Sensitivity analysis of key environmental fate parameters used in PETRORISK version 6.02 for the environmental risk assessment of petroleum substances

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Introduction

A review of the environmental and physicochemical methodologies used in the PetroTox and Hydrocarbon Block Method (HBM) tools was conducted by RIVM on the behalf of ECHA (ECHA, 2012). A number of uncertainties with respect to the physical-chemical, environmental fate and ecotoxicological parameters were identified and inconsistencies in the use of parameters generated from PetroTox and HBM, and their subsequent use in PETRORISK version 6.02, were also identified. This study investigates the potential effect of uncertainty on environmental exposure, for three environmental fate parameters identified in the review published by ECHA. In particular, the effect of variation in the octanol-water partition coefficient (Kow) and Henry's Law Constant on environmental exposure was investigated and the effect of uncertainty in the bioconcentration factor (BCF) on secondary poisoning and humans *via* the environment was also considered. Results for two aromatic hydrocarbons, C_9 aromatic hydrocarbons and C_{11} aromatic hydrocarbons, are summarised here.

Method

- PETRORISK version 6.02 calculates PEC's according to the substance emission rate and the corresponding fate factor for each environmental compartment. Fate factors are reported for each environmental compartment at the local, regional and continental scales for each substance in the 'Concawe library'. Fate factors reported in PETRORISK v6.02 are calculated using the EU TGD spreadsheet model adapted for the hydrocarbon block method (EUTGDsheetvs123 HB 20080715.xls, van de Meent, 2008).
- In this investigation, the 'Concawe library' within the HBM EU TGD spreadsheet has been amended for three separate environmental fate parameters according to recommendations in the ECHA review:
  - Octanol-water partition coefficient (Kow)
  - Henry's Law Constant (HLC)
  - Bioconcentration factor (BCF)
- Kow values in the current 'Concawe library' of the HBM EU TGD spreadsheet are calculated from KOWWIN estimates and experimental values, where available. In this investigation the current Kow values in the 'Concawe library' have been replaced with Kow values generated from SPARC 4.2.
- Henry's Law Constant (HLC) values in the current 'Concawe library' of the HBM EU TGD spreadsheet are calculated using the HenryWin v3.20 model and experimental values, where possible. The HLC values generated from SPARC 4.2 (expected to be more conservative) were used to replace the current HLC values in the 'Concawe library'.
- Bioconcentration factor's (BCF) in the current version of the 'Concawe library' are estimated from BCFWin v2.16. More conservative BCF values are generated in the updated version of the software, BCFBAF v3.00. These more conservative BCF values were used to update the current BCF values in the 'Concawe library'.
- Fate factors assuming 100% release to waste water, 100% release to air and 100% release to soil, have been generated for each change in environmental fate parameter (Kow, HLC and BCF) for all substances in the 'Concawe library'. Where release to waste water was modelled, application of sewage sludge to soil was assumed.
- Human intake fractions, used to estimate exposure to man via the environment have also been generated.

Preliminary results

Results for 2 aromatic hydrocarbons, C_9 aromatic hydrocarbons and C_{11} aromatic hydrocarbons, have been summarised. The substituents assumed to be present in each hydrocarbon have been generated from PETRORISK version 6.02.

<u>Henry's Law Constant:</u> changes in fate factors for C_9 aromatics and C_{11} aromatics appear to be very minor.

<u>Bioconcentration factor:</u> small decreases in fate factors for fish, fish eating predators and top predators, resulted with BCF values estimated using BCFBAF v3.00 for both C_9 aromatics and some C_{11} aromatics. Small decrease in human intake factors for C_{11} aromatics were calculated.

<u>Octanol-water partition coefficient:</u>

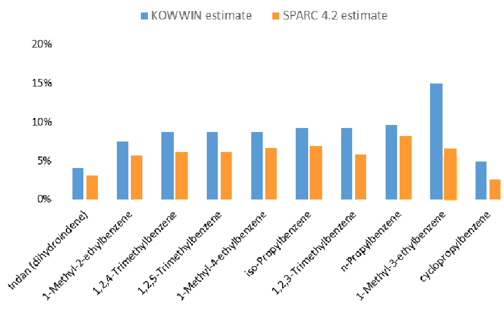

Figure 1. Estimated % of C_9 aromatic constituents in sewage sludge with varying Kow (100% release to water)

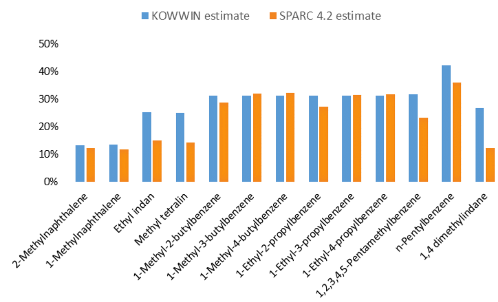

Figure 2. Estimated % of C_{11} aromatic constituents in sewage sludge with varying Kow (100% release to water)

- Small decreases were calculated in the fraction estimated to partition to sewage sludge for C_9 aromatics and some C_{11} aromatics.
- Small decreases were calculated in fate factors for sludge, soil and sediment for C_9 aromatics and some C_{11} aromatics.

Next Steps:

- Run updated fate factors in PETRORISK version 6.02 to investigate the impact on PECs.
- Investigate impact of Kow, HLC and BCF on a wider range of hydrocarbon types including higher carbon numbers.
- Investigate effects of degradation rates on soil, sediment, STP according to ECHA review.

Acknowledgements: Emiel Rorije, Expertise Centre for Substances (SEC), National Institute for Public Health and the Environment (RIVM)

References:

[1] van de Meent (2008), Environmental fate factors and human intake fractions for exposure and risk calculation of petroleum products with the hydrocarbon block method, Reports Environmental Science no 322, Netherlands Center for Environmental Modeling

[2] ECHA (2012), Emiel Rorije, Eric M.J. Verbruggen & Joop A. de Knecht, Service Request on a critical review of the environmental and physicochemical methodologies commonly employed in the environmental risk assessment of petroleum substances in the context of REACH registrations, Framework Contract No ECHA/2008/2 Reference No ECHA/2008/02/SR30