Development of the Hydrocarbon Block Method for environmental risk assessment of petroleum substances

TU282

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This poster is number 1 of a series of 5 posters on the risk assessment of petroleum substances. See also posters TU283, 284, 285 & 286

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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 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 (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:

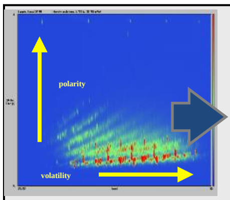
1. Analyse substance composition & variability
2. Select HBs to describe product composition
3. Compile relevant physic-chemical & fate property for HBs
4. Estimate environmental emissions of HBs throughout product lifecycle stages
5. Characterize fate factors & intake fractions of HBs
6. Determine environmental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

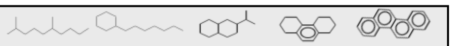
Grouping

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, foots oils, unrefined and acid treated oils, aromatic extracts, heavy fuel oils, petrolatums, 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 described by Carbon Number and hydrocarbon class. Examples of classes include n- and isoalkanes, n-cyclopentanes and n-cyclohexanes, mono- , di- and polynaphthenics, mono-, di- and polyaromatics etc. An example of such an analysis is given below in Figure 1.





HB	C#	n-P wt%	i-P wt%	n-CC6 wt%	i-N wt%	Di-N wt%	Poly-N wt%	MoAr wt%	NMAr wt%	DiAr wt%	NDiAr wt%	PolyAr wt%
1	3-5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	6-8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	9-11	0.1	0.2	0.0	0.3	0.2	0.0	0.1	0.4	0.4	0.1	0.0
4	12-14	2.1	2.9	0.3	3.3	1.6	0.0	1.4	1.6	0.9	0.6	0.3
5	15-17	4.6	9.1	1.1	7.6	4.2	0.0	3.0	2.2	1.0	0.4	0.4
7	etc	"	"	"	"	"	"	"	"	"	"	"

Figure 1. High resolution blocking scheme in PETRORISK 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 HC5 (HC5 = hazard concentration affecting 5% of the species)
- WWTP HC5
- Sediment HC5

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.

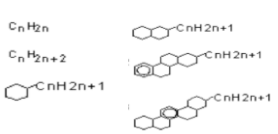


Figure 2. Example structures from Quann (1998)

For each structure, using the models in either SPARC or EPIWEB, 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 PETRORISK derives PECs, PNECs and RCRs for the representative hydrocarbons.

Estimating emissions to the environment

The emissions to the environment in PETRORISK are estimated using four different elements:

- The composition in the hydrocarbon blocks mapped to the CONCAWE library
- Emission factors and operating conditions contained in the ESIG spERCs (hard-coded)
- Fate Factors and Intake Fractions calculated using EUSES (hard-coded)
- Use/tonnage information for all relevant uses of petroleum substances

The emission factors were estimated based on spERCs which have been standardized in order to include process and use knowledge available in the petroleum industry. The further work describing these is to be seen in Poster 4 in this series (Leon Paumen).

Characterising fate factors and intake fractions (see poster TU285)

Based on the work described by van de Meent, SETAC 2007, environmental fate factors and human intake fractions were derived according to the the EU Technical Guidance Documents for risk assessment (EU, 2003). Environmental fate factors and human intake fractions of the 1500 individual library substances were combined into fate factors and intake fractions of hydrocarbon blocks. For this purpose, the EU TGD spreadsheet model by the Netherlands Center for Environmental Modeling (Van de Meent et al., 2005), which makes use of the original spreadsheet models SimpleTreat 3.1 (Struijs et al., 2003) and SimpleBox 3.0 (Den Hollander et al., 2004) were used.

Determining environmental exposure (see poster TU285)

Using the emission data and the fate factors, as described above, it then becomes possible to calculate the environmental concentrations of the hydrocarbons, as required by the risk assessment, see figure 2.

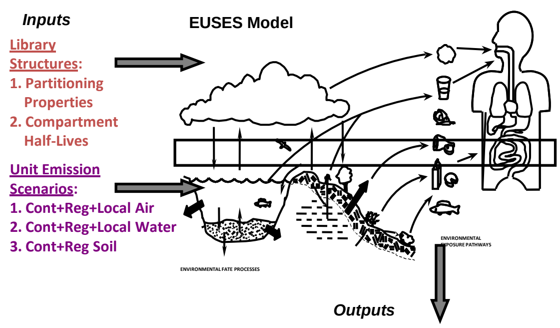


Figure 2. Assessing environmental exposures according to EUSES

Assessing environmental effects of hydrocarbons (see poster TU284)

The effects of the hydrocarbons, are predicted using the Target Lipid Model. 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.

Evaluation of risks (see poster TU285)

The evaluation of the risks for the petroleum substances which then brings together all these approaches is then conducted via an excel based model, PETRORISK, see poster 4 of this series.
PETRORISK contains the following elements;

- Clear packaging of relevant input information:
  - Product composition (2d-gc)
  - Life cycle information:
    - Tonnage (EU, fraction regional, local)
    - SpERC emission factors
    - Local operating conditions (DF, WWTP flow, duration)
  - Product library
    - Structures used in calculation & associated properties
- Output worksheets:
  - Multimedia distribution (TGD)
  - Regional assessment
  - Local assessment
  - Site-specific assessment for manufacturing use scenario
    - Production/Use questionnaire data

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; TU 283, 284, 285 and 286.

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Quann, 1998,

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