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IBRACS Calculator for estimating the risk of PAH pollution in strong sorbing, impacted soils and sediments

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1. Introduction

Traditional risk assessments of PAHs in soils and sediments are not suited for areas that are impacted by soots, coals and residues from industrial activities, such as gas-production, metal smelting, and mining. For these areas, PAHs sorb much stronger to the soil/sediment-media than they would in "pristine" areas, due to the presence of strong sorbing residues and black carbon. The PAHs thereby exhibit a lower bioavailability and lower leachability, and therefore reduced risk compared to what traditional risk assessments would assess, as traditional risk assessment do not account for the presence of strong sorbing phases.

The IBRACs calculator is a simple tool to assess risk, in both "pristine" soils as well as impacted soils (in which the presence of strong sorbing phases are confirmed). For impacted soils, the model bases risk on the measured or estimated, *bioavailable pore-water concentration of PAHs*, which has been the parameter most strongly linked to several soil and sediment microfauna (worms, amphopods, etc.) (USEPA, 2003; Verbruggen, 2012; Arp et al., 2014).

The model takes one of the following as input:

1) Soil concentrations of the 16 priority PAHs (the most typical)
2) or freely-dissolved pore water concentrations of the 16 priority PAHs

In site-specific risk assessments (Tier 3 level) we recommend to determine the pore water concentration of PAHs, e.g. using passive sampler methods like the POM method (e.g. Arp et al., 2014)

For each soil sample, the calculator will provide a toxic unit (TU) score. A TU value of 1 (or log TU of 0) indicates that the bioavailable PAH levels in the soil porewater are the equivalent to that a regulatory benchmark. In the calculator, three types of regulatory benchmarks are considered (Verbruggen, 2012; USEPA, 2003):

RIVM MPCeco: The proposed Dutch benchmark indicating maximum permissible concentration (MPC), where no risk is considered imminent to the soil ecosystem (similar to a PNEC).

RIVM SRC: The proposed Dutch benchmark where a serious risk concentration (SRC) is expected.

USEPA FCVsediment: The US EPA's final chronic value (FCF) for sediments, in which chronic effects to benthic species are expected (recommended for use in sediments).

The larger a TU value is greater than 1, the larger the bioavailable porewater concentrations are than a regulatory benchmark, and therefore the great the potential risk.

Note that RIVM method proposed two ways of estimating MPCeco and SRC. The first method, referred to as the "Single PAH" method, does not assume that the toxicities of individual PAHs are additive, and is derived by single-species PAH toxicity experiments. The "All PAH" method assumes that all PAHs have an effect on organisms through baseline narcosis, and therefore it combines all toxicity data on a per lipid basis before deriving toxicity values. Therefore we have developed the "Single-PAH" calculator and the "All PAH" calculator, to reflect these two approaches, i.e. one excel version for each approach. The USEPA FCV sediment levels (in both calculators) were derived using assumption that all PAHs act on sediment microfauna through baseline toxicity, similar to the "All PAH" method.

2. To use the calculator

Choose if you want to use the "Single-PAH" or "All-PAH" calculator version as described above.

2.1 Input data

2.1.1 Benchmarks based on total soil concentration of PAHs

a. In the tab "Soil Concentrations (Input)", input sample names on row 8.
b. If available, add the mass fraction of organic carbon (f_{OC} = mass OC/mass soil dry weight) in row 10 (otherwise use the default value of 0.058). Note that if mass fraction of organic matter (f_{OM}) is available, the typical f_{OC}/f_{OM} ratio is 0.58.
c. Add the soilconcentrations of PAHs in rows 12-27.

2.1.2 Benchmarks based on freely-dissolved pore-water data

a. In the tab "Water Concentrations (Input)", input sample names on row 8.
b. Add the pore water concentrations of PAHs in rows 12-27.
c. If you have determined the pore water concentrations using the POM method (Arp et al., 2014), the tab "POM-water converter" can be used to calculate the freely-dissolved pore water concentrations. The K_d values used for POM-water partitioning are given in tab "Benchmarks".

2.2 Output Data

2.2.1 Benchmarks based on the input of PAH soil concentrations

The different benchmarks for "Pristine" soils or sediments are reported in the tab "Soil TU - Pristine Soils", and the different benchmarks for "Impacted" soils or sediments are reported in the tab "Soil TU – Impacted Soils". The following is a description of these tabs

a. **Rows 2-14:** A summary table for output TU data for all PAHs present.

b. **Rows 17 - 80:** The TU calculations for individual PAHs are presented.

Values for "pristine" soils (or sediments), are based on recommended RIVM values for soils (RIVM MPC and RIVM SRC) or USEPA values for sediments (USEPA FCV). Values for "impacted" soils are based on pore water concentrations estimated using the "Koc-Coal tar model" (see Arp et al., 2014). The pore water concentrations (rows 78 – 98 of the "Soil TU – Impacted Soils" tab) were calculated using the given f_{OC} and the OC-water partition coefficients, K_{TOC} values, as presented in the tab "Benchmarks". These estimated porewater concentrations are then compared with the fresh water / porewater benchmarks from RIVM and USEPA-. Note, this way of calculating benchmarks is inherent with a higher degree of uncertainty compared to assessing benchmarks directly from freely-dissolved pore water concentrations. Thus, it should be a considered as a second choice compared to a direct determination of pore water concentration, but could be justified if, for example, a rapid estimate is needed.

2.2.2 Benchmarks based on freely-dissolved pore water concentrations

The different benchmarks are reported in tab "Water TU Calc".

a. **Rows 2-14:** A summary table for output data based on recommended RIVM values for soils (RIVM MPC and RIVM SRC) or USEPA values for sediments (USEPA FCV). The TU calculations for individual PAHs are presented on rows 17-77.

For more information about the theory and practical applications of the IBRACS TU calculators we refer to IBRACS final report which can be downloaded from IBRACS homepage http://projects.swedgeo.se/ibracs/.

3. References

Arp, H. P. H., S. Lundstedt, S. Josefsson, G. Cornelissen, A. Enell, A.-S. Allard and D. B. Kleja (2014). "Native Oxy-PAHs, N-PACs, and PAHs in Historically Contaminated Soils from Sweden, Belgium, and France: Their Soil-Porewater Partitioning Behavior, Bioaccumulation in Enchytraeus crypticus, and Bioavailability." Environmental Science & Technology. 48, 11187−11195.

USEPA (2003). "Equilibrium Partitioning Sediment Guidelines (ESBs) for the Protection of Benthic Organisms: PAH Mixtures." Office of Science and Technology and Office of Research and Development, U.S. Environmental Protection Agency: Washington, DC.

Verbruggen, E.M.J. (2012). Environmental risk limits for polycyclic aromatic hydrocarbons (PAHs). RIVM report 607711007/2012

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