

# Predicting ecotoxicity of coal tar asphalt in soils

---

Toxic Units of modelled bioavailable concentrations of Polycyclic Aromatic Hydrocarbons

# How does PAHs spread from coal tar asphalt?

- Leaching from bound subbase is limited
  - Limited contact with water
  - Small specific surface
- Asphalt particulates
  - Spreadable
  - Large specific surface



# Spread of particulate coal tar asphalt

- Road works
- Intermediate storage
- Heavy traffic induced road breakage
- Exposed coal tar asphalt in the surface course

# Basis for risk assessment

$$\sum_{i \in PAH16} PAH_i \longrightarrow \sum_{i \in PAH16} \frac{\text{Bioavailable concentration of } PAH_i}{EC50_i}$$

# Toxicity model for risk assessment

## Toxic Units (TU)

- Concentration addition
  - Suitable for PAHs
- Flexibility in measure of toxicity
  - Predictive (EC50)
  - Protective (NOEC, EC5)
- Adjust for bioavailability
  - Modelled
  - Measured

$$TU = \sum_i \frac{\text{Concentration}_i}{\text{Toxic concentration}_i}$$

$$TU = \sum_i \frac{\text{Concentration}_i}{EC50_i}$$

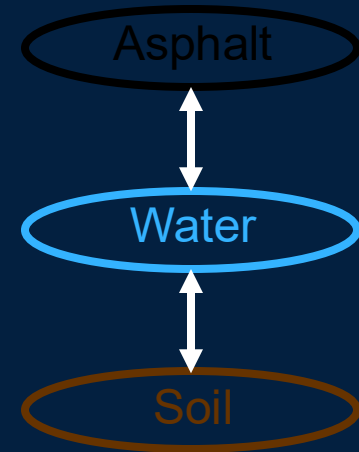
$$TU = \sum_i \frac{\text{Concentration}_i}{NOEC_i}$$

$$TU = \sum_{i \in PAH16} \frac{\text{Modelled bioavailable concentration}_i}{EC50_i}$$

# Equilibrium model for bioavailability

Assumptions:

- PAH in equilibrium between asphalt, water, and soil
- The equilibrium partitioning is linear
- The water phase is negligible for the mass balance
- Partitioning to soil follows  $K_D = f_{SOC}K_{SOC}$
- Equivalence between freely dissolved and bioavailable PAHs

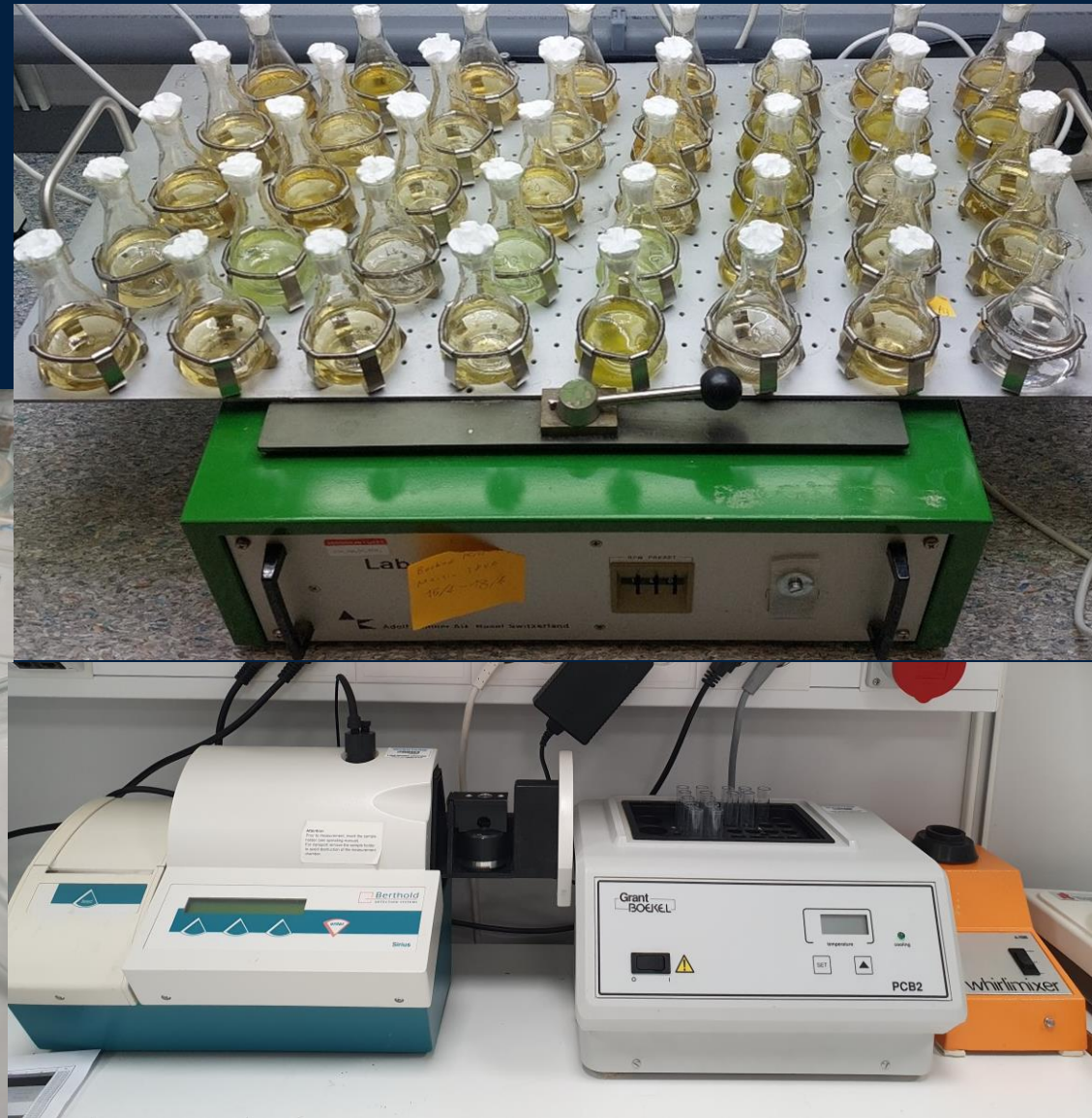


$$\text{Modelled bioavailable concentration}_i = \frac{\text{Mass}_{\text{Asphalt}} * \text{Concentration PAH in asphalt}_i}{K_{\text{Coal tar binder},i} \text{Mass}_{\text{Coal tar binder}} + K_{\text{SOC},i} f_{\text{SOC}} \text{Mass}_{\text{Soil}}}$$

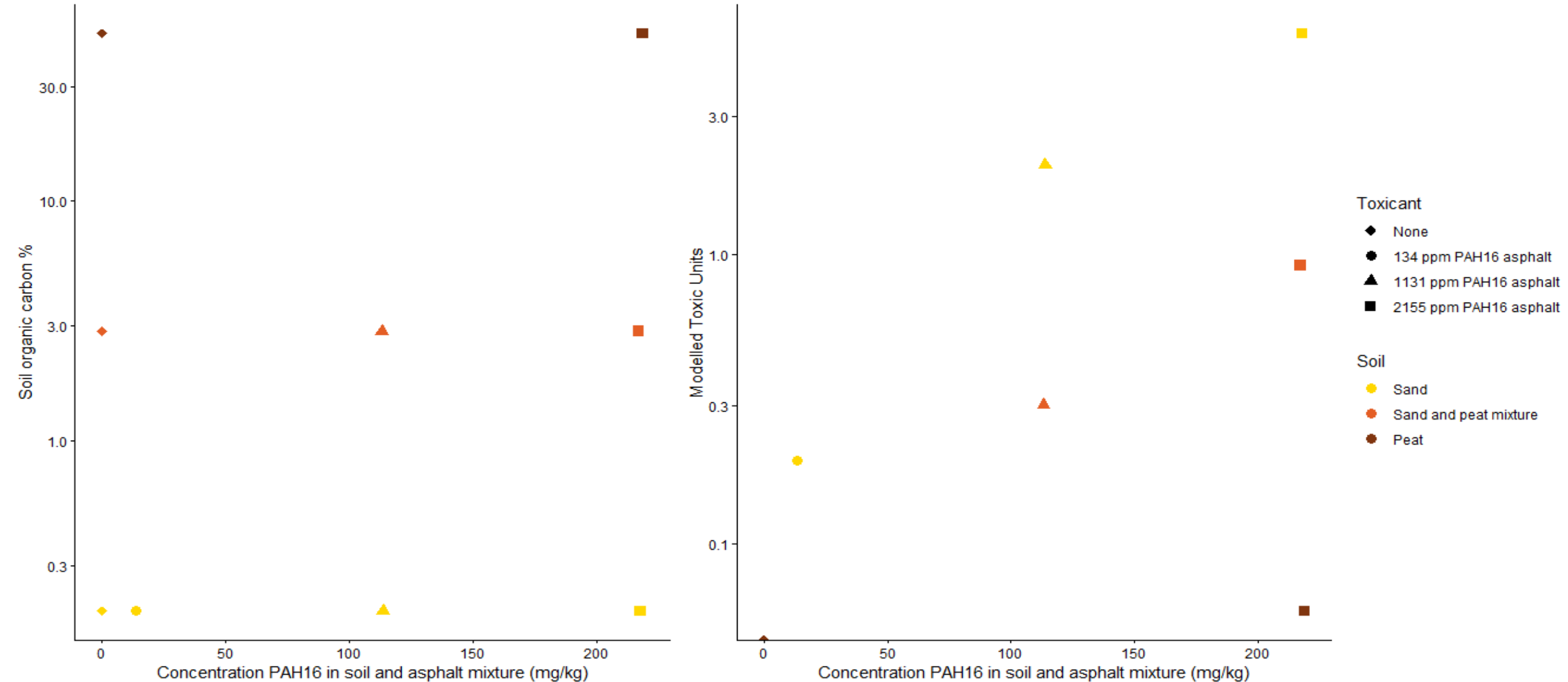
# Testing the model

Column leaching followed by three ecotoxicology tests:

1. Seedling germination test
2. Algae reproduction test
3. Bioluminescence test



# Experimental design



# Equilibrium partitioning model vs column leaching

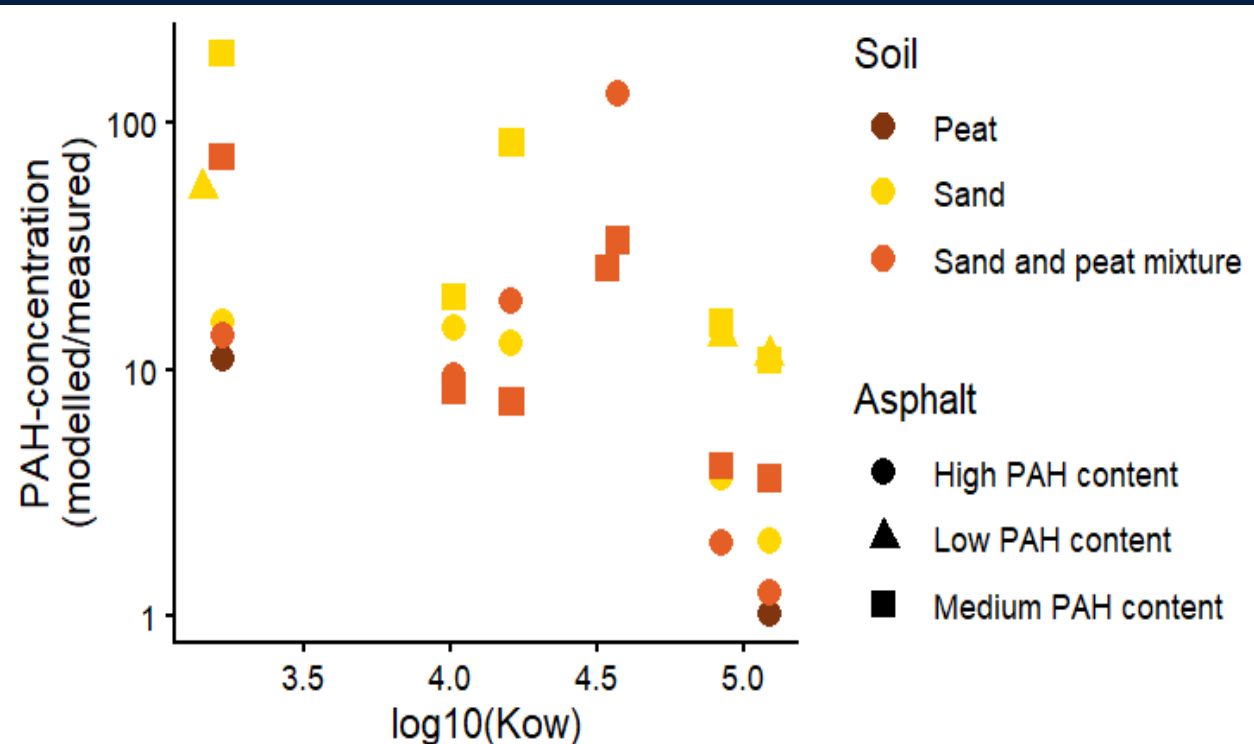
Leaching is overestimated

Negative relationship between:

- Overestimation and  $K_{OW}$
- Overestimation and soil organic carbon

I.e. less sorption -> greater overestimation

Modelled equilibrium partitioning compared to column test



# Ecotoxicity results

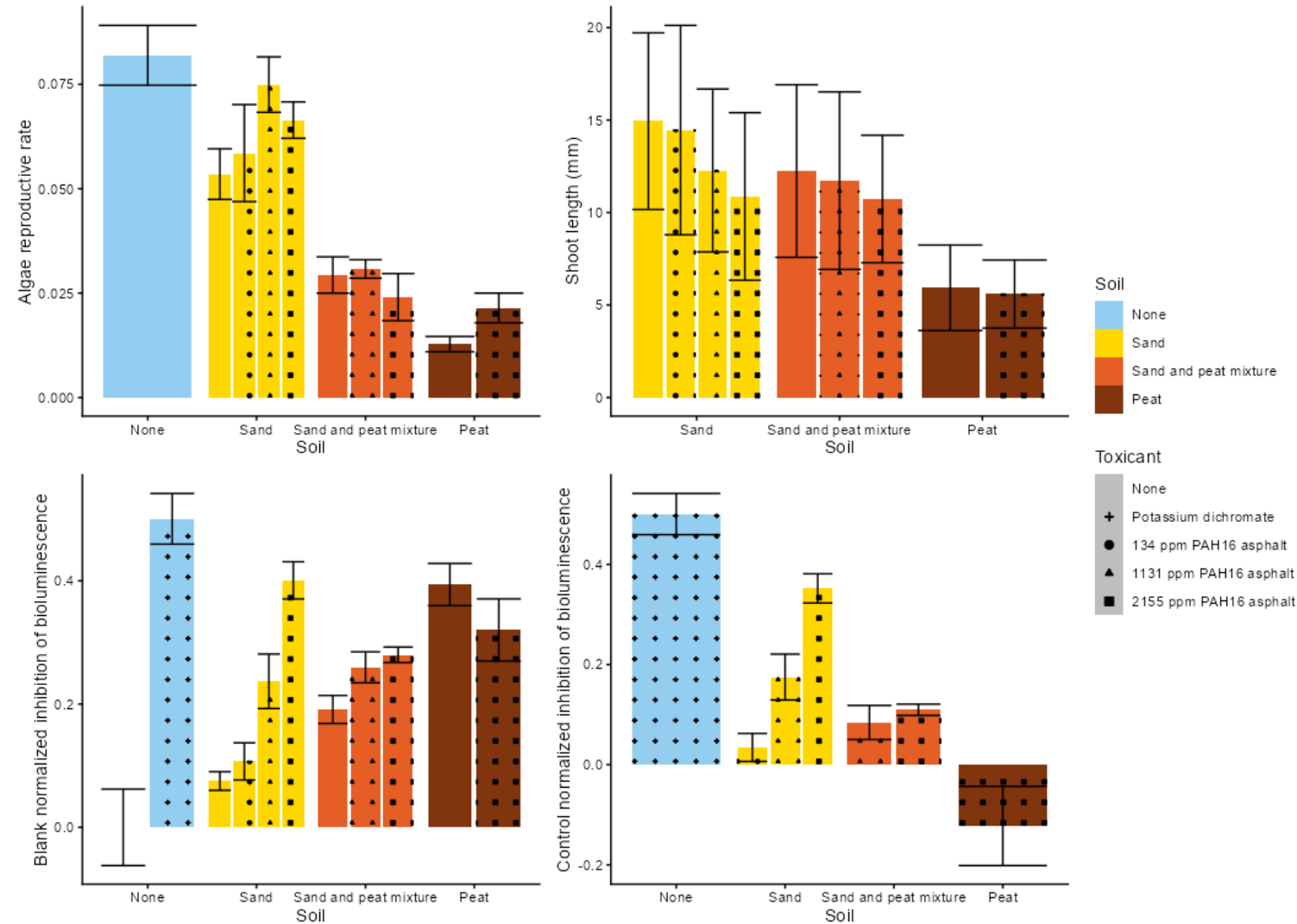
Soil type had bigger impact than asphalt

The algae were stimulated by PAH16

The shoots were inhibited PAH16

Bioluminescence was inhibited by PAH16

The inhibition was ameliorated by peat

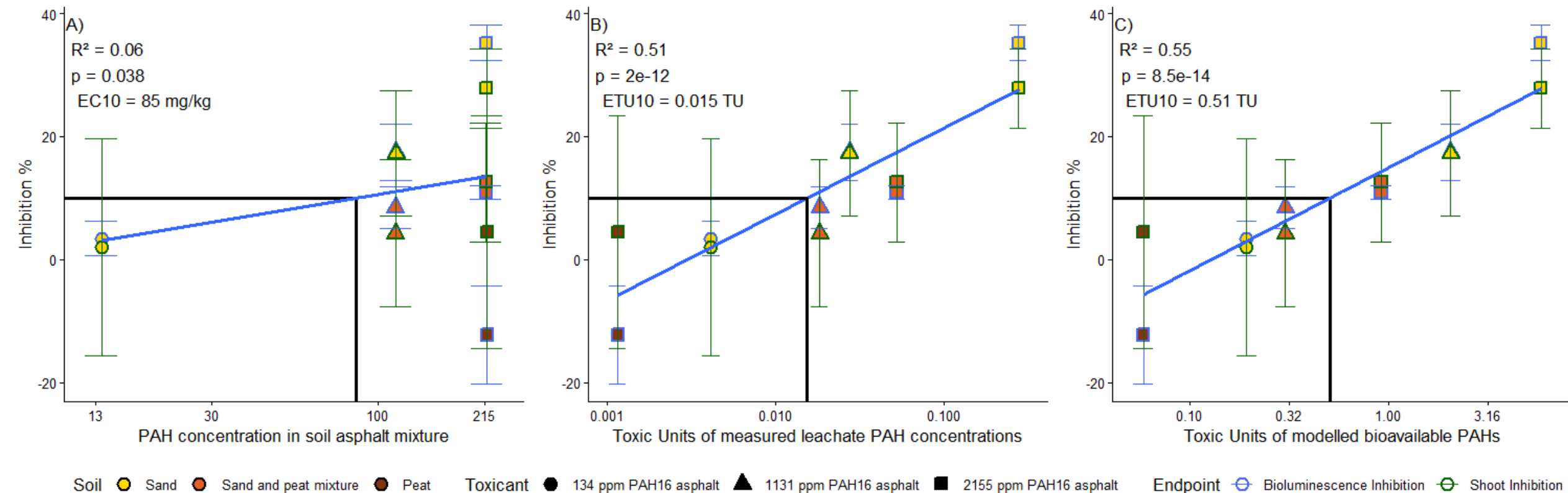


# Results

No correlation between total concentration and inhibition

Strong correlation between leachate concentrations and inhibition

Best correlation between modelled concentrations and inhibition



# Usage

## Low tier site specific risk assessments

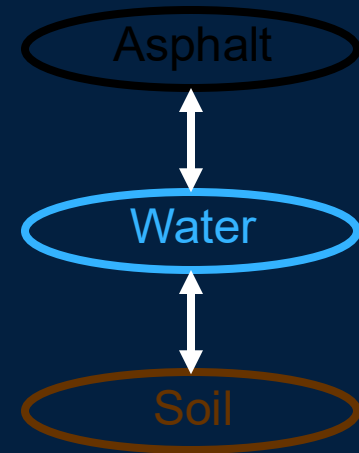
### How to do it:

Define your system, measure the asphalts PAH-content and the soil organic carbon content, estimate amount of asphalt, plop it into excel.

### Use case examples:

Risk assessments of actual or potential spread of particulate coal tar asphalt

Assessment of risk reduction measures



# Usage – Excel tool

**Asphalt Contamination Toxicity Calculator**

This is an early release of a toxicity calculator that has been developed for use in low tier risk assessments of contamination of soils by coal tar asphalt particles. It is based on research by Martin Oscar Larsson, Ivan Carabante, Hans Peter Arp and Jurate Kumpiene. It can be freely used and distributed.

| PAH                   | Asphalt Concentration (g/kg or µg/g) | PAH                   | C_Free (µg/L) | SRC_Eco_Water      | MPC_Eco_Water |
|-----------------------|--------------------------------------|-----------------------|---------------|--------------------|---------------|
| naphthalene           | 1.60                                 | naphthalene           | 15.168        | 0.029              | 0.015         |
| acenaphthylene        | 2.05                                 | acenaphthylene        | 2.489         | 0.035              | 0.027         |
| acenaphthene          | 0.42                                 | acenaphthene          | 0.525         | 0.005              | 0.001         |
| fluorene              | 2.10                                 | fluorene              | 1.184         | 0.010              | 0.007         |
| phenanthrene          | 14.50                                | phenanthrene          | 2.705         | 0.063              | 0.057         |
| anthracene            | 4.85                                 | anthracene            | 0.604         | 0.144              | 1.438         |
| fluoranthene          | 24.00                                | fluoranthene          | 0.240         | 0.020              | 0.167         |
| pyrene                | 20.50                                | pyrene                | 0.214         | 0.051              | 2.212         |
| benz[a]anthracene     | 10.85                                | benz[a]anthracene     | 0.023         | 0.007              | 0.619         |
| chrysene              | 8.70                                 | chrysene              | 0.018         | 0.011              | 0.161         |
| benzo[b]fluoranthene  | 10.00                                | benzo[b]fluoranthene  | 0.010         | 0.007              | 0.433         |
| benzo[k]fluoranthene  | 10.00                                | benzo[k]fluoranthene  | 0.007         | 0.008              | 0.465         |
| benzo[a]pyrene        | 11.25                                | benzo[a]pyrene        | 0.005         | 0.006              | 0.570         |
| indeno[123cd]pyrene   | 5.70                                 | indeno[123cd]pyrene   | 0.001         | 0.002              | 0.611         |
| dibenz[a,h]anthracene | 2.45                                 | dibenz[a,h]anthracene | 0.000         | 0.001              | 0.555         |
| benzo[ghi]perylene    | 5.20                                 | benzo[ghi]perylene    | 0.001         | 0.005              | 0.633         |
| <b>SUM</b>            | <b>134.17</b>                        | <b>Sum PAH-16</b>     | <b>23.194</b> | <b>Toxic Units</b> | <b>0.404</b>  |

| Material | Mass % in the modelled system | Organic carbon content (TOC g/g) |
|----------|-------------------------------|----------------------------------|
| Asphalt  | 10                            | 0.05                             |
| Soil     | 90                            | 0.00194                          |

| Term          | Explanation                                                                                                                                                                                                                                    |
|---------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| C_Free        | Freely dissolved concentration in pore water at equilibrium.                                                                                                                                                                                   |
| Toxic Units   | The sum of freely dissolved concentrations of PAH-16 normalized by their toxicity so that TU < 1 means the mixture toxicity is below the toxic effect threshold used (SRC_Eco_Water or MPC_Eco_Water) and TU > means it is above the threshold |
| SRC_Eco_Water |                                                                                                                                                                                                                                                |
| MPC_Eco_Water | Maximum Permissible Concentration                                                                                                                                                                                                              |

Available via: <https://www.ltu.se/en/research/research-subjects/waste-science-and-technology/research-projects/research-in-waste-science-and-technology/2023-12-06-spread-and-toxicity-of-pah-from-tar-asphalt-roads>

## In conclusion

Equilibrium models of bioavailability of PAHs are conservative  
and

Toxic Units are suitable for modelling ecotoxic effects of complex mixtures of PAHs  
thus

Toxic Units of equilibrium modelled bioavailable PAH:s are conservative, flexible, and  
predictive

Finally:

Whilst conservative, the equilibrium assumption greatly reduces expected toxicity

Only amount of asphalt, it's PAH-content and the SOC% is necessary for the modelling

# Kontakt

---

Martin Oscar Larsson  
[Martin.Larsson@ltu.se](mailto:Martin.Larsson@ltu.se)  
+46737053435

