Understanding WAF results used for the assessment of aquatic toxicity (CRANCS project)

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INTRODUCTION

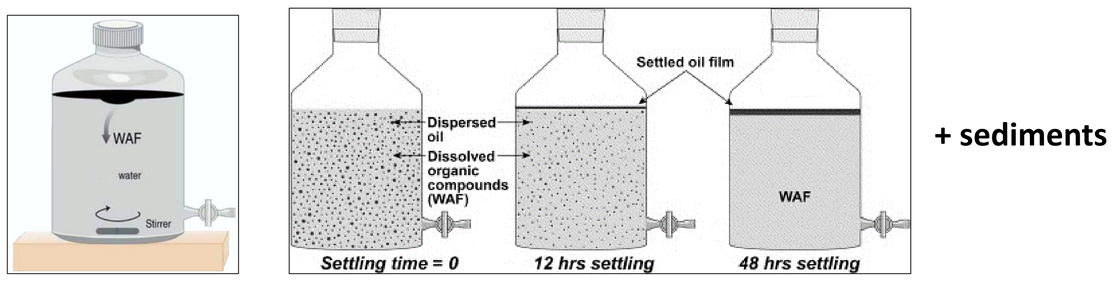
Various methodologies can be applied to perform an Environmental Risk Assessment for Natural Complex Substances (NCS) which are complex multi-constituent substances. While it is generally recognised that ecotoxicity studies can be performed using the Water Accommodated Fraction (WAF) method (OECD, 2000) at least for Classification and Labelling purposes, there is some concern that results of such studies cannot be easily validated or interpreted. Their interpretation is often considered as ambiguous, and a workable method to transform the effect loading result to derive a meaningful PNEC (Predicted No Effect Concentration) for environmental risk assessment where it is compared to a PEC (Predicted Environmental Concentration) currently does not exist.

CRANCS stands for **C**ompartmentalised **R**isk **A**ssessment for **N**atural **C**omplex **S**ubstances

OBJECTIVE : to develop a predictive method for environmental risk assessment in aqueous medium exposed to NCS1 (eg. essential oils for which >90% is characterised).
The main characteristic of CRANCS is to provide a more realistic picture of the distribution of a mixture and each of their constituents when they are released into the aquatic environment.

WAF concept within CRANCS

Due to the high hydrophobicity of many constituents in NCS, the WAF method is used in the CRANCS project in order to maximise dissolution in the aqueous phase to reach a thermodynamic equilibrium. The WAF is performed with and without sediment (Figure 1).



+ sediments

Figure 1: Illustration of experimental WAF methodology

METHOD AND RESULTS

The partitioning between pelagic and benthic phase of an artificial equimolar mixture of 4 constituents was studied. The chemicals chosen are known to be very stable in aquatic media in order to monitor their concentrations. The experimental results were compared to the predicted values using a thermodynamically based iSafeRat WAF calculation using the Partition Equilibrium Method (Bicherel & Thomas, 2021) and sediment partitioning calculation proposed for use for mono-constituents in the REACH regulation.

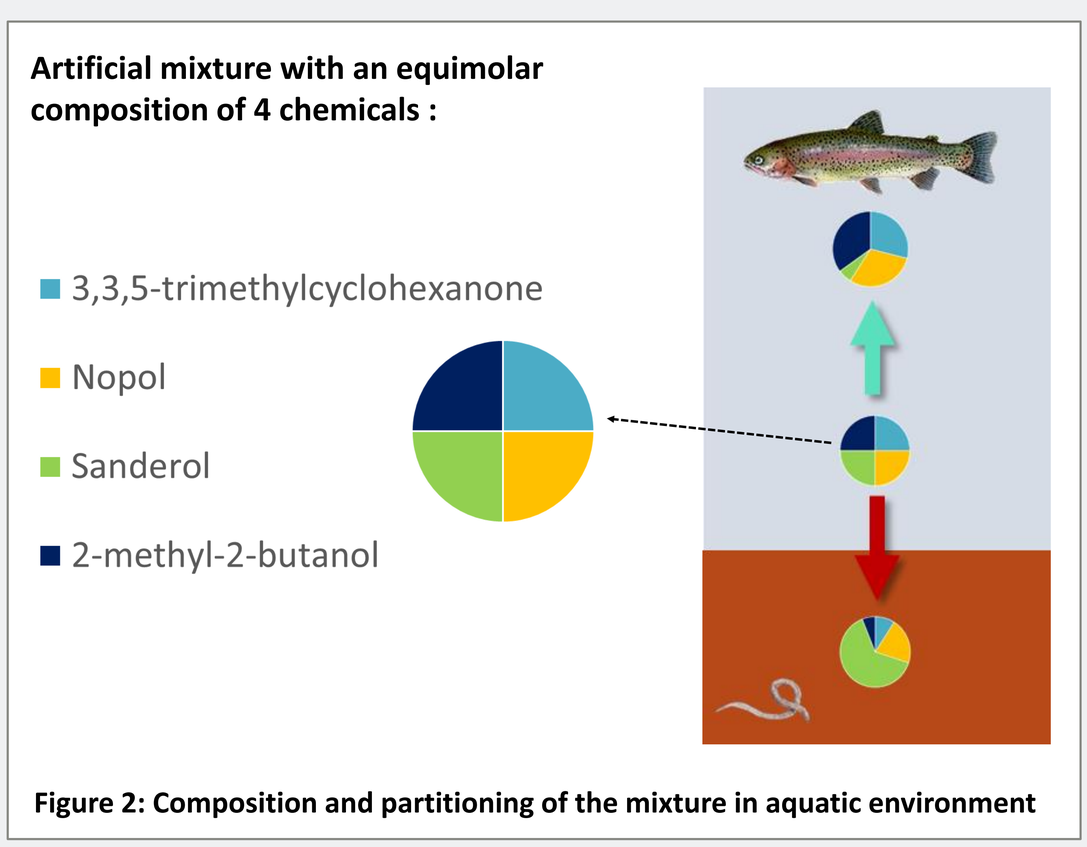
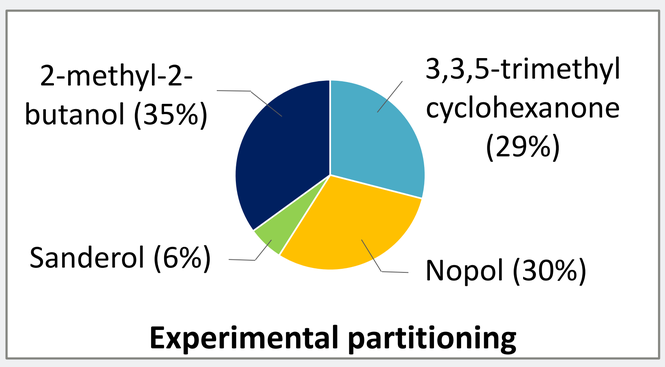
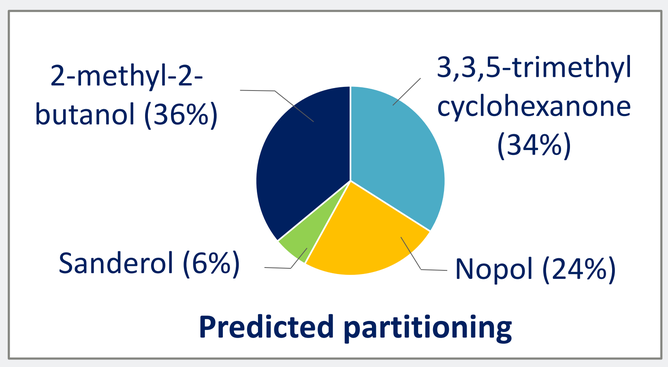


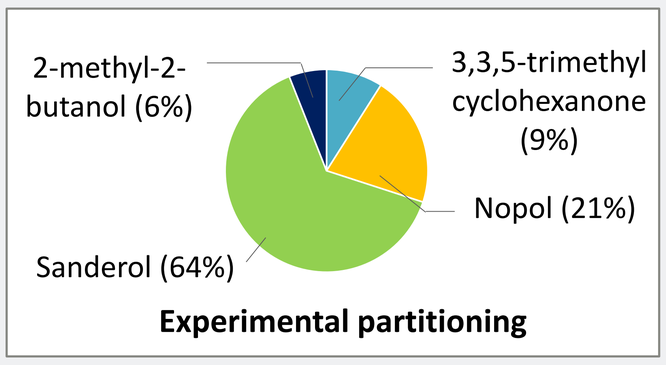
Figure 2: Composition and partitioning of the mixture in aquatic environment

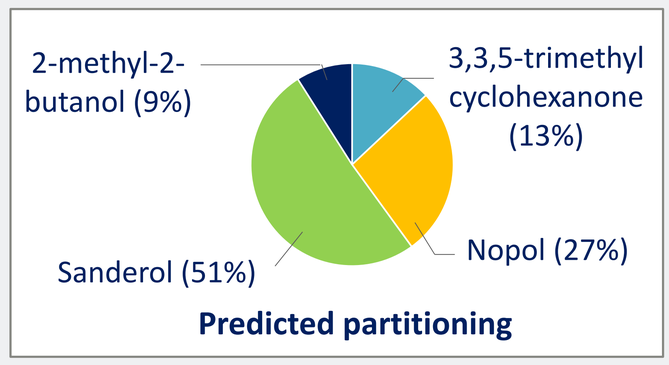
Pelagic compartment





Benthic compartment (*sediments*)





The toxicity of the WAF of the mixture has been tested on daphnids : before the partitioning and after the partitioning. Providing the toxicities and the concentrations of each constituents can be predicted, it is possible to calculate the WAF toxicity for both cases (Table 1).

Toxicity to daphnids*	Experimental toxicity	Predicted toxicity (KREATiS)
Before partitioning	5.31 mg/L	4.5 mg/L
After partitioning	8.348 mg/L	11 mg/L

Table 1: Toxicity of the artificial mixture to daphnids before and after presence of sediments.
*as 48h-Lethal Loading rate for 50% effect

CONCLUSION

The results showed that:

- The iSafeRat® WAF method accurately predicted aqueous WAFs both before and after sediment addition.
- The WAF method allowed the constituents of a mixture to reach a stable equilibrium concentration between pelagic and benthic phases.
- The concentrations of each constituent in both phases can be accurately predicted by calculation.
- WAF toxicity in the sediment can also be predicted by the iSafeRat® calculation method developed by KREATiS.

REFERENCES

OECD. [OECD] (2000) OECD series on testing and assessment Number 23. Guidance document on aquatic toxicity testing of difficult substances and mixtures. ENV/JM/MONO(2000)
Pascal Bicherel, Paul Thomas (2021). Aquatic Toxicity Calculation of Mixtures: A Chemical Activity Approach Incorporating a Bioavailability Reduction Concept. Environ. Sci. Technol. 2021 https://doi.org/10.1021/acs.est.1c04389
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