Abstract
CONCAWE has been conducting a programme assessing the risks to man and the environment of petroleum substances complying with the requirements of REACH. The substances have been grouped according to their intended use and exposed to the environment. The approach adopted for assessing the environmental fate and effects of these categories is based on the Hydrocarbon Block Method (HBM) as described in the Technical Guidance supporting REACH. The approach that CONCAWE has adopted reflects the comprehensive nature of the single substance approaches normally used, but allows for the complex nature of petroleum substances. The HBM has been used for all categories requiring an environmental risk assessment. The poster describes the basic approach and introduces the overall strategy:

1. Analysis substance composition & variability
2. Select HBS to describe product composition
3. Compile relevant physico-chemical & fate property for HBS
4. Estimate environmental emissions of HBS throughout product lifecycle stages
5. Characterize fate factors & intake fractions of HBS
6. Determine environmental exposure to HBS
7. Assess environmental effects of HBS
8. Evaluate individual and aggregate risk of HBS

Grouping
The substances assessed in the programme were grouped according to previous work, in which the substances were grouped for classification purposes. These groupings were subsequently amended to account for use. The groupings were:

- Low boiling point naphthas, kerosenes, gas oils – vacuum and hydrocracked, straight run, cracked and other gas oils, highly refined and other lubricant base oils, feet oils, unrefined and acid treated oils, aromatic extracts, heavy fuel oils, petroleumums, paraffin and hydrocarbon waxes, slack waxes and bitumens.

Substance analysis & hydrocarbon block assignment (see poster TU283)

The risk assessment process starts with analysis of the substances to be assessed, which in the case of petroleum substances is a complex process, and for the lighter products, involves GCxGC assessment (see poster 2 in this series, Eadsforth et al). This method, known as the high resolution approach, yields data enabling the substances to be assigned to the appropriate hydrocarbon class. Examples of classes include n- and isoparaffins, n-cycloparaffins and n-cycloalkanes, mono-, di- and polyphenothics, mono- di- and polyaromatics etc. An example of such an analysis is given below in Figure 1.

Figure 1. High resolution blocking scheme in PETRO Risks derived from GCxGC analysis

The "CONCAWE library"

Each hydrocarbon block included in the compositional matrix is defined using a set of representative hydrocarbon structures with specific physico-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 HCS (HCS = hazard concentration affecting 5% of the species)
- WWTP HCS
- Sediment HCS

The basic structures derived for this library of representative structures were based on Quann (1998) who described over 100 families of hydrocarbons present in petroleum substances, see Figure 2 for examples, from which over 1500 structures were described covering the carbon number range of C4 – C41. The structures were arranged into families of 16 hydrocarbon classes which correspond to their basic structure, but also align to the classes that can be analysed by GCxGC, if using this approach.

Figure 2. Example structures from Quann (1998)

For each structure, using the models in either SPARC or EPINWEB, the properties above were derived. Also fate factors (see TU284) were derived for all these structures.

The % composition of each of the blocks is then distributed evenly among the representative components included in the block. The risk assessment subsequently performed using PETRO RISK derives PECS, PNEDs and RCRs for the representative hydrocarbons.

References


Quann, 1998.