Hydrocarbon Block Petroleum Substances risk assessment - Summary and Conclusions, including further work

TU286

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This poster is number 5 of a series of 5 posters on the risk assessment of petroleum substances. See also posters TU282, 283, 284 & 285

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Abstract

CONCAWE has been conducting a programme assessing the risks of petroleum substances to man and the environment to comply with the REACH legislation. The substances have been grouped according to previously agreed categories for classification, with consolidation based on composition and intended use. The approach adopted for assessing the environmental fate and effects of these categories is based on the Hydrocarbon Block Method. This method has been used for all categories. Although all the petroleum substances have been registered under REACH, in the process of conducting these risk assessments the results have been addressed and research needs for furthering the approach taken, identified and initiated. The poster will describe the outcome under REACH and the research now being undertaken to improve the assessment of the environmental fate and effects of petroleum substances. Covering:

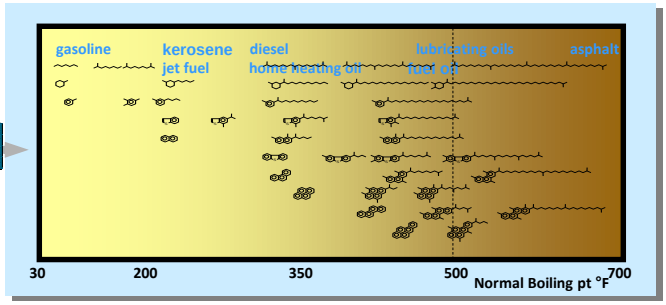
- Summary of the Petroleum substances for which risk assessments were conducted and key recommendations for further work
- Further work aimed at refining the Hydrocarbon Block Method and its constituent parts

Outcome of the Risk Assessments

Risk assessments were conducted on low boiling point naphthas, kerosene's, gas oils – vacuum and hydrocracked, straight run, cracked and other gas oils, highly refined and other lubricant base oils, foots oils, unrefined and acid treated oils, aromatic extracts, heavy fuel oils, petrolatums, paraffin and hydrocarbon waxes, slack waxes and bitumen. As described in other posters, the PETRORISK model was used to conduct an initial tier 1 risk assessment. Based on the findings addressing environmental impact, there were no uses of petroleum substances that were flagged as being unsafe. However, there were some refineries, for which it was necessary to conduct a higher tier assessment using local site conditions and knowledge. To ensure that the substances were being safely produced. Consequently, there are now projects on-going to improve understanding of the emissions of hydrocarbons and follow the fate of hydrocarbon blocks through refinery treatment processes.

In the course of conducting the substance risk assessments there were indications that the NPTL model, upon which both PETRORISK depend for the effects assessment (PNEC) and environmental fate parameters, used in PETRORISK for deriving the PEC, were in need of further refinement. These are further discussed below.

The "CONCAWE library" (see poster TU 283)



The approach summarised below is described in further details in Poster 2 of this series (TU 283). Each hydrocarbon block included in the compositional matrix is defined using a set of representative hydrocarbon structures with specific physical-chemical and fate properties. The properties included in the CONCAWE library are:

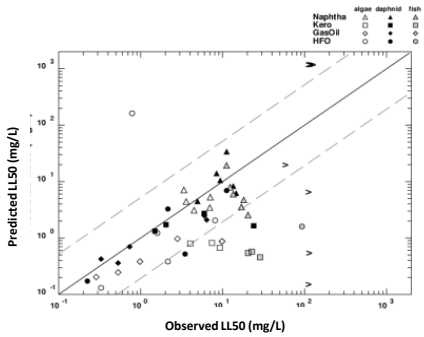
- Water solubility (estimated using SPARC)
- Henry's Law Constant (estimated using SPARC)
- logKow (estimated using SPARC)
- logKoc
- Air, Water, Wastewater Treatment Plant (WWTP), Soil and Sediment half-lives (BioHCWin)
- Aquatic HC5 (HC5 = hazard concentration affecting 5% of the species)
- WWTP HC5
- Sediment HC5

The basic structures were based on Quann (1998) who described over 100 families of hydrocarbons present in petroleum substances, see Figure 1 for examples, from which over 1500 structures were described covering the carbon number range of C4 – C41. However, as noted in a recent report issued by RIVM*, the library does not contain any hetero-hydrocarbons other than those with sulphur. Thus O and N derived hydrocarbons are not represented. This was originally considered to not be critical as the concentrations of these structures is believed to fairly low, less than 2%. However, given the recent interest expressed in these structures CONCAWE are now looking for data on the type of structures, the quantity that they may be present and environmental fate and effect data on such structures, to ensure they are adequately covered by the other structures in the library.

Improvements required to the PNEC derivation (see poster TU 284)

The effects of the hydrocarbons, are predicted using the Target Lipid Model (see poster 3 of this series). The model contains a database of TLM parameters for 55 individual organisms including freshwater and marine fish, invertebrate and algal endpoints. The TLM accounts for acute effects by a non-specific toxicity mode of action (e.g., narcosis) such as exhibited by hydrocarbons that are found in petroleum substances. The TLM uses critical target lipid body burdens (CTLBB) to model the toxicological sensitivity of different organisms. Empirical Acute to Chronic Ratios (ACR) are used for predicting chronic effects regardless of the underlying mechanism [16]. The approach is modified by accounting for the reduced bioavailability of high logKow chemicals, e.g. logKow >6. Based on the Species Sensitivity Distribution from the data it then is possible to derive an HC5, upon which the PNEC may be based.

The figure shows the ability of the model to predict toxicity of petroleum substances.



In considering improvements to the NPTL, there are three areas that stand out as requiring further improvements;

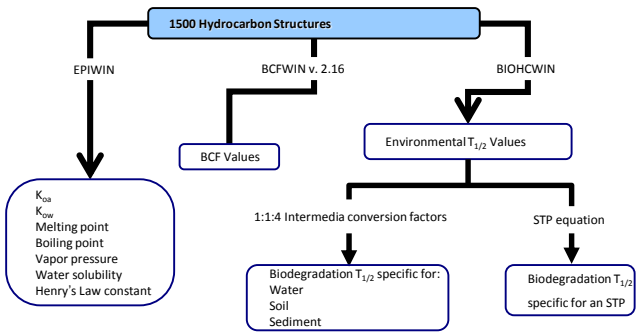
1. Enhancing the data base of Acute:Chronic data to support the ACR used, both in terms of quality and quantity of data
2. Increasing the number of species that the are described by the data used, to support the use of the HC5 and an application factor of 1.
3. Demonstration that the HC5 was protective for all components in petroleum substances including PAHs.

To achieve these aims, activities are now being planned for further testing, to increase the species database, the ACR database, and address statistical concerns of the methodology.

Improvements required for deriving the PEC (see poster TU 285)

The properties required for the calculation of a substances PEC (see figure) are;

1. Physical-chemical parameters : water solubility, vapour pressure, logKow. The melting point and boiling point may also be used.
2. Environmental fate parameters: abiotic and biotic ½ life, bioconcentration factor



Physical-chemical parameters:

The physical-chemical parameters are estimated for the structures in the library using QSAR, either SPARC or EPIWEB. However, as the models developed it was obvious that the use of these different systems may cause confusion and that the differences that exist between the two modelling systems for predictions of the parameters lead to concerns about the approach. Consequently, CONCAWE are investigating whether to re-parametise the PETROTOX/PETRORISK models using only one of the QSAR systems.

Environmental fate parameters:

Aquatic biodegradation ½ life : the model used to predict the primary ½ life for the hydrocarbon structures is BIOHCWIN. This model was originally developed using available information in 2005. At the time it was recognised that the model required further data on the ½ lives of typical hydrocarbons, and this is now being developed.

Extrapolation to soil & sediment : the data to support the extrapolation factors used in PETRORISK are limited and further data is now being generated to support the factors of 1:1:4.

Conclusion

The approaches adopted for the environmental risk assessment of petroleum substances has been outlined. The details are contained in other posters in this series (see below). As a result of the risk assessments conducted to meet the requirements of REACH, various improvements to the models were needed and are now being addressed.

* Rorije, E *et al., 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, ECHA/2008/02/SR30, RIVM/DHI, 2012*