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Concentration unit mistakes in health risk assessment of polycyclic aromatic hydrocarbons in soil, sediment, and indoor/road dust

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KEYWORDS

PAHs, cancer risk, exposure factors, ILCR, dimensional analysis, Monte Carlo

1 Introduction

Polycyclic aromatic hydrocarbons (PAHs) are primarily released into the environment by oil spills and incomplete combustion (Sojinu et al., 2010; Patel et al., 2020). Since the presence of these chemical substances causes a significant concern due to their ubiquitous impacts on human health (Mallah et al., 2022), many published research articles have recently been devoted to the occurrence, fate, and associated human health risks of PAHs in the environment (Table 1).

The carcinogenic risk of PAHs is significant as exposure to these compounds has been linked to an increased risk of developing cancer, i.e., increased incidences of lung, skin, and bladder cancers, which are associated with occupational exposure to PAHs (Mallah et al., 2022). Therefore, cancer health risk assessment (HRA) for PAHs is a critical tool for safeguarding public health by quantifying risk, identifying vulnerable populations, guiding environmental regulations, and evaluating intervention efficacy (Hussain et al., 2018).

A modern approach to HRA includes a variety of methods (Zhou et al., 2022; Zhang et al., 2023). In any case, the equations that connect the cancer risk index with the concentration levels of PAHs, the duration of exposure, and the frequency of exposure are the basis for risk assessment (Grellier et al., 2015). The vast majority of researchers in the HRA of PAHs in soil and related media (sediment, road dust, and indoor dust) use the USEPA based methodology (USEPA, 1991) for incremental lifetime cancer risk (ILCR) assessment due to exposure to PAHs through ingestion, inhalation, and dermal routes. This exposure is quantified using the following equations:

$$ILCR_{Ingestion} = \frac{Cs \times CSF_{Ingestion} \times \sqrt[3]{(BW/70)} \times IR_{Ingestion} \times EF \times ED}{BW \times AT \times 10^{6}}$$
(1)

$$ILCR_{Inhalation} = \frac{Cs \times CSF_{Inhalation} \times \sqrt[3]{(BW/70)} \times IR_{Inhalation} \times EF \times ED}{BW \times AT \times PEF}$$
 (2)

$$ILCR_{Dermal} = \frac{Cs \times CSF_{Dermal} \times \sqrt[3]{(BW/70)} \times SA \times AF \times ABS \times EF \times ED}{BW \times AT \times 10^{6}}$$
(3)

where Cs is the sum of converted PAH concentrations according to toxic equivalents (TEF) of benzo (a) pyrene (BaP) (also reffered to as BaP-TEQ or TEQ), while the exposure factors and their most frequently used values for are as follows: $CSF_{Ingestion}$, $CSF_{Inhalation}$, and CSF_{Dermal} are the carcinogenic slope factors of BaP and are 7.3, 3.85, and 25 (kg × day)/mg, respectively; BW is body weight assumed to be 15 kg for children and 70 kg for adults; AT is

TABLE 1 PAH concentration levels in soil, sediment, and road/indoor dust and ILCR values derived.

No.	Reference	Unitsª	ΣPAHs (ppb)	CS ^b or TEQ ^b (ppb)	Sample matrix	Cs ^c taken	ILCR⁴	ILCRe
1	Zhang et al. (2019)	mg/kg	9329	n.a	urban soil	UCL(90%)	4.9×10^{-6}	6.49 × 10 ⁻⁶
2	Tarafdar and Sinha (2019)	mg/kg	n.a	1656	roadside dust	mean	1.823×10^{-5}	1.37 × 10 ⁻⁵
3	Priya Ghosh and Maiti (2020)	mg/kg	1478	n.a	roadside soil	mean	1.237×10^{-6}	1.34 × 10 ⁻⁶
4	Qi et al. (2020)	mg/kg	137	n.a	soil	mean	4.77×10^{-6}	1.99 × 10 ⁻⁷
5	Qu et al. (2020)	mg/kg	460	49	park soil	mean	1.84×10^{-7}	1.86 × 10 ⁻⁷
6	Zhang et al. (2020)	mg/kg	499.47	20.59	urban soil	mean	0.85×10^{-4}	3.88 × 10 ⁻⁸
7	Zhang et al. (2021)	mg/kg	58.12	n.a	soil	mean	4.11×10^{-8}	8.45 × 10 ⁻⁸
8	Siemering and Thiboldeaux (2021)	mg/kg	2060	n.a	urban soil	UCL(95%)	1.67×10^{-6}	1.88 × 10 ⁻⁶
9	Ailijiang et al. (2022)	mg/kg	3304	733	park soil	mean	2.783 × 10 ⁻⁶	2.73 × 10 ⁻⁶
10	Wu et al. (2023)	mg/kg	149.63	14.71	soil	mean	4.67×10^{-8}	1.53 × 10 ⁻⁷
11	Tanić et al. (2023)	mg/kg	55	n.a	park soil	UCL(95%)	5.5 × 10 ⁻⁹	1.50 × 10 ⁻⁸
12	Wang et al. (2024)	mg/kg	278.91	n.a	soil	mean	2.1×10^{-8}	2.41 × 10 ⁻⁷
13	Sun et al. (2024)	mg/kg	56,420	4650	soil	mean	1.46×10^{-5}	3.25 × 10 ⁻⁵
14	Wang et al. (2011)	μg/kg	4800	548	urban dust	UCL(95%)	2.92×10^{-6}	4.53 × 10 ⁻⁶
15	Chen et al. (2013)	μg/kg	8171	n.a	roadside soil	mean	2.37×10^{-5}	1.22 × 10 ⁻⁵
16	Jiang et al. (2014)	μg/kg	4630	300	street dust	mean	1.93×10^{-6}	2.48 × 10 ⁻⁶
17	Soltani et al. (2015)	μg/kg	1074.58	90.88	road dust	mean	4.85×10^{-4}	4.85 × 10 ⁻⁷
18	Gereslassie et al. (2018)	μg/kg	138.72	34.55	soil	mean	3.5×10^{-6}	2.68×10^{-6}
19	Najmeddin et al. (2018)	μg/kg	2183	128.49	street dust	mean	6.2×10^{-4}	2.58 × 10 ⁻⁷
20	Wang et al. (2018)	μg/kg	2052.6	423.86	urban soil	mean	2.53×10^{-5}	1.41 × 10 ⁻⁵
21	Parra et al. (2020)	μg/kg	2211	307.4	soil	mean	3.64×10^{-3}	3.85 × 10 ⁻⁶
22	Mohamadian Geravand et al. (2022)	μg/kg	557.73	19.311	street dust	mean	5.52×10^{-5}	1.53 × 10 ⁻⁷
23	Roy et al. (2022)	μg/kg	13,124	1930	railroad soil	max	3.81×10^{-5}	3.09 × 10 ⁻⁵
24	He et al. (2023)	μg/kg	629.83	93.65	urban soil	mean	1.23×10^{-6}	1.23 × 10 ⁻⁶

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TABLE 1 (Continued) PAH concentration levels in soil, sediment, and road/indoor dust and ILCR values derived.

No.	Reference	Unitsª	ΣPAHs (ppb)	CS ^b or TEQ ^b (ppb)	Sample matrix	Cs ^c taken	ILCR ^d	ILCR ^e
25	Odali et al. (2023)	μg/kg	9810	2180	indoor dust	mean	4.61×10^{-1}	2.01 × 10 ⁻⁵
26	Ali et al. (2017)	ng/g	14,200	305	workshop dust	mean	2.54×10^{-3}	1.49 × 10 ⁻⁶
27	Hu et al. (2017)	ng/g	463.08	32.34	soil	max	1.53×10^{-6}	4.02 × 10 ⁻⁷
28	Ke et al. (2017)	ng/g	890.85	n.a	park soil	max	1.13×10^{-2}	1.25 × 10 ⁻⁵
29	Fu et al. (2018)	ng/g	733.5	n.a	soil	max	8.81 × 10 ⁻⁴	2.26 × 10 ⁻⁶
30	Gope et al. (2018)	ng/g	9688	1422	street dust	max	1.5×10^{-5}	1.56 × 10 ⁻⁵
31	Ghanavati et al. (2019)	ng/g	11,766	951	street dust	max	5.07×10^{-3}	5.08 × 10 ⁻⁶
32	Dreij et al. (2020)	ng/g	5466	n.a	park soil	mean	4.06×10^{-5}	1.35 × 10 ⁻⁵
33	Gope et al. (2020)	ng/g	5491	693	street dust	max	3.4×10^{-6}	7.62 × 10 ⁻⁶
34	Mihankhah et al. (2020)	ng/g	566	36.4	urban dust	mean	2.89×10^{-4}	2.89 × 10 ⁻⁷
35	Apiratikul et al. (2021)	ng/g	4376.93	661.03	urban soil	max	7.57×10^{-6}	7.87 × 10 ⁻⁶
36	Besis et al. (2021)	ng/g	4650	838	house dust	median	9.20×10^{-7}	1.94 × 10 ⁻⁶
37	Jia et al. (2021)	ng/g	688	n.a	soil	mean	2.37×10^{-7}	2.06 × 10 ⁻⁷
38	Shi et al. (2021)	ng/g	932	124	soil	mean	n.a	3.19 × 10 ⁻⁷
39	Cai et al. (2022)	ng/g	219	n.a	soil	mean	10 ⁻⁶ -10 ⁻⁵	1.81 × 10 ⁻⁶
40	Shukla et al. (2022)	ng/g	3748.23	647.9	roadside soil	mean	6.2×10^{-3}	6.17 × 10 ⁻⁶
41	Zhang et al. (2022)	ng/g	508.41	n.a	outdoor soil	mean	1.91 × 10 ⁻⁵	6.46 × 10 ⁻⁷
42	Bigović et al. (2022)	ng/g	271.49	21.7	agricultural soil	mean	1.59×10^{-5}	2.30 × 10 ⁻⁷
43	Wu et al. (2022)	ng/g	2673	268	road dust	mean	1.43 × 10 ⁻⁶	1.43 × 10 ⁻⁶
44	Ambade et al. (2023)	ng/g	5867.4	n.a	urban soil	mean	1.56×10^{-7}	7.46 × 10 ⁻⁶
45	Grmasha et al. (2023)	ng/g	9723.9	1933	sediment	max	1.53×10^{-2}	1.53 × 10 ⁻⁵
46	Liang et al. (2023)	ng/g	434	110	park soil	median	1.09 × 10 ⁻⁷	5.57 × 10 ⁻⁷
47	Miao et al. (2023)	ng/g	593.39	n.a	sediment	max	7.35×10^{-4}	1.29 × 10 ⁻⁶
48	Cui et al. (2023)	ng/g	2441.29	213.61	soil	mean	8.05 × 10 ⁻⁶	3.38 × 10 ⁻⁶

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TABLE 1 (Continued) PAH concentration levels in soil, sediment, and road/indoor dust and ILCR values derived.

No.	Reference	Unitsª	ΣPAHs (ppb)	CS ^b or TEQ ^b (ppb)	Sample matrix	Cs ^c taken	ILCR⁴	ILCR ^e
49	Sankar et al. (2023)	ng/g	3256.74	430.51	soil	mean	3.67×10^{-3}	3.64 × 10 ⁻⁶
50	Gbeddy et al. (2020)	g/g	n.a	492	road dust	mean	1.51×10^{-5}	2.62 × 10 ⁻⁶

afor Cs in Eqs 1-3.

the average time for carcinogenic effects 70 years \times 365 days = 25,550 days; the EF value of 350 days/year is exposure frequency for children and adults; ED is exposure duration (24 years for adults and 6 years for children); IR $_{\rm Ingestion}$ is the soil/sediment/dust intake rate at 100 mg/day for adults and 200 mg/day for children; IR $_{\rm Inhalation}$ is the inhalation rate (20 m³/day for adults and 10 m³/day for children); SA is the dermal surface exposure (5,700 cm²/day for adults and 2,800 cm²/day for children); AF is the dermal adherence factor (0.07 mg/cm²) for adults and (0.2 mg/cm²) for children; ABS value of 0.13 (unitless) is the absorption efficiency factor of PAHs by the human body through dermal contact of soil particles; PEF is the particle emission factor (1.36 \times 10° m³/kg). The aggregate ILCR is the sum of all three ILCR routes.

Eqs 1–3 were used in all cited references in Table 1, except for the correction term $\sqrt[3]{(BW/70)}$, which was omitted in some articles. This term has little influence on the calculated ILCR. Nevertheless, when performing the ILCR for adults and taking the BW to be 70 kg, then $\sqrt[3]{(BW/70)}$ is reduced to number one. In the equations for the ingestion and inhalation routes, sometimes, instead of 10^6 , a conversion factor (CF) is written, which has the same value. The exposure factor values for some of the parameters differ depending on the receptor type (resident, worker, recreator, etc.), age and gender, or location in the world. In many articles, the impact of PAHs on residents divided into two age groups (adults and children) has been evaluated.

The concentrations of PAHs in soil are typically measured using gas chromatographic separation of individual PAHs followed by quantification of the separated PAHs by mass spectrometry (Soursou et al., 2023). These concentrations are expressed as the mass of an individual PAH (nanograms, micrograms, or milligrams) per soil mass (gram or kilogram), i.e., ng/g, µg/kg, or mg/kg. Also, units written as parts per billion (ppb) or parts per million (ppm) may be encountered.

Having analyzed the published works on the presence of PAHs in the soil, sediment, and road/indoor dust and the associated risk, inconsistencies were encountered in the expression of the concentration levels of PAHs in Eqs 1–3 and the results of the health risk estimates derived. Namely, a critical problem among some published articles arises from the use of different units for the concentration values (Cs) of PAHs in soil, sediment, and/or dust.

2 Dimensional analysis

In addition to published articles in which the concentration of PAHs in Eqs 1-3 was expressed in mg/kg (ppm) (Refs. 1-13 in

Table 1); there are a significant number of articles published in reputable international journals in which the concentrations in these equations are expressed in $\mu g/kg$ (ppb) (Refs. 14–25, Table 1) or ng/g (ppb) (Refs. 26–49, Table 1); and there is one case where the concentration is expressed in g/g (Ref. 50, Table 1) without correctly matching/converting the units of the remaining variables/constants in the equations. Because of these disparities in the units for Cs in Eqs 1–3, the estimated human health risk may be tremendously different.

This article aims to clarify this issue. If we start from the fact that, except for concentration (Cs), there is a consensus in units for all other exposure factors in Eqs 1-3, a simple dimensional analysis can resolve this dilemma. This analysis is shown in Eqs 4-6.

$$(-) = \frac{\binom{\frac{1}{kg}}{kg} \times \binom{\frac{2a}{kg} \times \frac{1}{2g}}{\frac{1}{kg}} \times \binom{\frac{1}{kg}}{\frac{1}{kg}} \times \binom{\frac{1}{kg}}{\frac{$$

On the left side of Eqs 4–6, we have ILCR, which is a unitless quantity, and on the right side, identical units have been crossed out according to the following methodology: 1a crosses out 1b, 2a crosses out 2b, 3a crosses out 3b, and so on. The conversion of mg to kg in Eqs 1, 3 is made using the conversion factor (10⁶ value).

When Cs is expressed in mg/kg in the equations, this method of subtraction results in the unitless final value on the right side of the equation. Conversely, if the concentration is expressed in µg/kg or ng/g, the dimensional analysis cannot equate the left and right sides of the equations. Based on this, it is correct to express the concentration of PAHs in the soil, sediment, and dust as mg/kg.

A good example is the case where we would have a BaP-TEQ concentration of 600 μ g BaP/kg, which is the Canadian soil quality guide value for PAHs (CCME, 2010). Calculated the total ILCR, using the aforementioned exposure factors, for 0.6 mg BaP/kg in Eqs 1–3 equals 5.71 \times 10⁻⁶, which is an acceptable cancer health risk with caution. However, if we take 600 μ g BaP/kg in Eqs 1–3 without any unit corrections, we will get

^bA fraction of 0.13 ΣPAHs, was used if TEQ, was not available.

^cMean, UCL(95%), Range or the first sample from the dataset; n.a.—not available.

dpublished in the cited reference.

 $^{^{}e}$ recalculated in this study using mg/kg instead of ng/g or μ g/kg.

ILCR = 5.71×10^{-3} . The latter is an unacceptable risk that requires urgent action.

3 Comparison of the risk assessment results

In line with the above example, the ILCR values from the cited articles were recalculated and compared with the reported ILCR values in the same articles. When the exposure factor values in the cited articles were not reported, the ILCR values were recalculated using the exposure factor values mentioned above.

Because some articles did not report TEQ values, an option that could have been taken was the worst possible case scenario (TEQ = Σ PAHs). However, this option was ruled out because the worst-case scenario was unrealistic. Instead, the TEQ values were approximated as a fraction of Σ PAHs, considering the data in Table 1. Thus, a fraction of 0.13 was derived as the average fraction of Σ PAHs contributing to the TEQ BaP. The standard deviation for this ratio is 0.063. It is important to note that the ratio of TEQ to total PAHs varies depending on the specific soil composition and the sources of contamination.

The calculated ILCR values in most cases differ from the ILCR values reported in the cited references within an order of magnitude. The main cause may lie in the uncertainty of the exposure factor values and the approximation of the TEQ values. Besides, the probabilistic HRA using Monte Carlo simulation used in some cited works resulted in a range of calculated ILCR values, whose mean values differ from the calculated ILCR values in this article. In some cases, ILCR and concentration values at the upper confidence level (UCL) of 90% or 95% were reported instead of the means. However, when the compared ILCR values differ by several orders of magnitude (underlined ILCR values in Table 1), this is primarily attributed to different units for Cs.

Interestingly, in some articles, the Cs units for the equations are written in ng/g or μ g/kg, and yet the results obtained are as if mg/kg was used. This means that only the description of the equations was incorrect. However, if one strictly follows the equations and the units reported, which some authors apparently did, then it can easily result in a difference of several orders of magnitude in ILCR values.

4 Conclusion

The reliance on assumptions of consistent exposure factor values and approximation of TEQ values are the main reasons for the differences in the reported and calculated ILCR values. Additionally,

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the study does not explicitly explore the potential factor and TEQ variations and uncertainties, which are integral components of the HRA equations. However, the mistake in the PAH concentration units in the HRA models may cause a difference of three orders of magnitude in the ILCR estimates for the same concentration level. It may result in inadequate decisions in managing the investigated soil and related media, including sediment, road dust, and household dust. To summarize, it is recommended that PAH concentrations be expressed in ILCR equations as mg/kg. This could help future research to avoid inconsistencies and errors in the units for the concentration of PAHs and, consequently, errors in the associated health risk estimate due to the presence of PAHs in soil, sediment, or dust. It is noteworthy that this article covers only a part of the published works in reputable international journals, mostly recently published articles and a few published quite ago that have been cited many times.

Author contributions

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