Explanation of PAH benchmark calculations using EPA PAH ESB approach
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The effects of PAHs are cumulative (additive to be more precise) across all of the PAH compounds in petroleum. When you measure a single PAH, phenanthrene, for example, only a small percentage of the aggregate effect of the petroleum-contaminated mixture is measured.

The "potency divisors" used in the calculation represent the amount of an individual chemical (ie phenanthrene), by itself, that can cause an adverse effect. So, if there was a spill that was nothing but pure phenanthrene, the "potency divisor" for phenanthrene would be the same as the effect level for phenanthrene alone, and one would just compare the two numbers.

PAH Benchmark Calculation for Water Samples
In the case of oil, phenanthrene is just one chemical that contributes to the overall potency of the petroleum mixture. To determine the overall effect of the petroleum in water, one must combine the contributions of all the individual chemicals in the petroleum mixture. The effect of the mixture can be calculated by simply adding together the fractional contributions of all of the components of the mixture. So to estimate the total effect of the mixture of PAHs in an oil sample, first you divide each of the individual compounds by the potency divisor (explained above), then the ratios are added together to calculate the combined toxicity. (See example calculation on page 5)

PAH Benchmark Calculation for Sediment Samples
To determine PAHs in sediment, it is important to factor in the amount of organic carbon in the sediment. When organic carbon is present in sediment, PAHs bind to the organic carbon, making the PAHs less available to aquatic life, thuis lessening their toxicity. For example, both sediments A and B have measured phenanthrene concentrations of 10,000 ug/kg dry weight. Sediment A has an organic carbon concentration of 1% and Sediment B has an organic carbon concentration of 2%. Sediment B is considered half as toxic as Sediment A, because Sediment B can bind twice the amount of phenanthrene than Sediment A.

In order to account for the differences in bioavailability, the dry weight-based PAH concentrations measured in sediment are divided by the organic carbon concentration. From the example above, the phenanthrene concentration of 10,000 ug/kg dry weight in Sediment A is divided by 0.01 (1%) kg organic carbon to equal 1,000,000 ug phenanthrene/kg organic carbon. The phenanthrene concentration of 10,000 ug/kg dry weight in Sediment B is divided by 0.02 (2%) kg organic carbonto equal 500,000 ug phenanthrene/kg organic carbon. Sediment B has a lower organic carbon-normalized phenanthrene concentration, reflective of the lower bioavailability of phenanthrene in Sediment B.

A more complex sediment example is as follows:

A sediment sample contains
9.23 ug/kg dry weight pyrene
10.00 ug/kg dry weight naphthalene
10.00 ug/kg dry weight phenanthrene
20.00 ug/kg dry weight fluoranthene
3.5% or 0.035 organic carbon concentration

1. Normalize the PAH concentrations by dividing by the fraction organic carbon:

(9.23 ug pyrene/kg dwt) / (0.035 kg organic carbon/kg dwt) = 263.7 ug pyrene/kg organic carbon
(10.00 ug naphthalene/kg dwt) / (0.0035 kg organic carbon/kg dwt) = 285.7 ug naphthalene/kg organic carbon
(10.00 ug phenanthrene/kg dwt) / (0.0035 kg organic carbon/kg dwt) = 285.7 ug phenanthrene/kg organic carbon
(20.00 ug fluoranthene/kg dwt) / (0.0035 kg organic carbon/kg dwt) = 571.4 ug fluoranthene/kg organic carbon

2. Divide these organic carbon-normalized values by their "potency divisors" from the sediment benchmark table. The chronic “potency divisors” are:

pyrene = 697,000 ug/kg organic carbon
naphthalene = 385,000 ug/kg organic carbon
phenanthrene = 596,000 ug/kg organic carbon
fluoranthrene = 707,000 ug/kg organic carbon

These calculations yield

(263.7 ug pyrene/kg organic carbon) / (697,000 ug/kg organic carbon) = 0.000378
(285.7 ug naphthalene/kg organic carbon) / (385,000 ug/kg organic carbon) = 0.000742
(285.7 ug phenanthrene/kg organic carbon) / (596,000 ug/kg organic carbon) = 0.000479
(571.4 ug fluoranthene/kg organic carbon) / (707,000 ug/kg organic carbon) = 0.000808

These numbers are basically the fraction of a chronically toxic concentration represented by that single compound. So the concentration of pyrene is basically 0.000378 or 0.0378% of the amount of pyrene alone that would be required to cause toxicity.

3. Add the individual fractional contributions of each PAH compound together, since the toxicity of the compounds are additive:

0.000378 pyrene + 0.000742 naphthalene + 0.000479 phenanthrene + 0.000808 fluoranthene =

0.002407

The chronic benchmark is exceeded when the sum exceeds 1.0. In this example, the PAH concentration in the sample is well below a toxic concentrations.

The previous example is based on four PAH compounds out of 100's that are in oil. To determine the combined potency or toxicity, the calculation procedure must be completed for all of the PAHs present in the sample. The potency of oil lies outside the dozen or so PAHs often measured.

In addition to PAHs, the BTEX compounds will also add to the overall potency of petroleum. While EPA is measuring for these chemicals in oil, it is unlikely that BTEX will remain in the samples by the time Deepwater Horizon petroleum reaches shore. This is because these chemicals are volatile, and quickly evaporate into the air when oil reaches the surface of the ocean. If there was BTEX chemicals left, it would add to the potency of the PAHs. The calculations are done exactly the same, but you just include the potency ratios (concentration/potency divisor) for those compounds in the sum also.

Consideration of samples without alkylated PAHs

When evaluating a sample in which the alkylated PAHs were not measured, you must compensate for their contribution by using "alkylation multipliers". These multipliers account for the unmeasured alkyl compounds that are missed. The multipliers were created based the reported analysis of the Dauphin Island tar ball from the current spill, but were then also checked against oil composition data from other sources, including the Exxon Valdez oil.

For example, the multiplier for naphthalene is 120. That is because this analysis shows that the concentrations of alkylated naphthalenes exceeds the concentration of naphthalene itself. The total potency of all the naphthalene compounds (alkylated and not),were calculated and compared to the ratio of the potency of naphthalene alone. This ratio was 118 (which was rounded to 120). In this case, 99.2% of the real potency of all naphthalene compounds is caused by alkyl-substituted naphthalenes rather than naphthalene itself. To account for this, the alkylation multipliers increase the concentration of naphthalene to account for the unmeasured material.

So, in the example calculation above, we had the organic carbon normalized concentrations calculated as:

(9.23 ug pyrene/kg dwt) / (0.035 kg organic carbon/kg dwt) = 263.7 ug pyrene/kg organic carbon

(10.00 ug naphthalene/kg dwt) / (0.0035 kg organic carbon/kg dwt) = 285.7 ug naphthalene/kg organic carbon

(10.00 ug phenanthrene/kg dwt) / (0.0035 kg organic carbon/kg dwt) = 285.7 ug phenanthrene/kg organic carbon
(20.00 ug fluoranthene/kg dwt) / (0.0035 kg organic carbon/kg dwt) = 571.4 ug fluoranthene/kg organic carbon

and alkylation multipliers apply to three of the four compounds as follows:

pyrene = 2.1
naphthalene = 120
phenanthrene = 6.8

So the concentrations adjusted for alkylation would be:

263.7 ug pyrene/kg organic carbon * 2.1 = 553.8 ug pyrene/kg organic carbon
285.7 ug naphthalene/kg organic carbon * 120 = 34280 ug naphthalene/kg organic carbon
285.7 ug phenanthrene/kg organic carbon * 6.8 = 1943 ug phenanthrene/kg organic carbon
571.4 ug fluoranthene/kg organic carbon * 1 (no multiplier) = 571.4 ug fluoranthene/kg organic carbon

Completing the calculation as above, these values are divided by the potency divisors:

(553.8 ug pyrene/kg organic carbon) / (697,000 ug/kg organic carbon) = 0.000795
(34280 ug naphthalene/kg organic carbon) / (385,000 ug/kg organic carbon) = 0.0890
(1943 ug phenanthrene/kg organic carbon) / (596,000 ug/kg organic carbon) = 0.00326
(571.4 ug fluoranthene/kg organic carbon) / (707,000 ug/kg organic carbon) = 0.000808

The sum of these is 0.094, which means it still meets the guideline (because the sum is less than 1), but it indicates a much higher level of contamination than in the original calculation. See example calculation on page 6.

Example PAH Water Benchmark Calculation

	Column A	Column B	Column C	Column D	Column E	Column F	Column G
CHEMICAL	Measured Concentration (ug/L)	Alkylation Multiplier	Alkyl Adjusted Concentration (ug/L)	Acute Potency Divisor (ug/L)	Chronic Potency Divisor (ug/L)	Acute Potency Ratio	Chronic Potency Ratio
Acenaphthene	0	1	0	232	55.8	0.00000	0.00000
Acenaphthylene	0	1	0	1,280	307	0.00000	0.00000
Anthracene	0	1	0	86.1	20.7	0.00000	0.00000
Benz(a)anthracene	0	1	0	9.28	2.23	0.00000	0.00000
Benzene	0	1	0	27,000	5,300	0.00000	0.00000
Benzo(a)pyrene	0	1	0	3.98	0.957	0.00000	0.00000
Benzo(b)fluoranthene	0	1	0	2.82	0.677	0.00000	0.00000
Benzo(e)pyrene	0	1	0	3.75	0.901	0.00000	0.00000
Benzo(g,h,i)perylene	0	1	0	1.83	0.439	0.00000	0.00000
Benzo(k)fluoranthene	0	1	0	2.67	0.642	0.00000	0.00000
Chrysene	0	5	0	8.49	2.04	0.00000	0.00000
Cyclohexane	0	1	0	1,900	374	0.00000	0.00000
Dibenz(a,h) anthracene	0	1	0	1.17	0.282	0.00000	0.00000
Ethylbenzene	0	1	0	4,020	790	0.00000	0.00000
Fluoranthene	**4.2**	1	4.2	29.6	7.11	0.14197	0.59072
Fluorene	0	14	0	164	39.3	0.00000	0.00000
Indeno(1,2,3-cd)pyrene	0	1	0	1.14	0.275	0.00000	0.00000
Isopropylbenzene	0	1	0	2,140	420	0.00000	0.00000
Methylcyclohexane	0	1	0	463	91.0	0.00000	0.00000
m-Xylene	0	1	0	3,560	700	0.00000	0.00000
Naphthalene	**3**	120	360	803	193	0.44828	1.86528
o-Xylene	0	1	0	3,560	700	0.00000	0.00000
Perylene	0	1	0	3.75	0.901	0.00000	0.00000
Phenanthrene	**1.5**	6.8	10.2	79.7	19.1	0.12802	0.53270
p-Xylene	0	1	0	3,560	700	0.00000	0.00000
Pyrene	**1.2**	2.1	2.52	42.0	10.1	0.05996	0.24950
Toluene	0	1	0	8,140	1,600	0.00000	0.00000

	TOTAL	0.778	3.238
Reported Concentrations	**DO NOT**		exceed acute benchmark because total value is less than 1
Reported Concentrations		**DO**	exceed chronic benchmark beccause total value is greater than 1

Legend
White = measured value from sample
Turquoise = given values
Tan = calculated values

STEP 1: Multiply Column A by Column B. The result is Column C.
STEP 2a: Divide Column C by Column D. The result is Column F.
STEP 2b: Divide Column C by Column E. The result is Column G.
STEP 3a: Sum Column F for Acute Benchmark Value.
STEP 3b: Sum Column G for Chronic Benchmark Value.

Example PAH Sediment Benchmark Calculation

Sediment TOC (mg/kg dwt)	35000

	Column A	Column B	Column C	Column D	Column E	Column F	Column G	Column H
CHEMICAL	Measured Concentrations (ug/kg dwt)	Organic Carbon Normalized Concentrations (ug/kg OC)	Alkylation Multiplier	Alkyl-Adjusted Concentrations (ug/kg OC)	Acute Potency Divisor (ug/kg Organic Carbon)	Chronic Potency Divisor (ug/kg Organic Carbon)	Acute Potency Ratio	Chronic Potency Ratio
Benzene	0	0	1	0	3,360,000	660,000	0.00000	0.00000
Cyclohexane	0	0	1	0	4,000,000	786,000	0.00000	0.00000
Ethylbenzene	0	0	1	0	4,930,000	970,000	0.00000	0.00000
Isopropylbenzene	0	0	1	0	5,750,000	1,130,000	0.00000	0.00000
m-Xylene	0	0	1	0	4,980,000	980,000	0.00000	0.00000
p-Xylene	0	0	1	0	4,980,000	980,000	0.00000	0.00000
o-Xylene	0	0	1	0	4,980,000	980,000	0.00000	0.00000
Methylcyclohexane	0	0	1	0	4,960,000	976,000	0.00000	0.00000
Toluene	0	0	1	0	4,120,000	810,000	0.00000	0.00000
Naphthalene	10	286	120	34286	1,600,000	385,000	0.02143	0.08905
Acenaphthylene	0	0	1	0	1,880,000	452,000	0.00000	0.00000
Acenaphthene	0	0	1	0	2,040,000	491,000	0.00000	0.00000
Fluorene	0	0	14	0	2,240,000	538,000	0.00000	0.00000
Phenanthrene	10	286	6.8	1943	2,480,000	596,000	0.00078	0.00326
Anthracene	0	0	1	0	2,470,000	594,000	0.00000	0.00000
Fluoranthene	20	571	1	571	2,940,000	707,000	0.00019	0.00081
Pyrene	9.23	264	2.1	554	2,900,000	697,000	0.00019	0.00079
Benz(a)anthracene	0	0	1	0	3,500,000	841,000	0.00000	0.00000
Chrysene	0	0	5	0	3,510,000	844,000	0.00000	0.00000
Perylene	0	0	1	0	4,020,000	967,000	0.00000	0.00000
Benzo(b)fluoranthene	0	0	1	0	4,070,000	979,000	0.00000	0.00000
Benzo(k)fluoranthene	0	0	1	0	4,080,000	981,000	0.00000	0.00000
Benzo(e)pyrene	0	0	1	0	4,020,000	967,000	0.00000	0.00000
Benzo(a)pyrene	0	0	1	0	4,020,000	965,000	0.00000	0.00000
Indeno(1,2,3-cd)pyrene	0	0	1	0	4,620,000	1,110,000	0.00000	0.00000
Dibenz(a,h) anthracene	0	0	1	0	4,660,000	1,120,000	0.00000	0.00000
Benzo(g,h,i)perylene	0	0	1	0	4,540,000	1,090,000	0.00000	0.00000
						TOTAL	0.023	0.094
						Reported Concentrations	DO NOT	**exceed acute benchmark because total value is less than 1**
						Reported Concentrations	DO NOT	**exceed chronic benchmark because value is less than 1**

Legend
White = measured value from sample
Turquoise = given values
Tan = calculated values

STEP 1: Divide Column A by TOC, then Multiply by 1,000,000. The result is Column B.
STEP 2: Multiply Column B by Column C. The result is Column D.
STEP 3a: Divide Column D by Column E. The result is Column G.
STEP 3b: Divide Column D by Column F. The result is Column H.
STEP 4a: Sum Column G for Acute Benchmark Value.
STEP 4b: Sum Column H for Chronic Benchmark Value.