 indicated in Fig. 4b suggests a relatively small fraction,
379 roughly 13% of the total mass escaping the cap and leaking into the subsurface, formed
380 the persistent, visible surface slick. This likely contributed to a low bias in early oil leak
381 rate estimates that relied upon visual observations of the surface slick (29).

382

383 **iv). Hydrocarbon flow into the subsurface plume.**

384 Subsurface hydrocarbon mass is estimated using measurements of dissolved
385 oxygen (DO) deficits in the deep hydrocarbon plumes. Kessler et al. (2011) integrated
386 the detected far-field plume DO deficits to estimate a total of $(3.5 \pm 0.5) \times 10^{10}$ moles of
387 oxygen were consumed during bacterial respiration of DWH hydrocarbons, using data
388 generated on research cruises in August-October 2010 after flow from the well had
389 ceased. They derived a similar value using the observed near-field relationship between

390 DO and the surfactant dioctyl sodium sulfosuccinate (DOSS) in the deep plumes (18-20).
391 This deficit in DO was sufficient to respire all emitted *DWH* methane in the official
392 estimate (1), plus substantial additional mass of non-methane hydrocarbons (19). A
393 hydrocarbon mass flux into the persistent deep plume of $(3.6 \pm 0.8) \times 10^6$ kg/day averaged
394 over the 83-day spill is calculated by scaling the integrated DO anomaly by the mass of
395 the dissolved compounds (Fig. 2b), the estimated mass of suspended droplets, and by O₂
396 respiration stoichiometry appropriate to each hydrocarbon in this mixture (Table S1).

397 This calculation assumes complete biodegradation to CO₂ of dissolved
398 hydrocarbons, of which methane (18, 19), ethane (21), propane (21), and isomers of
399 butane (17) account for 89% of the mass (Table S1). It further assumes that by the
400 August-September cruise dates all hydrocarbon mass was biodegraded (Table S1). The
401 biodegraded fraction of hydrocarbons has not been directly measured, and it is likely to
402 have been negligible for the heaviest hydrocarbons; thus, the calculation represents a
403 lower limit to hydrocarbon mass flow into the deep plume. We note that deriving
404 hydrocarbon mass from the observed DO anomaly is sensitive to the assumed
405 composition and extent of biodegradation of the subsurface plume. Error limits
406 encompassing these sensitivities are estimated by assuming a range of 5 to 25% for the
407 heavy *n*-alkane fractions (shaded region in Fig. 3d), leading to a range of 13 to 43%
408 calculated for the plume mass initially transported in the form of suspended oil droplets.
409 Under these assumptions, the calculated mass flow of $(3.6 \pm 0.8) \times 10^6$ kg/day into the
410 subsurface plumes was the primary flow path for leaked *DWH* hydrocarbons, as shown in
411 Fig. 4d, and was composed primarily of dissolved species.

412

413 **v). Composition data constrain hydrocarbon release into the environment**

414 A total DO-removing potential in the deep plume of (0.041 ± 0.008) moles O₂/g
415 of hydrocarbon is calculated (Table S1) from the deep plume chemical composition,
416 above. Dividing this into the total integrated DO anomaly of $(3.5 \pm 0.5) \times 10^{10}$ moles O₂
417 removed over the 83 days of the spill results in an average daily environmental
418 hydrocarbon release into the water column of $(10.1 \pm 2.0) \times 10^6$ kg/day (Fig. 5; Table S1).
419 This hydrocarbon mass flow rate based on the available chemical data agrees, within the
420 uncertainties, with the official estimate of environmental release by subtracting recovered
421 amounts from the official flow rate of $(10.3 \pm 1.2) \times 10^6$ kg/day of gas and oil estimated for
422 June 10, 2010 based on physical and optical data (1).

423

424 **Discussion.**

425 Although the totals agree quantitatively, we note that the sum of chemically
426 detected mass flows along individual transport pathways (Fig. 4d) is lower than the
427 average environmental release rate inferred from the DO anomaly. While the simplified
428 model shown in Fig. 1 is generally consistent with the available subsurface and
429 atmospheric chemical data, it does not rule out additional mass transported outside of the
430 deep plumes but not yet detected in the chemical data. A specific gravity < 1 is expected
431 for the mixture remaining after removal of soluble species; thus, dissolution alone is not
432 expected to cause suspended droplets to descend out of the deep plume. A potential
433 transport pathway could instead involve gradual ascent, on hours-to-days time scales,
434 after the initial trapping of small hydrocarbon droplets into the deep plume (8), which
435 would distribute the corresponding hydrocarbon mass into a larger volume of the

436 subsurface as a function of rise velocity, thus droplet size. Absent measured data
437 throughout the full range of permitted drop sizes, a model study is needed to determine
438 what fraction of the total leaked mass could be represented by the size range of initially
439 trapped droplets that subsequently exited the plume on relevant time scales.

440 Analysis of the chemical data provides an independent estimate of total
441 hydrocarbon mass flow rate against which other estimates based on physical (1, 12) or
442 optical (13, 30) methods can be compared (Fig. 5). Beyond the flow rate, the chemical
443 data provide critical information on initial environmental distribution of the different
444 mixtures resulting from transport of hydrocarbons emitted from the leaking well (e.g.,
445 Fig. 4). The information provided by a cooperative subsurface, surface, and airborne
446 chemical sampling program should therefore be an integral part of a systematic response
447 to future deepwater blowouts. Strategic cooperation during a response would
448 significantly improve the ability to quantify leaking mass and environmental impacts of
449 future spills, and would further provide a means to track and quantify the effects of
450 deliberate intervention measures, subsurface dispersant application, and well and sea-
451 floor integrity after cessation of flow. With sufficient advance preparation, joint airborne
452 and subsurface chemical sampling could provide a national rapid-response capability to
453 promptly assess deepwater well leak rates, especially for those in remote and Arctic
454 regions (2).

455

456 **Materials and Methods**

457 Leaking fluid was collected into isobaric gas-tight samplers by ROV from directly
458 within the lower marine riser package (LMRP) (5). Subsequent analyses of the gas and

459 oil composition were conducted in parallel using gas chromatography with flame
460 ionization detection (GC-FID) by Geomark Research Ltd. (www.geomarkresearch.com),
461 Alpha Analytical Laboratory (www.alphalab.com), and by WHOI with similar results (5).

462 Atmospheric hydrocarbon samples were acquired by sampling air into evacuated
463 stainless-steel canisters carried aboard three surface vessels, F/V *Eugenie*, R/V *Pelican*,
464 and R/V *Thomas Jefferson*; similar canisters were used on June 08 and 10 during two
465 DWH survey flights of a chemically-instrumented NOAA P-3 research aircraft (2). All
466 atmospheric samples taken aboard the vessels and aircraft flights were subsequently
467 analyzed by GC-FID or GC-mass spectrometry at the University of California at Irvine
468 (24).

469

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478 P-3 oil spill survey flights were funded in part by NOAA and in part by a U.S. Coast
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481 that helped improve the manuscript.

482

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- 556

557 **Figure legends**

558

559 **Figure 1. a).** Scale diagram of surfacing hydrocarbon plume dimensions; the
560 atmospheric plume data are consistent with a surface source area of ~1.6 km diameter.

561 **b).** Gaussian fits to hydrocarbon composition data, and corresponding full widths at half
562 maximum (FWHM) from crosswind P-3 aircraft transects of the evaporating plume 10
563 km downwind of DWH; data from a single transect are shown as an example. **c).** Data

564 above the detection limit (>5 parts per trillion by volume (pptv)) from all *DWH* plume
565 transects show no evidence for different populations of *n*-C₄ through *n*-C₈ alkanes
566 relative to *n*-C₉ (different volatilities & solubilities). **d).** Data >5 pptv from all transects
567 show no evidence for different populations of C₇ and C₈ aromatics relative to *n*-alkanes
568 of the same carbon number (similar volatilities, different solubilities).

569

570 **Figure 2. a).** Pre-spill Macondo reservoir hydrocarbon mass fraction (mass of compound
571 per mass of reservoir fluid) (2) plotted versus leaking fluid hydrocarbon mass fraction
572 measured during the spill in mid-June (5). Each data point represents an individual
573 hydrocarbon compound; several are labeled for illustration. Data for methane (CH₄)
574 through *n*-undecane (C₁₁H₂₄) are shown, comprising 38% of the total mass of the leaking
575 fluid. The dashed line (blue) has a slope of unity; the slope of a linear-least-squares fit
576 (red) is, within estimated errors, not significantly different than unity. **b).** Lower panel:
577 Atmospheric hydrocarbon mass enhancement ratios to measured 2-methylheptane (open
578 symbols) from research vessels and aircraft reflect the undissolved and volatile
579 components of the leaking fluid (black bars). Upper panel: Fractions in air (open
580 symbols) are the atmospheric enhancement ratios normalized to the expected ratio to 2-
581 methylheptane in the leaking fluid. The dissolved fraction (filled squares) is calculated
582 from the June 10, 2010 data.

583

584 **Figure 3. a).** Subsurface near-field plume data (blue) from Table 2 in Joye *et al.* (2010),
585 normalized to measured methane, compared to the composition of leaking gas and oil
586 (black) and the composition inferred for the mixture dissolved from the promptly

surfacing mass (red). The seven most concentrated samples ($\text{CH}_4 > 45,000 \text{ nM}$) sampled within 5 km of the well were averaged; the isobutane and *n*-butane data were transposed, and isomer-specific pentane data were apportioned according to their relative abundance in the leaking fluid. **b).** As in **a)** using subsurface plume data from Camilli *et al.* (2010) normalized to measured benzene. **c).** As in **a)** using subsurface BTEX plume data $>5\mu\text{g/L}$ of seawater from Hazen *et al.* (2010) normalized to measured toluene. **d).** As in **a)** using subsurface *n*-alkane plume data $>2.5 \mu\text{g/L}$ of seawater from Hazen *et al.* (2010) normalized to measured toluene. The average and range of (0.15 ± 0.10) used to scale the DO observations are shown by the dashed line and shading, respectively.

596

Figure 4. a). Evaporated hydrocarbon composition after 2 days (blue bars), **b).** surface oil slick composition after 2 days (black bars), and **c).** dissolved hydrocarbon composition (red bars). The leaking hydrocarbon composition from CH_4 through $n\text{-C}_{39}$ (black line) is shown in each panel for comparison. **d).** Schematic (not to scale) of hydrocarbon mass flows in the marine environment; values are calculated for June 10, 2010 in millions of kilograms per day.

603

Figure 5. The left-hand bar shows *DWH* hydrocarbon mass flow, in millions of kilograms for June 10, 2010, along different environmental transport pathways calculated using the chemical composition data. The middle bar shows the calculated release into the Gulf averaged over the spill duration, and the right-hand bar shows the official estimate of total hydrocarbon mass flow averaged over the spill.

Figure 1.

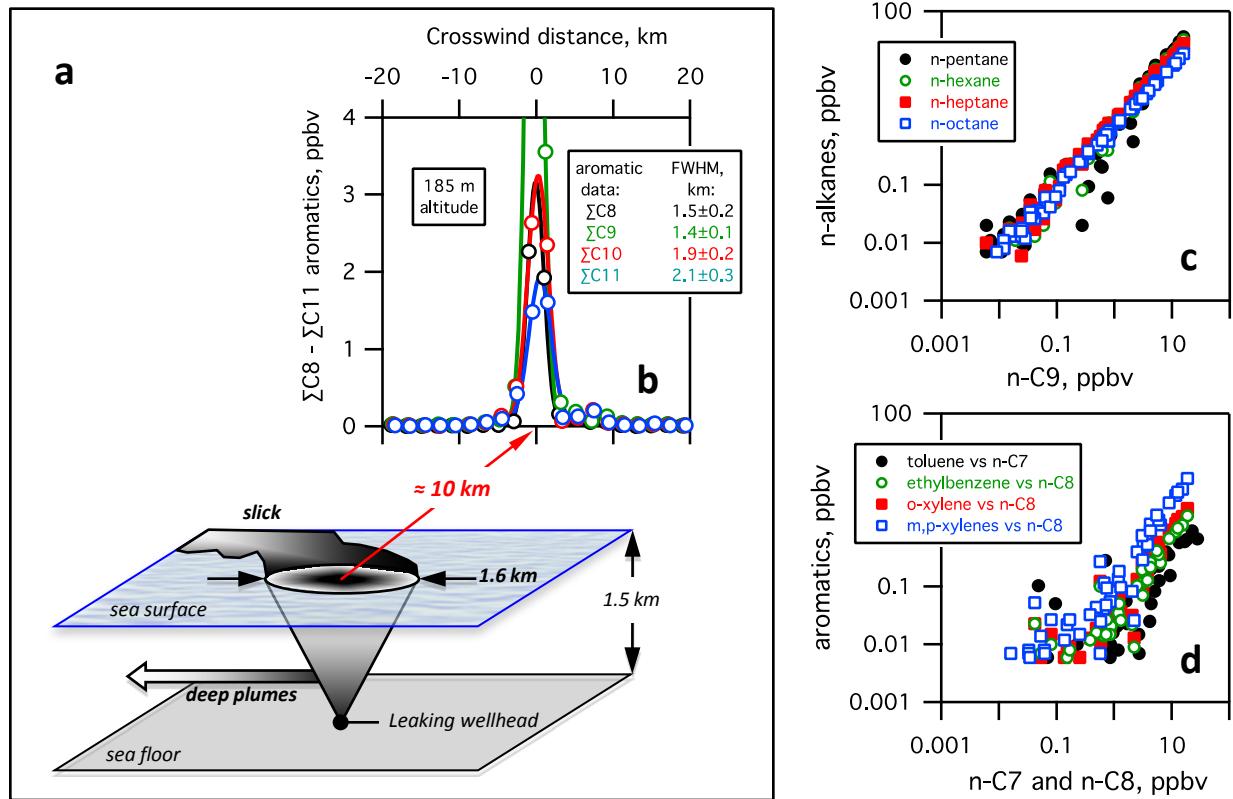


Figure 2.

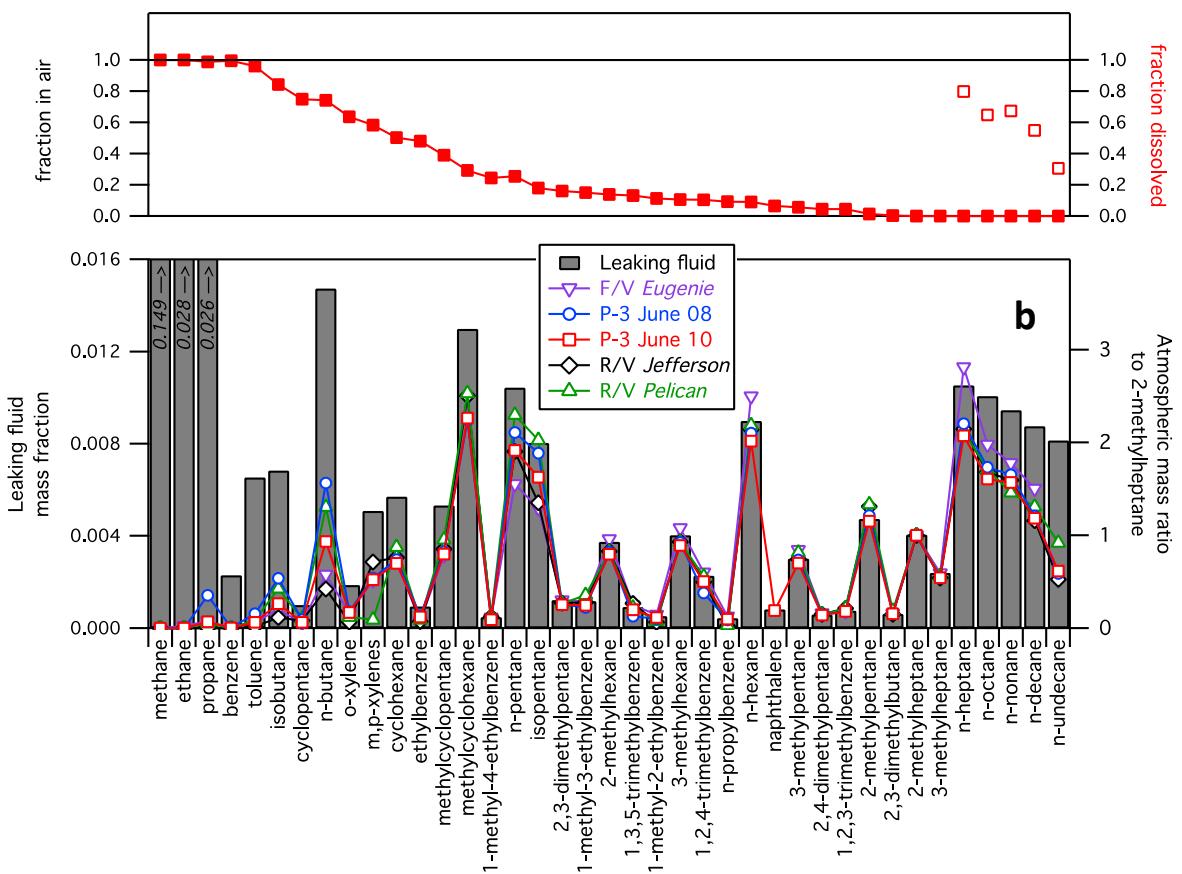
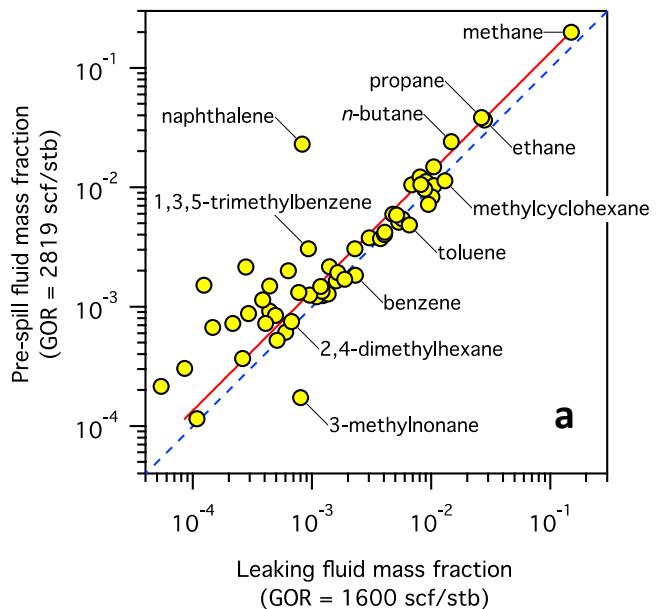


Figure 3.

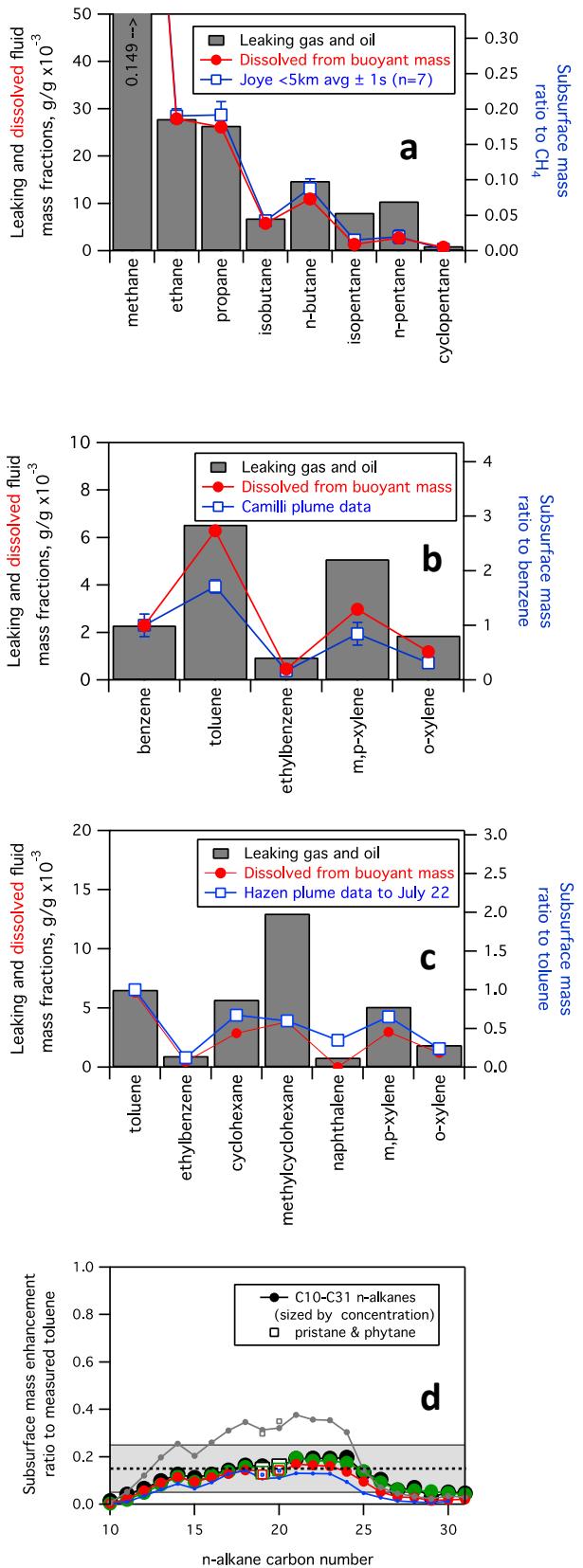


Figure 4.

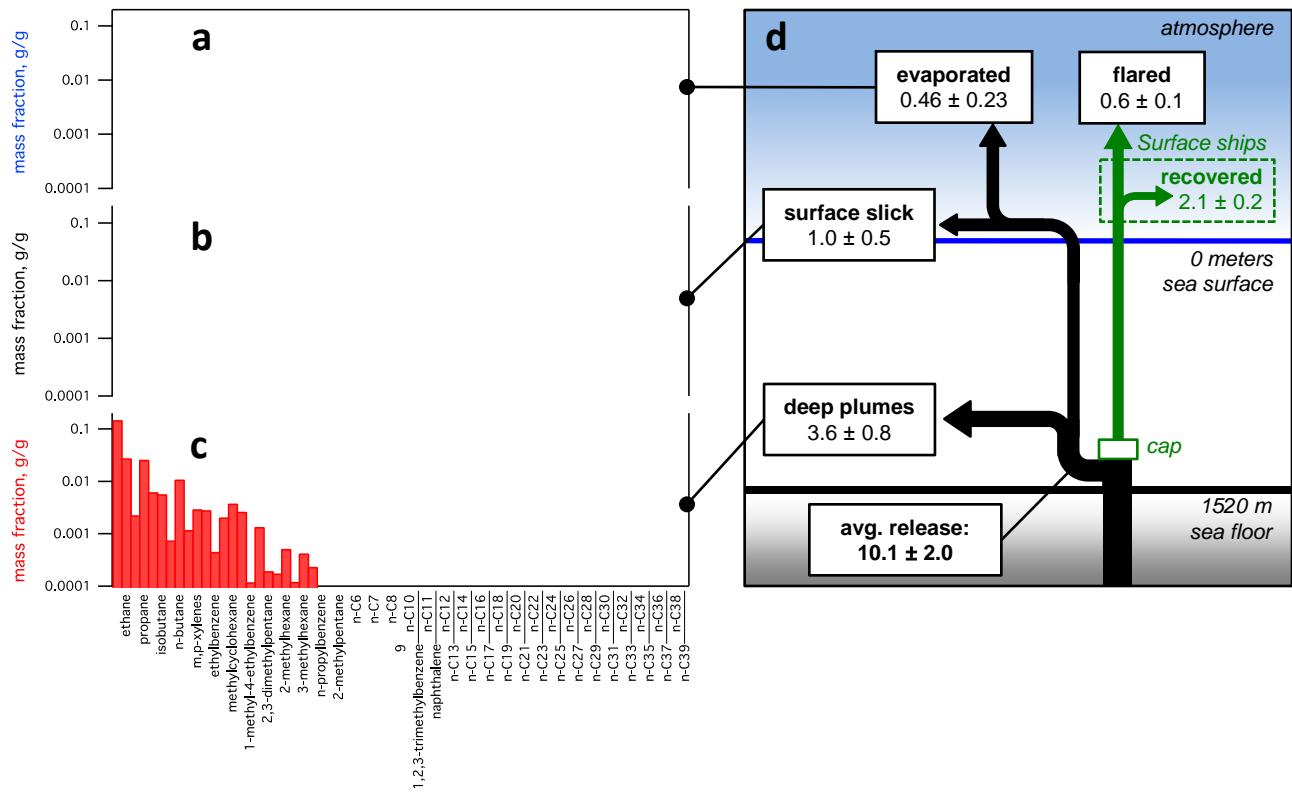
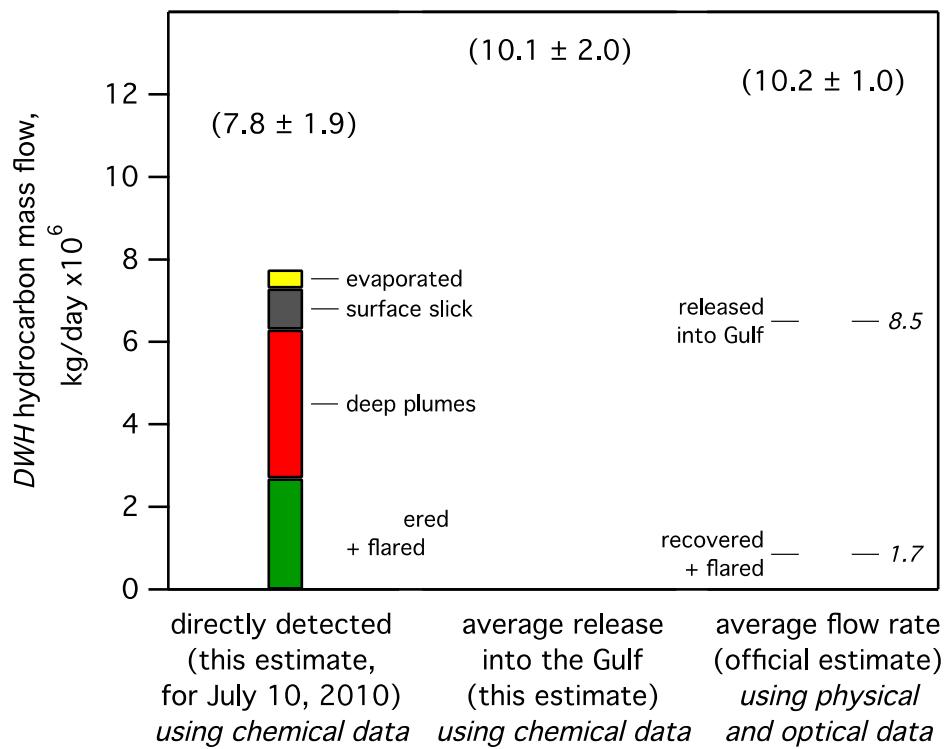


Figure 5.



Supplemental figures

1 **SI Figure captions.**

2

3 **Fig. S1.** Lower panel: Time series showing official estimate of total Macondo well flow
4 rate of oil (black circles) and oil plus gas (red circles); red shading denotes 10%
5 uncertainties stated for these estimates. Rates of oil recovery (black line) and oil plus gas
6 recovery (red line) to surface ships are also shown. Upper panel: dates of ship cruises
7 and aircraft flights used in this report. Dates for ship cruises following closure of the
8 well are not shown.

9

10 **Fig. S2.** A Gaussian fit to the evaporating plume VOC signal detected by the P-3 aircraft
11 at 10 km downwind (black line, with peak values offscale at 22 ppbv) was used to
12 parameterize atmospheric plume simulations of a series of successively larger source
13 areas (colored lines). Simulated source areas were assumed to be circular and
14 homogeneous; other source distributions would give rise to larger atmospheric
15 enhancements. The simulations show the P-3 would have detected an equal VOC mass
16 evaporating over a 1000-fold larger area with a plume signal-to-noise of approximately
17 60 (red line), based on instrument sensitivities and the measured background alkane and
18 aromatic concentrations of 10 ± 10 pptv in the upwind Gulf marine boundary layer.

19

20 **Fig. S3. a).** Simulated oil drop rise times as a function of drop diameter; data (blue
21 circles) are from the Oil Budget Calculator Appendix 7, Table 1 (1). Average diameters
22 of droplets (black squares) for the range of surfacing times derived in the text are
23 calculated by extrapolating from a fitted line to the OBC data. **b).** Oil drop size

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“Chemical data quantify Deepwater Horizon hydrocarbon flow rate and environmental distribution”

2

24 distribution (red dashed line) extrapolated from a fit to data (blue circles) from Delvigne
25 and Sweeney (1988) Figure 9, and the corresponding mass distribution (black).

26

27 **Fig. S4. a).** Lower panel: Comparison of leaking fluid mass fraction (black bars) (2)
28 and pre-spill reservoir fluid mass fraction (red squares) (3). Upper panel: Ratio of pre-
29 spill mass fraction to leaking fluid mass fraction; axis range shows a factor of ± 2 . **b).**
30 Atmospheric mass fluxes of hydrocarbons measured on June 10, 2010 are shown for
31 soluble (blue), insoluble and volatile (red) and less volatile (black) compounds as a
32 function of the leaking fluid mass fraction. Benzene, ethane, and methane data are off
33 scale due to negligible or zero atmospheric flux.

34

35 **Fig. S5. a).** Fraction of *n*-alkanes remaining in the surface oil slick predicted from the
36 volatility distribution of the oil mixture. **b).** GC-FID traces (courtesy of C. Carmichael,
37 WHOI) of the liquid oil fraction of the leaking fluid (2) (upper trace) and of a fresh oil
38 sample collected 1.4 km from *Enterprise* in the surface oil slick (lower trace).

39

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48

49

Figure S1.

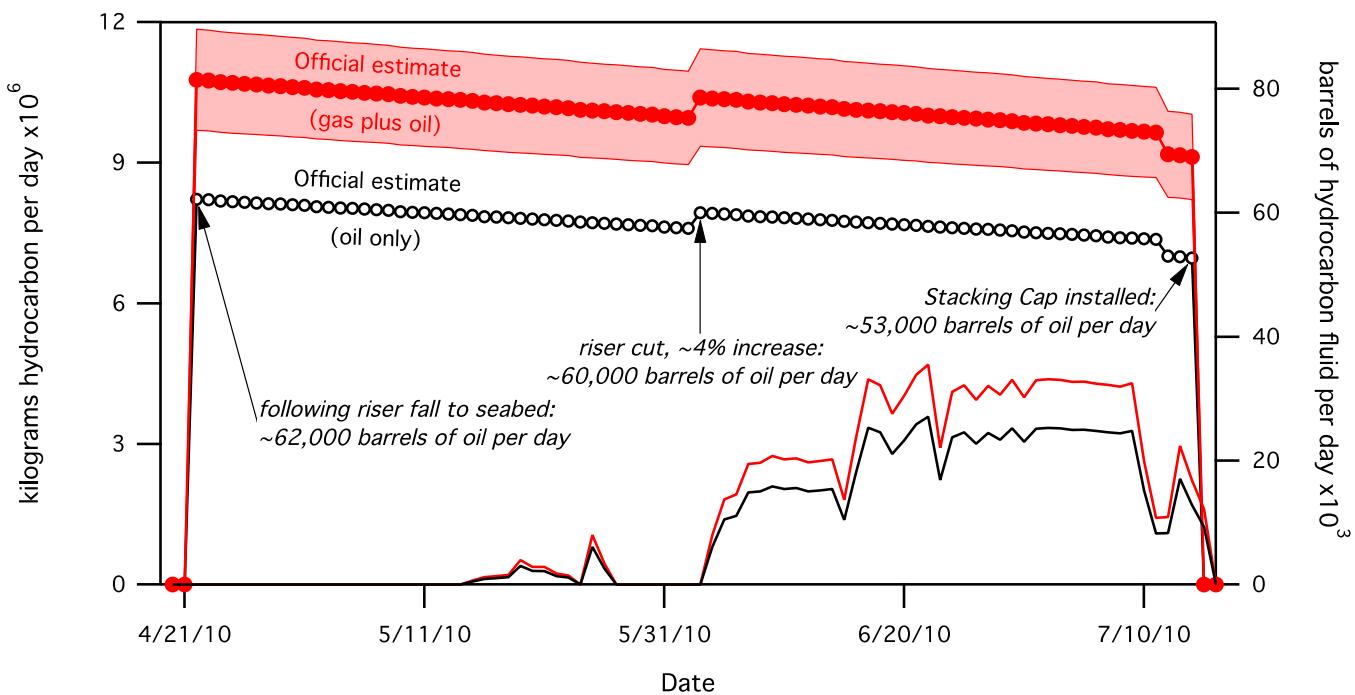
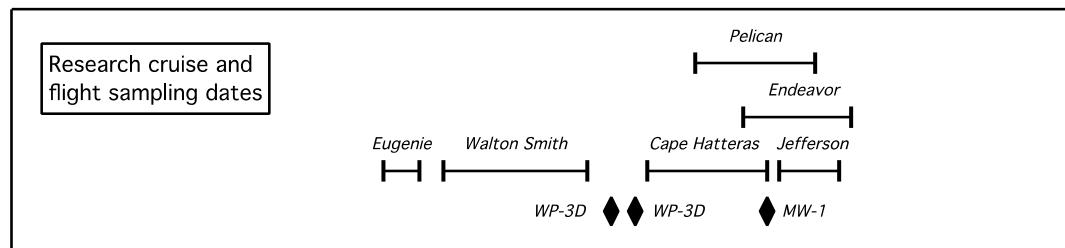


Figure S2.

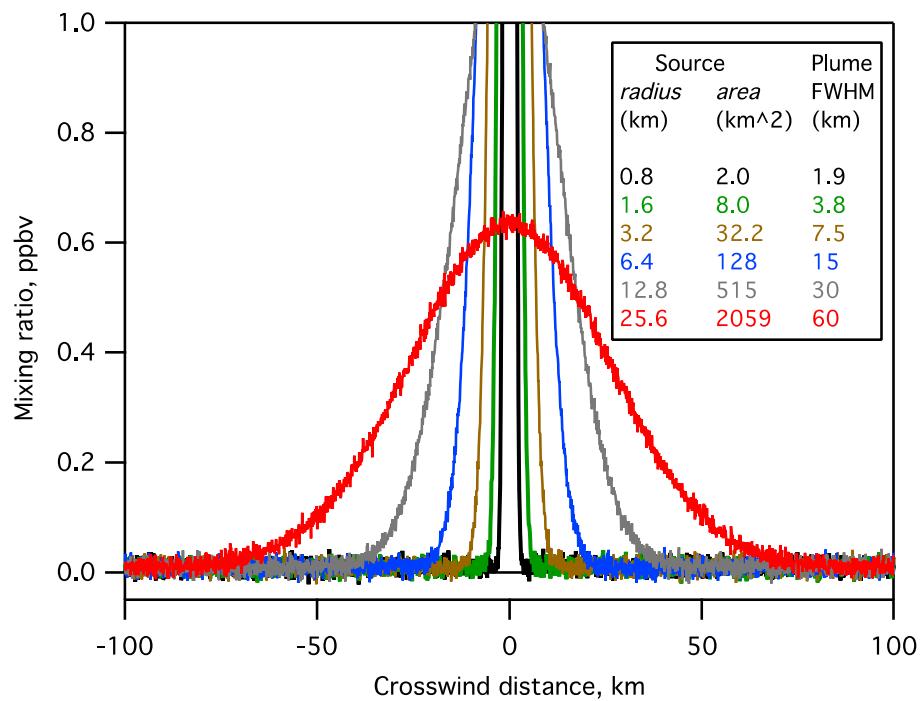


Figure S3.

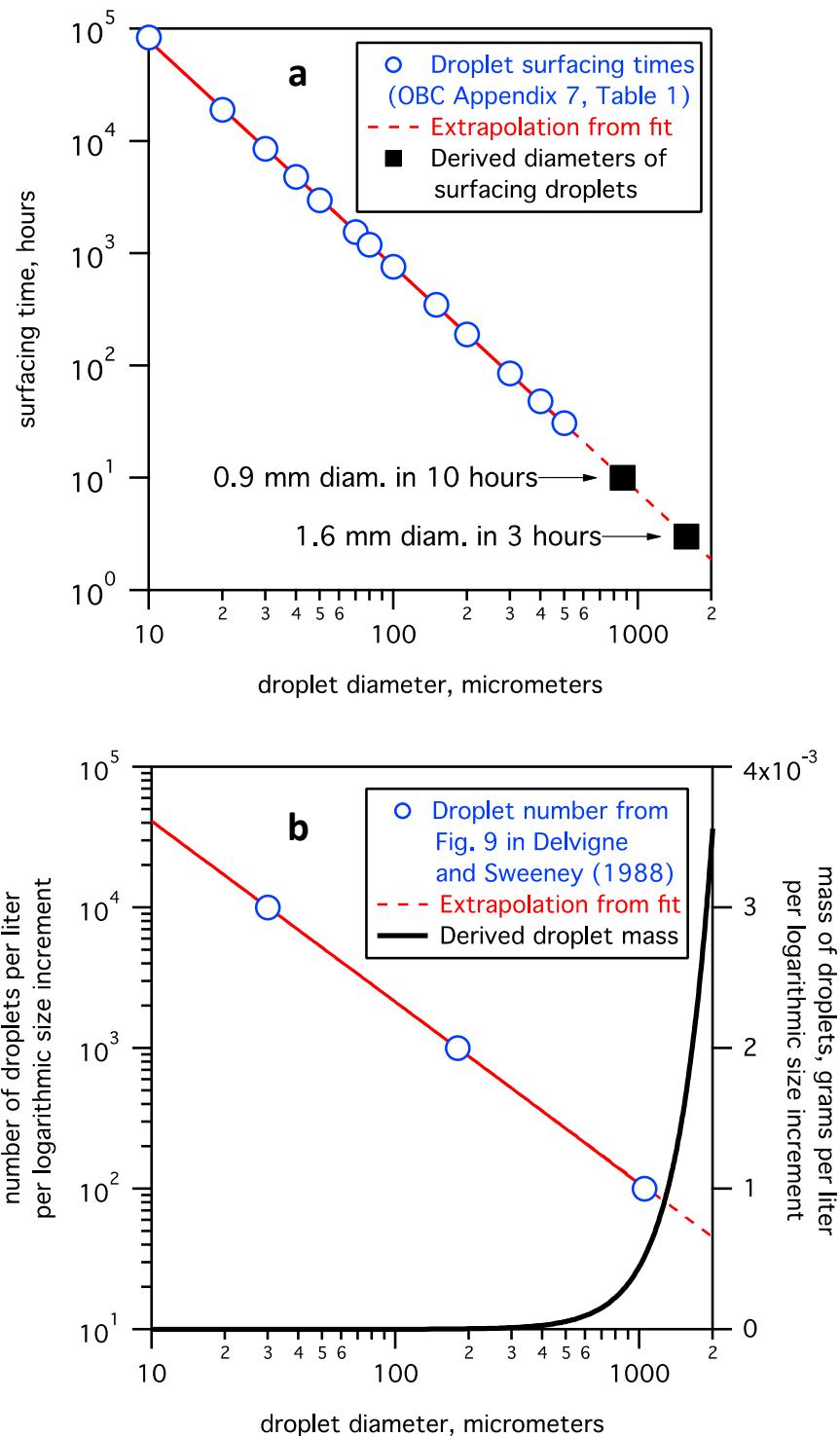


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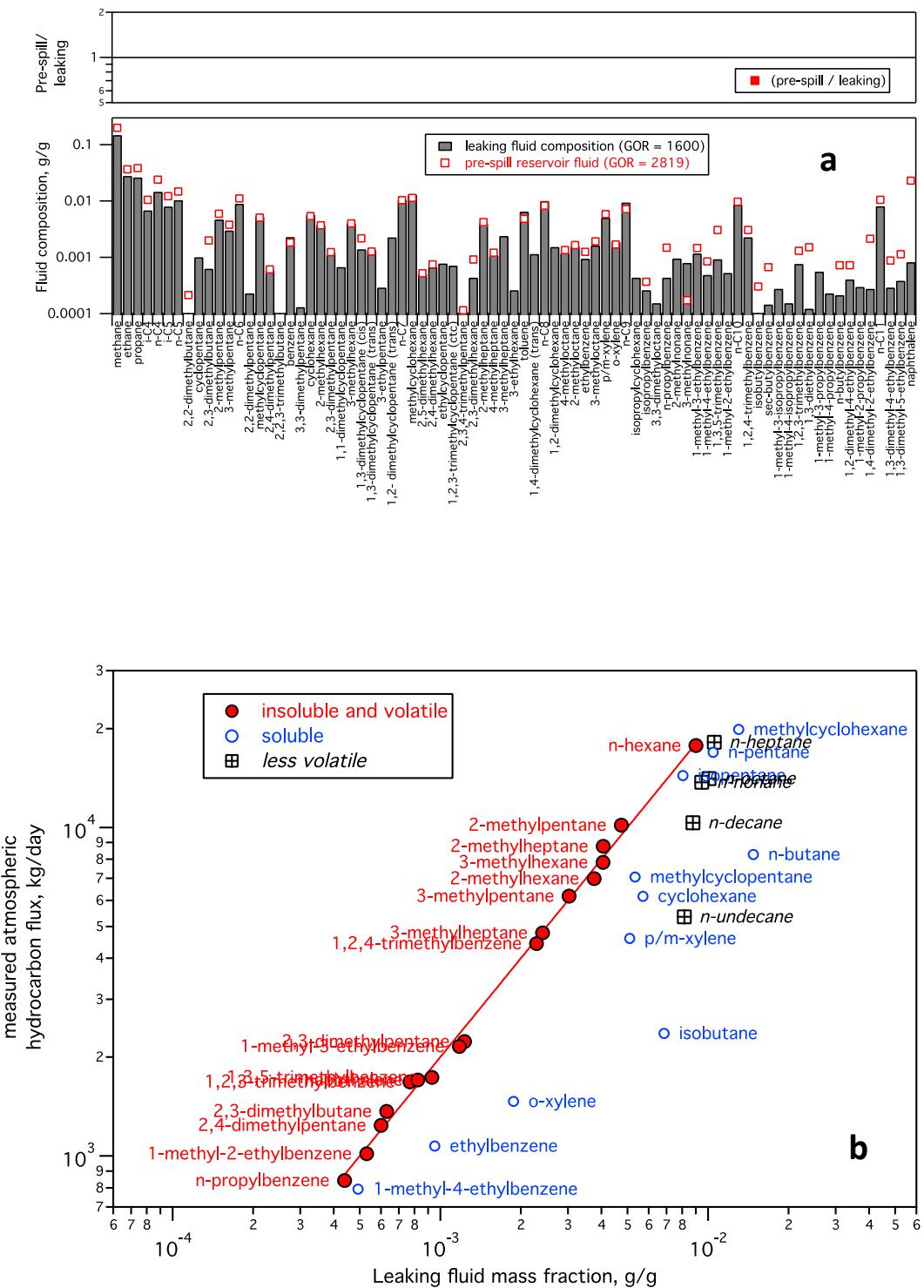


Figure S5.

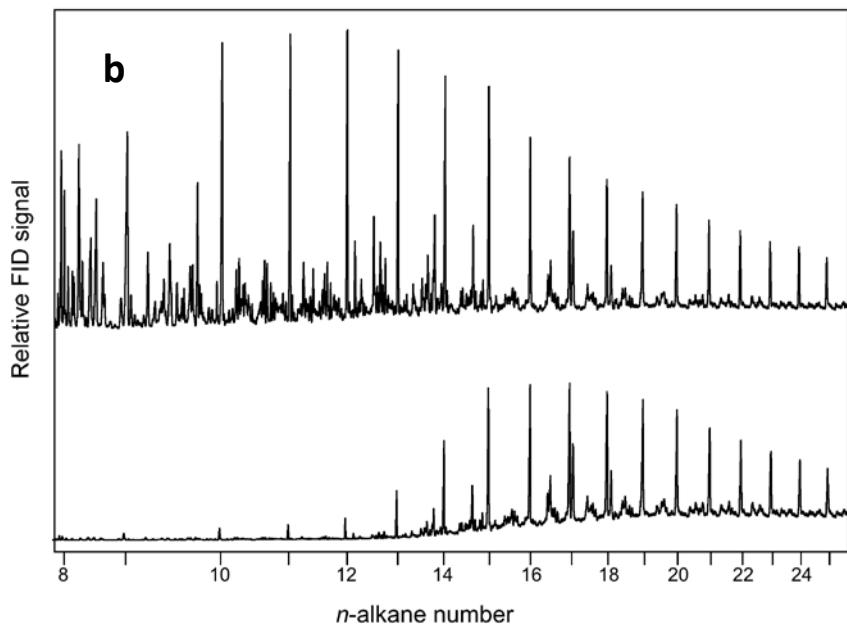
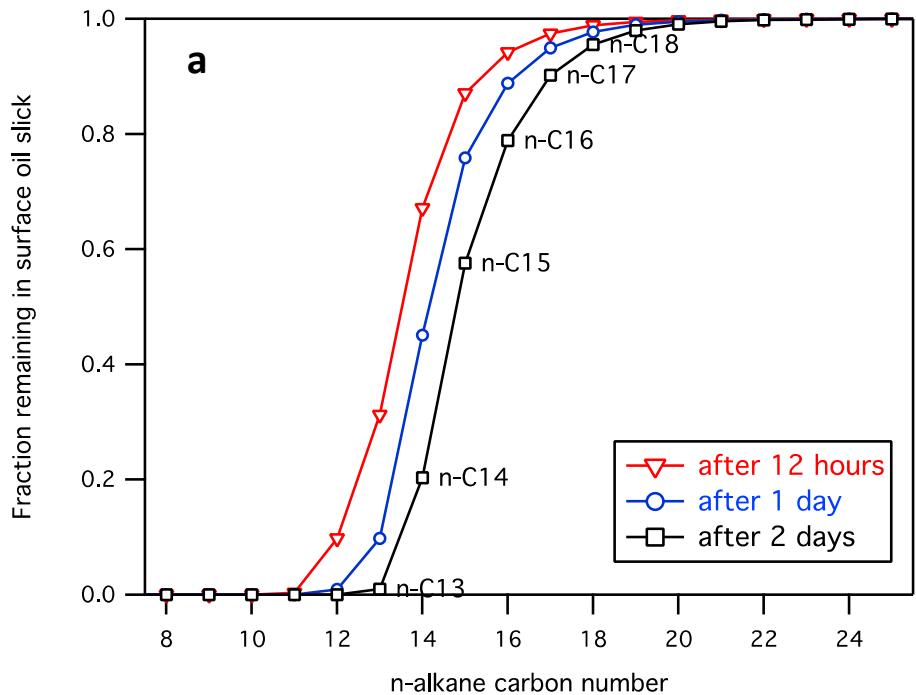


Table S01.

Compound	Molec. weight (g/mol)	Mass fraction in leaking fluid (g/g _{Total})	Fraction dissolved ^a	Stoichio-metric Ratio O ₂ :HC ^b	DO removing potential of soluble hydrocarbons (mol O ₂ /g _{Total})	DO removing potential of insoluble hydrocarbons (mol O ₂ /g _{Total}) ^c	Mass of dissolved HCs - Low (g) ^d	Mass of dissolved HCs - High (g) ^e	Mass of insoluble HCs - Low (g) ^f	Mass of insoluble HCs - High (g) ^g
	MW _i	M _i	F _i	S _i	(F _i *M _i *S _i)/MW _i	((1-F _i)*M _i *S _i)*0.15*0.961)/(MW _i *F _x)				
methane	16.042	0.14957	1	2.0	1.865E-02	0	1.31E+06	1.70E+06	0.00E+00	0.00E+00
ethane	30.069	0.02787	1	3.5	3.245E-03	0	2.44E+05	3.17E+05	0.00E+00	0.00E+00
propane	44.096	0.02642	0.9893	5.0	2.964E-03	1.496E-05	2.29E+05	2.97E+05	1.16E+03	1.50E+03
benzene	78.112	0.00230	0.9952	7.5	2.197E-04	4.987E-07	2.00E+04	2.60E+04	4.55E+01	5.91E+01
toluene	92.138	0.00654	0.9610	9.0	6.141E-04	1.167E-05	5.50E+04	7.15E+04	1.05E+03	1.36E+03
<i>i</i> -C ₄	58.122	0.00684	0.8431	6.5	6.453E-04	5.619E-05	5.05E+04	6.57E+04	4.40E+03	5.72E+03
<i>n</i> -C ₄	58.122	0.01474	0.7423	6.5	1.224E-03	1.987E-04	9.58E+04	1.25E+05	1.56E+04	2.02E+04
cyclopentane	70.133	0.00101	0.7501	7.5	8.078E-05	1.260E-05	6.61E+03	8.60E+03	1.03E+03	1.34E+03
<i>o</i> -xylene	106.165	0.00188	0.6360	10.5	1.180E-04	3.160E-05	1.04E+04	1.36E+04	2.80E+03	3.64E+03
<i>p/m</i> -xylene	106.165	0.00510	0.5840	10.5	2.944E-04	9.812E-05	2.61E+04	3.39E+04	8.68E+03	1.13E+04
cyclohexane	84.159	0.00570	0.5025	9.0	3.066E-04	1.420E-04	2.51E+04	3.26E+04	1.16E+04	1.51E+04
ethylbenzene	106.165	0.00095	0.4814	10.5	4.539E-05	2.288E-05	4.02E+03	5.22E+03	2.02E+03	2.63E+03
methylcyclopentane	84.159	0.00533	0.3904	9.0	2.225E-04	1.625E-04	1.82E+04	2.37E+04	1.33E+04	1.73E+04
methylcyclohexane	98.186	0.01299	0.2935	10.5	4.078E-04	4.593E-04	3.34E+04	4.34E+04	3.76E+04	4.89E+04
1-methyl-4-ethylbenzene	120.192	0.00049	0.2448	12.0	1.203E-05	1.736E-05	1.05E+03	1.37E+03	1.52E+03	1.98E+03
<i>i</i> -C ₅	72.149	0.00805	0.2557	8.0	2.282E-04	3.108E-04	1.80E+04	2.34E+04	2.45E+04	3.19E+04
<i>n</i> -C ₅	72.149	0.01045	0.1697	8.0	1.966E-04	4.500E-04	1.55E+04	2.02E+04	3.55E+04	4.62E+04
2,3-dimethylpentane	100.202	0.00123	0.1605	11.0	2.168E-05	5.304E-05	1.73E+03	2.25E+03	4.23E+03	5.50E+03
1-methyl-3-ethylbenzene	120.192	0.00118	0.1502	12.0	1.764E-05	4.670E-05	1.55E+03	2.01E+03	4.09E+03	5.32E+03
2-methylhexane	100.202	0.00375	0.1393	11.0	5.737E-05	1.659E-04	4.57E+03	5.95E+03	1.32E+04	1.72E+04
1,3,5-trimethylbenzene	120.192	0.00093	0.1321	12.0	1.227E-05	3.772E-05	1.08E+03	1.40E+03	3.31E+03	4.30E+03
3-methylhexane	100.202	0.00404	0.1055	11.0	4.683E-05	1.858E-04	3.73E+03	4.85E+03	1.48E+04	1.93E+04
1,2,4-trimethylbenzene	120.192	0.00228	0.1039	12.0	2.370E-05	9.558E-05	2.08E+03	2.70E+03	8.38E+03	1.09E+04
<i>n</i> -propylbenzene	120.192	0.00044	0.0932	12.0	4.077E-06	1.856E-05	3.57E+02	4.65E+02	1.63E+03	2.12E+03
1,2,3-trimethylbenzene	120.192	0.00077	0	12.0	0	3.591E-05	0.00E+00	0.00E+00	3.15E+03	4.09E+03
2,2-dimethylbutane	86.175	0.00005	0	9.5	0	2.776E-06	0.00E+00	0.00E+00	2.20E+02	2.87E+02
2,3-dimethylbutane	86.175	0.00063	0	9.5	0	3.252E-05	0.00E+00	0.00E+00	2.58E+03	3.36E+03

Table S01.

2-methylpentane	86.175	0.00474	0	9.5	0	2.447E-04	0.00E+00	0.00E+00	1.94E+04	2.53E+04
3-methylpentane	86.175	0.00302	0	9.5	0	1.558E-04	0.00E+00	0.00E+00	1.24E+04	1.61E+04
<i>n</i> -C ₆	86.175	0.00900	0	9.5	0	4.640E-04	0.00E+00	0.00E+00	3.68E+04	4.79E+04
2,2-dimethylpentane	100.202	0.00023	0	11.0	0	1.185E-05	0.00E+00	0.00E+00	9.45E+02	1.23E+03
2,4-dimethylpentane	100.202	0.00060	0	11.0	0	3.080E-05	0.00E+00	0.00E+00	2.46E+03	3.19E+03
2,2,3-trimethylbutane	100.202	0.00005	0	11.0	0	2.369E-06	0.00E+00	0.00E+00	1.89E+02	2.46E+02
3,3-dimethylpentane	100.202	0.00013	0	11.0	0	6.713E-06	0.00E+00	0.00E+00	5.35E+02	6.96E+02
1,1-dimethylcyclopentane	98.186	0.00068	0	10.5	0	3.385E-05	0.00E+00	0.00E+00	2.77E+03	3.60E+03
1,3-dimethylcyclopentane (<i>cis</i>)	98.186	0.00140	0	10.5	0	7.001E-05	0.00E+00	0.00E+00	5.73E+03	7.45E+03
1,3-dimethylcyclopentane (<i>trans</i>)	98.186	0.00136	0	10.5	0	6.809E-05	0.00E+00	0.00E+00	5.57E+03	7.24E+03
3-ethylpentane	100.202	0.00029	0	11.0	0	1.501E-05	0.00E+00	0.00E+00	1.20E+03	1.56E+03
1,2-dimethylcyclopentane (<i>trans</i>)	98.186	0.00228	0	10.5	0	1.139E-04	0.00E+00	0.00E+00	9.32E+03	1.21E+04
<i>n</i> -C ₇	100.202	0.01053	0	11.0	0	5.410E-04	0.00E+00	0.00E+00	4.31E+04	5.61E+04
2,5-dimethylhexane	114.229	0.00051	0	12.5	0	2.598E-05	0.00E+00	0.00E+00	2.08E+03	2.70E+03
2,4-dimethylhexane	114.229	0.00067	0	12.5	0	3.425E-05	0.00E+00	0.00E+00	2.74E+03	3.56E+03
ethylcyclopentane	98.186	0.00078	0	10.5	0	3.885E-05	0.00E+00	0.00E+00	3.18E+03	4.13E+03
1,2,3-trimethylcyclopentane (ctc)	112.213	0.00072	0	12.0	0	3.577E-05	0.00E+00	0.00E+00	2.93E+03	3.81E+03
2,3,4-trimethylpentane	114.229	0.00011	0	12.5	0	5.511E-06	0.00E+00	0.00E+00	4.41E+02	5.73E+02
2,3-dimethylhexane	114.229	0.00044	0	12.5	0	2.244E-05	0.00E+00	0.00E+00	1.79E+03	2.33E+03
2-methylheptane	114.229	0.00406	0	12.5	0	2.078E-04	0.00E+00	0.00E+00	1.66E+04	2.16E+04
4-methylheptane	114.229	0.00109	0	12.5	0	5.590E-05	0.00E+00	0.00E+00	4.47E+03	5.81E+03
3-methylheptane	114.229	0.00241	0	12.5	0	1.232E-04	0.00E+00	0.00E+00	9.86E+03	1.28E+04
3-ethylhexane	114.229	0.00026	0	12.5	0	1.338E-05	0.00E+00	0.00E+00	1.07E+03	1.39E+03
1,4-dimethylcyclohexane (<i>trans</i>)	112.213	0.00115	0	12.0	0	5.770E-05	0.00E+00	0.00E+00	4.72E+03	6.14E+03
<i>n</i> -C ₈	114.229	0.01007	0	12.5	0	5.157E-04	0.00E+00	0.00E+00	4.12E+04	5.36E+04
1,2-dimethylcyclohexane	112.213	0.00153	0	12.0	0	7.655E-05	0.00E+00	0.00E+00	6.27E+03	8.15E+03
4-methyloctane	128.255	0.00121	0	14.0	0	6.165E-05	0.00E+00	0.00E+00	4.94E+03	6.43E+03
2-methyloctane	128.255	0.00159	0	14.0	0	8.128E-05	0.00E+00	0.00E+00	6.52E+03	8.47E+03
3-methyloctane	128.255	0.00164	0	14.0	0	8.364E-05	0.00E+00	0.00E+00	6.71E+03	8.72E+03
<i>n</i> -C ₉	128.255	0.00946	0	14.0	0	4.830E-04	0.00E+00	0.00E+00	3.87E+04	5.03E+04

Table S01.

isopropylcyclohexane	126.239	0.00044	0	13.5	0	2.193E-05	0.00E+00	0.00E+00	1.79E+03	2.33E+03
isopropylbenzene	120.192	0.00026	0	12.0	0	1.221E-05	0.00E+00	0.00E+00	1.07E+03	1.39E+03
3,3-dimethyloctane	142.282	0.00015	0	15.5	0	7.837E-06	0.00E+00	0.00E+00	6.30E+02	8.19E+02
2-methylnonane	142.282	0.00096	0	15.5	0	4.898E-05	0.00E+00	0.00E+00	3.94E+03	5.12E+03
3-methylnonane	142.282	0.00080	0	15.5	0	4.075E-05	0.00E+00	0.00E+00	3.27E+03	4.26E+03
1-methyl-2-ethylbenzene	120.192	0.00053	0	12.0	0	2.478E-05	0.00E+00	0.00E+00	2.17E+03	2.82E+03
<i>n</i> -C ₁₀	142.282	0.00876	0	15.5	0	4.467E-04	0.00E+00	0.00E+00	3.59E+04	4.67E+04
isobutylbenzene	134.218	0.00008	0	13.5	0	3.980E-06	0.00E+00	0.00E+00	3.46E+02	4.50E+02
sec-butylbenzene	134.218	0.00015	0	13.5	0	6.874E-06	0.00E+00	0.00E+00	5.98E+02	7.78E+02
1-methyl-3-isopropylbenzene	134.218	0.00028	0	13.5	0	1.303E-05	0.00E+00	0.00E+00	1.13E+03	1.47E+03
1-methyl-4-isopropylbenzene	134.218	0.00015	0	13.5	0	7.236E-06	0.00E+00	0.00E+00	6.30E+02	8.19E+02
1,3-diethylbenzene	134.218	0.00012	0	13.5	0	5.789E-06	0.00E+00	0.00E+00	5.04E+02	6.55E+02
1-methyl-3-propylbenzene	134.218	0.00056	0	13.5	0	2.641E-05	0.00E+00	0.00E+00	2.30E+03	2.99E+03
1-methyl-4-propylbenzene	134.218	0.00023	0	13.5	0	1.085E-05	0.00E+00	0.00E+00	9.45E+02	1.23E+03
<i>n</i> -butylbenzene	134.218	0.00022	0	13.5	0	1.013E-05	0.00E+00	0.00E+00	8.82E+02	1.15E+03
1,2-dimethyl-4-ethylbenzene	134.218	0.00041	0	13.5	0	1.918E-05	0.00E+00	0.00E+00	1.67E+03	2.17E+03
1-methyl-2-propylbenzene	134.218	0.00030	0	13.5	0	1.411E-05	0.00E+00	0.00E+00	1.23E+03	1.60E+03
1,4-dimethyl-2-ethylbenzene	134.218	0.00028	0	13.5	0	1.303E-05	0.00E+00	0.00E+00	1.13E+03	1.47E+03
<i>n</i> -C ₁₁	156.308	0.00815	0	17.0	0	4.147E-04	0.00E+00	0.00E+00	3.34E+04	4.34E+04
1,3-dimethyl-4-ethylbenzene	134.218	0.00029	0	13.5	0	1.375E-05	0.00E+00	0.00E+00	1.20E+03	1.56E+03
1,3-dimethyl-5-ethylbenzene	134.218	0.00038	0	13.5	0	1.809E-05	0.00E+00	0.00E+00	1.57E+03	2.05E+03
naphthalene	128.171	0.00082	0	12.0	0	3.604E-05	0.00E+00	0.00E+00	3.37E+03	4.38E+03
C ₁ -naphthalenes	142.197	0.00178	0	13.5	0	7.923E-05	0.00E+00	0.00E+00	7.30E+03	9.50E+03
C ₂ -naphthalenes	156.224	0.00218	0	15.0	0	9.774E-05	0.00E+00	0.00E+00	8.91E+03	1.16E+04
C ₃ -naphthalenes	170.250	0.00162	0	16.5	0	7.356E-05	0.00E+00	0.00E+00	6.64E+03	8.64E+03
C ₄ -naphthalenes	184.277	0.00070	0	18.0	0	3.197E-05	0.00E+00	0.00E+00	2.87E+03	3.72E+03
1,2,3,4-tetramethylbenzene	134.218	0.00033	0	13.5	0	1.556E-05	0.00E+00	0.00E+00	1.35E+03	1.76E+03
<i>n</i> -C ₁₂	170.335	0.00722	0	18.5	0	3.669E-04	0.00E+00	0.00E+00	2.96E+04	3.84E+04
<i>i</i> -C ₁₃	184.361	0.00178	0	20.0	0	9.014E-05	0.00E+00	0.00E+00	7.27E+03	9.46E+03
<i>i</i> -C ₁₄	198.388	0.00130	0	21.5	0	6.588E-05	0.00E+00	0.00E+00	5.32E+03	6.92E+03
<i>n</i> -C ₁₃	184.361	0.00638	0	20.0	0	3.239E-04	0.00E+00	0.00E+00	2.61E+04	3.40E+04
<i>i</i> -C ₁₅	212.415	0.00130	0	23.0	0	6.582E-05	0.00E+00	0.00E+00	5.32E+03	6.92E+03

Table S01.

<i>n</i> -C ₁₄	198.388	0.00584	0	21.5	0	2.959E-04	0.00E+00	0.00E+00	2.39E+04	3.11E+04	
<i>i</i> -C ₁₆	226.441	0.00221	0	24.5	0	1.117E-04	0.00E+00	0.00E+00	9.04E+03	1.17E+04	
<i>n</i> -C ₁₅	212.415	0.00559	0	23.0	0	2.832E-04	0.00E+00	0.00E+00	2.29E+04	2.98E+04	
fluorene	166.219	0.00013	0	15.5	0	5.702E-06	0.00E+00	0.00E+00	5.35E+02	6.96E+02	
C ₁ -fluorenes	180.245	0.00034	0	17.0	0	1.493E-05	0.00E+00	0.00E+00	1.39E+03	1.80E+03	
C ₂ -fluorenes	194.272	0.00050	0	18.5	0	2.227E-05	0.00E+00	0.00E+00	2.05E+03	2.66E+03	
C ₃ -fluorenes	208.298	0.00045	0	20.0	0	2.003E-05	0.00E+00	0.00E+00	1.83E+03	2.37E+03	
<i>n</i> -C ₁₆	226.441	0.00467	0	24.5	0	2.366E-04	0.00E+00	0.00E+00	1.91E+04	2.49E+04	
<i>i</i> -C ₁₈	254.494	0.00149	0	27.5	0	7.541E-05	0.00E+00	0.00E+00	6.11E+03	7.94E+03	
<i>n</i> -C ₁₇	240.468	0.00411	0	26.0	0	2.081E-04	0.00E+00	0.00E+00	1.68E+04	2.19E+04	
pristane	268.521	0.00241	0	29.0	0	1.216E-04	0.00E+00	0.00E+00	9.86E+03	1.28E+04	
dibenzothiophene	184.258	0.00008	0	14.0	0	2.733E-06	0.00E+00	0.00E+00	3.15E+02	4.09E+02	
C ₁ -dibenzothiophenes	198.285	0.00026	0	15.5	0	9.560E-06	0.00E+00	0.00E+00	1.07E+03	1.39E+03	
C ₂ -dibenzothiophenes	212.311	0.00037	0	17.0	0	1.383E-05	0.00E+00	0.00E+00	1.51E+03	1.96E+03	
C ₃ -dibenzothiophenes	226.338	0.00030	0	18.5	0	1.138E-05	0.00E+00	0.00E+00	1.22E+03	1.58E+03	
C ₄ -dibenzothiophenes	240.364	0.00018	0	20.0	0	7.183E-06	0.00E+00	0.00E+00	7.56E+02	9.82E+02	
phenanthrene	178.229	0.00031	0	16.5	0	1.332E-05	0.00E+00	0.00E+00	1.26E+03	1.64E+03	
C ₁ -phenanthrenes	192.256	0.00076	0	18.0	0	3.334E-05	0.00E+00	0.00E+00	3.12E+03	4.05E+03	
C ₂ -phenanthrenes	206.282	0.00083	0	19.5	0	3.672E-05	0.00E+00	0.00E+00	3.40E+03	4.42E+03	
C ₃ -phenanthrenes	220.309	0.00058	0	21.0	0	2.589E-05	0.00E+00	0.00E+00	2.38E+03	3.09E+03	
C ₄ -phenanthrenes	234.336	0.00028	0	22.5	0	1.243E-05	0.00E+00	0.00E+00	1.13E+03	1.47E+03	
<i>n</i> -C ₁₈	254.494	0.00335	0	27.5	0	1.695E-04	0.00E+00	0.00E+00	1.37E+04	1.78E+04	
phytane	282.547	0.00144	0	30.5	0	7.261E-05	0.00E+00	0.00E+00	5.89E+03	7.65E+03	
<i>n</i> -C ₁₉	268.521	0.00297	0	29.0	0	1.500E-04	0.00E+00	0.00E+00	1.22E+04	1.58E+04	
<i>n</i> -C ₂₀	282.547	0.00259	0	30.5	0	1.309E-04	0.00E+00	0.00E+00	1.06E+04	1.38E+04	
fluoranthene	202.251	0.00000	0	18.5	0	1.974E-07	0.00E+00	0.00E+00	1.89E+01	2.46E+01	
pyrene	202.251	0.00002	0	18.5	0	6.581E-07	0.00E+00	0.00E+00	6.30E+01	8.19E+01	
C ₁ -	216.277	0.00012	0	20.0	0	5.322E-06	0.00E+00	0.00E+00	5.04E+02	6.55E+02	
fluoranthenes/pyrenes	C ₂ -	230.304	0.00019	0	21.5	0	8.395E-06	0.00E+00	0.00E+00	7.87E+02	1.02E+03
fluoranthenes/pyrenes	C ₃ -	244.330	0.00021	0	23.0	0	9.143E-06	0.00E+00	0.00E+00	8.50E+02	1.11E+03
fluoranthenes/pyrenes	C ₄ -	258.357	0.00015	0	24.5	0	6.822E-06	0.00E+00	0.00E+00	6.30E+02	8.19E+02
fluoranthenes/pyrenes	<i>n</i> -C ₂₁	296.574	0.00211	0	32.0	0	1.063E-04	0.00E+00	0.00E+00	8.63E+03	1.12E+04
	<i>n</i> -C ₂₂	310.601	0.00185	0	33.5	0	9.311E-05	0.00E+00	0.00E+00	7.56E+03	9.82E+03
	<i>n</i> -C ₂₃	324.627	0.00158	0	35.0	0	7.989E-05	0.00E+00	0.00E+00	6.49E+03	8.43E+03
	<i>n</i> -C ₂₄	338.654	0.00140	0	36.5	0	7.056E-05	0.00E+00	0.00E+00	5.73E+03	7.45E+03
benz[<i>a</i>]anthracene		228.288	0.00002	0	21.0	0	6.618E-07	0.00E+00	0.00E+00	6.30E+01	8.19E+01
chrysene		228.288	0.00008	0	21.0	0	3.640E-06	0.00E+00	0.00E+00	3.46E+02	4.50E+02

Table S01.

C ₁ - benz[a]anthracenes/ chrysenes	242.314	0.00018	0	22.5	0	8.016E-06	0.00E+00	0.00E+00	7.56E+02	9.82E+02
C ₂ - benz[a]anthracenes/ chrysenes	256.341	0.00022	0	24.0	0	9.767E-06	0.00E+00	0.00E+00	9.13E+02	1.19E+03
C ₃ - benz[a]anthracenes/ chrysenes	270.368	0.00015	0	25.5	0	6.446E-06	0.00E+00	0.00E+00	5.98E+02	7.78E+02
<i>n</i> -C ₂₅	352.680	0.00115	0	38.0	0	5.814E-05	0.00E+00	0.00E+00	4.72E+03	6.14E+03
<i>n</i> -C ₂₆	366.707	0.00102	0	39.5	0	5.153E-05	0.00E+00	0.00E+00	4.19E+03	5.44E+03
<i>n</i> -C ₂₇	380.734	0.00085	0	41.0	0	4.300E-05	0.00E+00	0.00E+00	3.49E+03	4.54E+03
<i>n</i> -C ₂₈	394.760	0.00064	0	42.5	0	3.214E-05	0.00E+00	0.00E+00	2.61E+03	3.40E+03
<i>n</i> -C ₂₉	408.787	0.00059	0	44.0	0	2.981E-05	0.00E+00	0.00E+00	2.42E+03	3.15E+03
<i>n</i> -C ₃₀	422.813	0.00051	0	45.5	0	2.555E-05	0.00E+00	0.00E+00	2.08E+03	2.70E+03
<i>n</i> -C ₃₁	436.840	0.00053	0	47.0	0	2.670E-05	0.00E+00	0.00E+00	2.17E+03	2.82E+03
<i>n</i> -C ₃₂	450.866	0.00043	0	48.5	0	2.167E-05	0.00E+00	0.00E+00	1.76E+03	2.29E+03
<i>n</i> -C ₃₃	464.893	0.00036	0	50.0	0	1.818E-05	0.00E+00	0.00E+00	1.48E+03	1.92E+03
<i>n</i> -C ₃₄	478.920	0.00027	0	51.5	0	1.354E-05	0.00E+00	0.00E+00	1.10E+03	1.43E+03
<i>n</i> -C ₃₅	492.946	0.00021	0	53.0	0	1.044E-05	0.00E+00	0.00E+00	8.50E+02	1.11E+03
<i>n</i> -C ₃₆	506.973	0.00018	0	54.5	0	8.894E-06	0.00E+00	0.00E+00	7.24E+02	9.41E+02
<i>n</i> -C ₃₇	520.999	0.00015	0	56.0	0	7.346E-06	0.00E+00	0.00E+00	5.98E+02	7.78E+02
<i>n</i> -C ₃₈	535.026	0.00013	0	57.5	0	6.572E-06	0.00E+00	0.00E+00	5.35E+02	6.96E+02
<i>n</i> -C ₃₉	549.053	0.00011	0	59.0	0	5.412E-06	0.00E+00	0.00E+00	4.41E+02	5.73E+02
<i>n</i> -C ₄₀	563.079	0.00010	0	60.5	0	5.024E-06	0.00E+00	0.00E+00	4.09E+02	5.32E+02
<i>n</i> -C ₄₁	577.106	0.00008	0	62.0	0	3.864E-06	0.00E+00	0.00E+00	3.15E+02	4.09E+02
<i>n</i> -C ₄₂	591.132	0.00010	0	63.5	0	5.023E-06	0.00E+00	0.00E+00	4.09E+02	5.32E+02
Totals	0.48017			0.02965		0.01164	2.18E+06	2.83E+06	9.48E+05	1.23E+06

Table S01.

Oxygen removing potential of ALL Plume HC's (mol O₂/g)^h	0.0413			
	<i>Low Estimate</i>	<i>High Estimate</i>	<i>average</i>	<i>plus-minus</i>
Total DO Anomaly (mol)ⁱ	3.000E+10	3.900E+10	3.450E+10	4.500E+09
Total environmental release (kg)^j	7.265E+08	9.445E+08	8.355E+08	1.090E+08
Total environmental release rate (kg/day)^k	8.753E+06	1.138E+07	1.007E+07	1.313E+06
Total soluble HC mass flow rate into deep plume (kg/day)^l	2.177E+06	2.830E+06	2.503E+06	3.265E+05
Total insoluble HC mass flow rate into deep plume (kg/day)^m	9.480E+05	1.232E+06	1.090E+06	1.422E+05
			<i>average</i>	<i>plus-minus</i>
		total deep plume mass	3.594E+06	3.562E+05

a Dissolved fraction set to zero for hydrocarbons less soluble than n-C₆

b Stoichiometric ratio of O₂:hydrocarbon normalized to hydrocarbon = 1

c Oxygen removing potential of **insoluble** hydrocarbon mass

0.15 = fraction trapped relative to toluene

0.9610 = fraction of toluene dissolved

F_x = ($\sum M_i - \sum (F_i * M_i)$) / (1 - $\sum (F_i * M_i)$) is the fraction of insoluble species characterized in the MW-1 sample

$\sum M_i$ = Sum of the mass fractions characterized in the MW-1 sample = 0.480169

d Mass of dissolved hydrocarbons - Low (g) = F_i x M_i x TFI

TFI = Total HC Mass Flow Rate - Low Estimate (kg/day)

e Mass of dissolved hydrocarbons - High (g) = F_i x M_i x TFH

TFH = Total HC Mass Flow Rate - High Estimate (kg/day)

f Mass of trapped hydrocarbons - Low (g) = ((1-F_i) x M_i x 0.15 x 0.9610 x TFI) / F_x

0.15 = fraction trapped relative to toluene

0.9610 = fraction of toluene dissolved

g Mass of trapped hydrocarbons - High (g) = ((1-F_i) x M_i x 0.15 x 0.9610 x TFH) / F_x

0.15 = fraction trapped relative to toluene

0.9610 = fraction of toluene dissolved

h sum of DO removing potential of soluble + insoluble HCs

i Kessler et al., (2011) Science, 331, 312-315.

j total DO anomaly / total DO removing potential *1000

k total environmental hydrocarbon mass released divided by 83 days of spill

l $\Sigma [F_i * M_i * \text{total release rate into deep plume}]$

m $\Sigma [(1-F_i) * M_i * 0.15 * 0.9610 * \text{total release rate into deep plume} / F_x]$