Applications of PETROTOX in hazard assessment of petroleum substances

Aaron Redman[1], Tom Parkerton[1], Mike Comber[2], Miriam León Paumen[3], Charles Eadsforth[4], Klaas den Haan[5]
[1]ExxonMobil Biomedical Sciences, New Jersey; [2]Mike Comber Consulting, UK; [3]ExxonMobil Petroleum and Chemical, Belgium;
[4]Shell Services International Limited, UK; [6]CONCAWE, Belgium

TU284

This poster is number 3 of a series of 5 posters on the risk assessment of petroleum substances

Abstract

PETROTOX is a spreadsheet model that related the composition of a petroleum substance to it's aquatic toxicity. This poster reports on validation activity since it's initial development (Redman et al 2005 PETROTOX – an aquatic toxicity model for petroleum substances. SETAC-Europe, The Hague, The Netherlands.) The model has been validated using composition and aquatic effects data for more than 100 individual substances across more than 15 major substances categories (e.g., fuels, lubricants, bitumen, etc.). In combination with passive sampling methods, PETROTOX is used to streamline testing programs by identifying candidate test substances (e.g., toxic vs. nontoxic) and test concentrations..

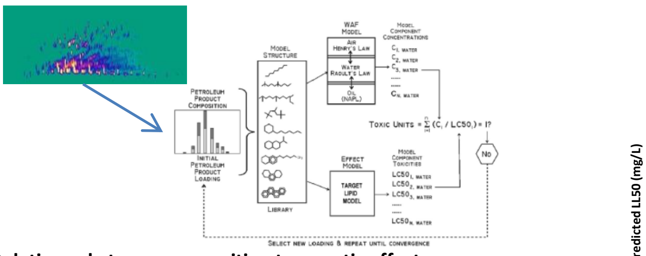
PETROTOX combines the hazard assessment strategies used on single chemicals with the hydrocarbon block approach to modeling complex substances:

- Blocks are defined by available analytical chemistry, which characterizes substances in terms of mass fractions for discrete blocks based on chemical class and physicochemical properties (e.g., C#, BP).
- It uses a library of 1500 representative structures as an extension of the CONCAWE hydrocarbon block method (HBM)
- Solubility estimated using multi-component dissolution model
- Toxicity is considered additive and modeled using toxic units based on the Target Lipid Model (TLM)
- Toxicity is assumed to be due to interaction of test organisms with dissolved phase hydrocarbons

Hydrocarbon blocks

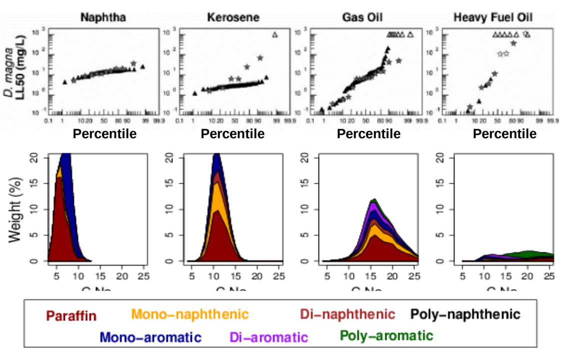
PETROTOX uses two different compositional resolution schemes depending on available analytical

- Low resolution (BP-based assignment) and High resolution (detailed C#-based assignment)
- Composition is mapped to library compounds for use in solubility and toxicity calculations



Relating substance composition to aquatic effects

Substance composition varies between and within categories. Mass weighting of Library structures provide response to variations in composition. Figure presents indirect verification of model applied to category data by comparing observed effects data (triangles) to predicted effect levels (stars).

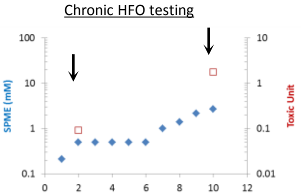


Screening with passive sampling and PETROTOX

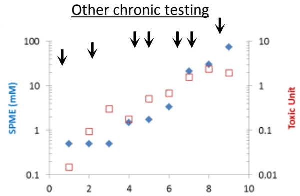
UVCB substances were screened with SPME and PETROTOX to identify candidate (toxic and non-toxic) substances for testing. Arrows indicate substances selected for further testing.

Substance ID	Class	Loading (mg/L)	SPME mM	TU, acute D.magna	Endpoint	ELxx (mg/L)	SPME mM	TU @ ELxx
MRD-11-104	HFO	1	Bdl	0.1	D.magna, 21d repro	>1.2	bdl	0.4
MRD-11-113	HFO	1	2.67	1.8	D.magna, 21d repro	0.1	1.17	2.7
MRD-07-909	HFO	100	21.4	1.6	D.magna, 2d LL50	2	5.9	0.9
MRD-07-910	HFO	100	30.3	2.3	D.magna, 2d LL50	3.2	14	1.7
MRD-07-911	HFO	100	74.3	1.9	D.magna, 2d LL50	10	28	1.2
MRD-08-346	DAE	100	10.9	0.3	D.magna, 21d repro	>0.1	0.04	0.6
MRD-08-347	DAE	100	Bdl	0.4	D.magna, 21d repro	>1	bdl	0.1
MRD-08-375	TDAE	100	Bdl	0.2	D.magna, 2d LL50	>100	bdl	0.8
MRD-08-385	UATO	10	6.05	0.4	D.magna, 21d repro	0.1	0.3	0.5
MRD-09-415	UATO	1	Bdl	0.001	D.magna, 21d repro	>1	bdl	0.003
MRD-09-435	LBO	1	Bdl	0.1	D.magna, 21d repro	3	0.1	0.7
MRD-08-383	foots oil	1	Bdl	0.0002	D.magna, 21d repro	>1.1	bdl	0.0
MRD-10-579	Gas Oil	100	111	3.9	D.magna, 2d LL50	1.35	40.0	1.9
MRD-10-604	Gas Oil	100	100	1.8	D.magna, 2d LL50	5.8	20.0	1.2
MRD-10-578	Gas Oil	100	404	6.1	D.magna, 2d LL50	0.7	40.0	1.0
MRD-10-595	Gas Oil	100	215	4.5	D.magna, 2d LL50	0.32	15.0	0.7

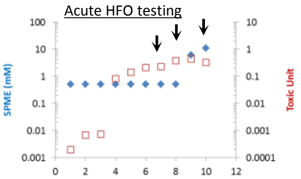
Chronic HFO testing



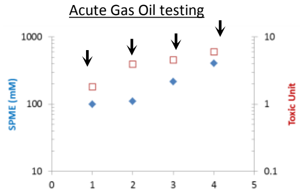
Other chronic testing



Acute HFO testing

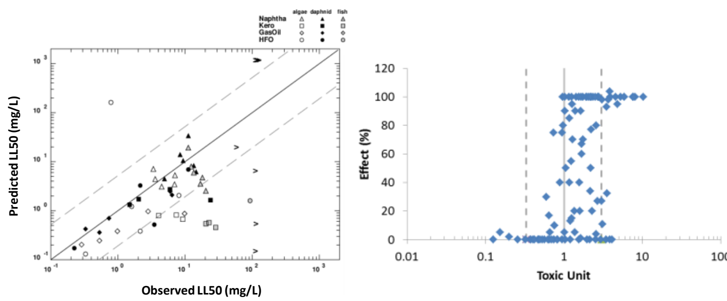


Acute Gas Oil testing



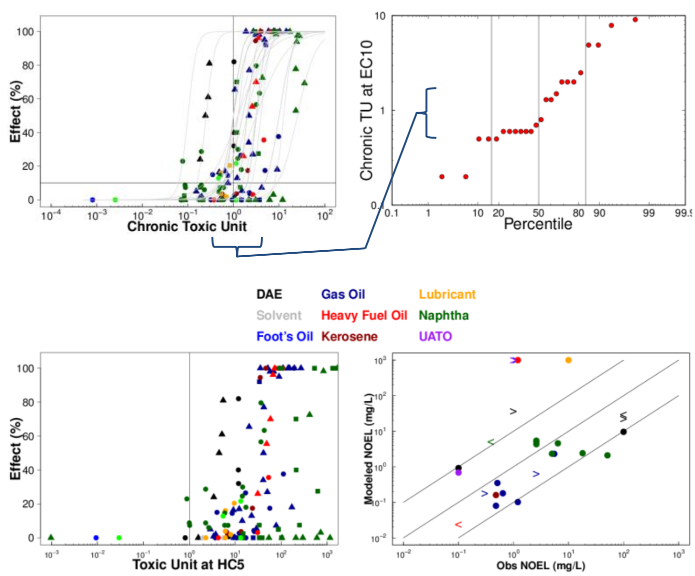
PETROTOX applied to acute exposures

- Modeled toxicity of >20 individual substances across 9 substance categories following exposures to invertebrates, fish and algae.
- Model-data comparisons agree within a factor of 3, consistent with uncertainties in model and data
- Figures provide verification of model through direct comparisons be predicted and observed median lethal loadings (LL50) and by comparing effects data to predicted toxic units (TU)



PETROTOX applied to chronic exposures

- Modeled toxicity of 21 individual substances across 9 substance categories following exposures to invertebrates (21d reproduction), fish (14 & 28d growth, survival) and algae (3d growth)
- Predicted TU-responses consistent with Chronic TUs and 90% of observed EC10s are ± 2x of TU=1 supporting assumed additivity in chronic exposures
- Predicted NOELs are generally conservative and accurate to ± 2x. Variability in this direct comparison is in part due to shallow TU-loading curve of these generally insoluble petroleum substances
- HC5 is protective of observed effects petroleum-bases UVCBs



Conclusion

- PETROTOX is considered fit for purpose of hazard assessment of petroleum-based UVCBs
- Observed acute and chronic toxicity are consistent with model and above modeled HC5

References

Redman et al 2012. PETROTOX: an aquatic toxicity model for petroleum substances *ETC* 31:2498
Redman et al 2014 Application to chronic exposures of HFO *ETC* accepted