

Industry view on PetCO approach for PBT assessment

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## Agenda



Concawe, and its activities to support REACH (3 slides)

Petroleum UVCBs (3 slides)

Petroleum substances under REACH (1 slide)

PBT assessment of petroleum substances/Concawe PBT report (2 slide)

PetCo, and Concawe support to PetCo (1 slide)

Persistence (2 slides)

**Bioaccumulation** (2 slides)

Summary (1 slide)



#### **Introduction to Concawe**

- <u>CON</u>servation of <u>C</u>lean <u>A</u>ir and <u>W</u>ater in <u>E</u>urope, established in 1963 in The Hague
- 40 member companies in 2019
- Concawe's mission is to conduct research to provide impartial scientific information in order to:
  - Improve scientific understanding of the environmental, health, safety and economic performance aspects of both petroleum refining and the distribution and sustainable use of refined products.
  - Assist the development of technically feasible and cost effective policies and legislation by EU institutions and Member States.
  - Allow informed decision making and cost effective legislative compliance by Association members.
- Concawe endeavours to conduct its activities with objectivity and scientific integrity
- Concawe seeks to uphold three key principles:

sound science, transparency and cost-effectiveness



#### Petroleum substances are UVCBs

Unknown or Variable composition, Complex reaction products and Biological materials

- **Crude oil:** a very complex and variable natural substance consisting of a wide range of saturated and unsaturated hydrocarbons
- Refining: (1) separation according to boiling point (distillation), (2) cracking high boiling hydrocarbons into more valuable short chains, (3) reforming saturated <> unsaturated, (4) removing impurities
- **Petroleum products:** need to meet performance specifications (e.g. jet fuel)



#### Petroleum refining (<u>https://www.concawe.eu/videos/</u>)





#### Unknown, Variable (and Complex) composition





## Petroleum substances (PS) under REACH

• PSs are fit into a finite and manageable number of EC numbers based on refinery process and basic physicochemical parameters

EC #	Substance	Description
265-060-4	Distillates (petroleum), light catalytic cracked	A complex combination of hydrocarbons produced by the distillation of products from a catalytic cracking process. It consists of hydrocarbons having carbon numbers <b>predominantly</b> in the range of C9 through C25 and boiling in the range of <b>approximately 150°C to 400°C</b> . It contains a <b>relatively large proportion of bicyclic</b> aromatic hydrocarbons.

- Petroleum substances are grouped into major product categories (currently 20)
  - e.g. kerosines, gas oils, base oils, aromatic extracts
- As an action under PetCo, Concawe has systematically removed all redundant and unsupported uses and PS
- Currently 185 active PS in use in EU, 44 of which are in wide dispersive use
- <u>Concawe 2019 REACH roadmap for petroleum substances</u>



#### Concawe has invested to develop environmental assessments for REACH

- Technical improvements: Water Accommodated Fraction (WAF), passive dosing/sampling, persistence testing, analytical methods
- Data generation: persistence, bioaccumulation and toxicity data, analytical compositional data
- Technical developments:
  - Hydrocarbon block method: grouping of hydrocarbons by carbon number
  - QSAR: Quantitative Structure Activity Relationship models
    - Persistence: active contribution to HCBioWin, a biodegradation prediction hydrocarbon specific model
    - Bioaccumulation: active contribution to update an expansion of BCFBAF model
    - Aquatic toxicity: Target Lipid Model updated with expanded database to meet guidelines for use of Species Sensitivity Distribution (SSD) approach in risk assessment
- We work collaboratively with regulators, institutes and Universities
- >10 Million Euro on ENV over 20 years, contributing to > 50 publications



### **Current projects**

Concawe is managing projects on environmental fate, toxicity and risk assessment projects - list of indicative projects:

- Primary degradation rates of radiolabelled hydrocarbons in soil, sediment, water (Fraunhofer 2019)
- Mixture effects of hydrocarbons on biodegradation (DTU, 2019)
- Temperature effects on biodegradation of hydrocarbons (DTU, 2020)
- Aerobic soil degradation and characterisation of NERs of <sup>14</sup>C-Phenanthrene (Fraunhofer, 2020)
- Aquatic toxicity of naphthenic monoaromatics (EMBSI, 2019) and heterocycles (EMBSI, 2020)
- Update of hazard (Petrotox) and risk (Petrorisk) assessment tools (2019)
- Update of Concawe PBT report (2019)
- Underpinning the GCxGC HCB relationship (2019)



#### **Concawe at PetCo**

- Initial PetCo Mandate to agree the approach for prioritization of registered PS is complete
- Actions realized by Concawe:
  - Updated use maps to include only relevant uses (44 substances in WSU)
  - Updated Substance identity of registered substances
  - Agreement to regularly update dossiers
  - Development of the Human health testing strategy [early 2018]
- Current PetCo mandate is to agree on regulatory steps for assessment of PetCo substances regarding SVHC roadmap
- Concawe would welcome a continuation of the collaborative approach to assessment of UVCBs:
  - Environmental strategy proposed by NL based on Hydrocarbon Block (HCB) Method
  - To keep a consistent strategy that can be applied on all HCBs and substances



### **PBT assessment of petroleum substances**

- REACH Annex XIII:
  - provides P, B and T criteria for <u>substances</u>: cut-offs for persistence half-lives, BCF and NOEC/EC10
  - "a <u>weight-of- evidence</u> determination using <u>expert judgement</u> shall be applied"
  - "based on data obtained under <u>relevant conditions</u>"
  - "Shall also take into account <u>relevant constituents</u> and transformation and/or degradation products"
- Scientific view:
  - released to the natural environment, constituents within a PS behave differently with respect to partitioning, degradation and toxicity
  - However, structurally similar constituents have similar environmental fate and behaviours
- Concawe and academics have revealed the limitations of current methods and the need to improve our knowledge of PBT assessments
- Concawe is actively engaged in further improving the science for both P and B assessments of constituents of petroleum substances



#### **Concawe PBT report**

• Groups 'similar' constituents into hydrocarbon blocks (HCB) for PBT assessment

<> different purpose than the HCB method developed in 1996 for environmental risk assessment

- 16 000 representative constituents (Kutsarova et al. 2019)
  - generated by computational/statistical model
  - 1 to 371 constituents/block
- Evidence based conclusions for every HCB
  - P, B and T predictions used alongside experimental data
  - Predictions are generally conservative
- Report first submitted with registrations in 2010
- Feedback provided by regulators in 2015
- Revised in 2016
- New revision will be released during 2019





## Persistence

- Weight of evidence approach on reliable data for every HCB obtained under relevant conditions:
  - P, B and T predictions used alongside experimental data
  - Experimental data, when available, are given more weight than model predictions
  - extrapolation of persistence conclusion to higher carbon numbers
  - Predictions are generally conservative

Hydrocarbon	Hydrocarbon class	C #	ŀ	lalf-life (da	Deference	
nyulocalboli			Predicted	Marine	Freshwater	Reference
biphenyl	<b>Di-aromatics</b>	12	31	11.6	2.8	Prince and Walters, 2007
C2-naphthalenes	<b>Di-aromatics</b>	12	14.2	8.8	-	Brakstad et al., 2015

3- phenylbicyclohexyl	Napthenic mono-aromatics	18	119	23	-	EMBSI (2009a)
dodecahydrochrysene	Napthenic mono-aromatics	18	954	95	-	EMBSI (2009a)
dodecahydro-terphenyl	Napthenic mono-aromatics	18	470	23	-	EMBSI (2009a)

#### • Concawe requests a clear, agreed methodology for persistence testing for PS



CH2 CH2

# **Persistence - 3 ring PAHs**

• Biodegradation half-lives are inherently variable (inoculum, conditions, experimental challenges) - need to consider all of the evidence

versus

• Large amount of experimental data available for 3-ring PAHs



**Figure:** experimentally determined, reliable aquatic half-lives (y-axis, in days) of 3-ring PAHs dosed at environmental relevant concentrations, with increasing carbon number (x-axis)



• Concawe is open to discuss extrapolation, as long as robust WoE-based persistence conclusions are extrapolated:



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# **Bioaccumulation**

- Weight of evidence approach on reliable data obtained under relevant conditions
- Annex XIII: "Information on the ability of the substance to biomagnify in the food chain, where possible expressed by biomagnification factors or trophic magnification factors"
- Concawe PBT report:
  - Fish bioaccumulation data used
  - experimental BCFs> experimental BMFs>predicted BCF data
  - BCFBAF predictions: Arnot-Gobas model (including metabolism) and LogKow-based regression model
  - BMF < 0.1 is considered not bioaccumulative
  - BSAFs and TMF as part of WoE

Hudrocorboo	Hudrosarban slass	c #	BCF		BMF	Reference
пустосатооп	Hydrocarbon class		Predicted	Measured	Measured	
3- phenylbicyclohexyl	Napthenic mono-aromatics	18	72/7586	-	1.09	EMBSI (2005d)
dodecahydrochrysene	Napthenic mono-aromatics	18	82/17700	4588	0.17	EMBSI (2008c)
<i>m</i> -dicyclohexylbenzene	Napthenic mono-aromatics	18	289/6610	1406	0.07	EMBSI (2008c)



#### Concawe requests a clear, agreed methodology for bioaccumulation testing for PS



# **Bioaccumulation - 3 ring PAHs**

- Parent compounds (phenanthrene, anthracene):
  - reliable, observed lipid normalised fish BCFs are in the range of 237-2240 L/kg
  - data do not support vB (RIVM report 601779002/2009)
- Alkylated 3-ring PAHs: available experimental data (up to C18) show notB



Concawe is open for further dialogue and potential related research activities



# **Summary**

- Concawe has a long history to improve understanding of environmental and health risks associated with the use of petroleum substances
- Hazard (PBT) assessment of petroleum substances is challenging and new approaches must be considered and incorporated into the assessment process
- Concawe's role remains focused on developing science of both hazard and risk assessment consistent with advances in science to safely manage petroleum substances
- Concawe welcomes the opportunity for continued collaboration to develop agreed methodologies, leading to robust hazard and risk assessment of petroleum substances
- Concawe acknowledges the support of RIVM in advising Concawe projects





#### www.concawe.eu

# Thank you for your attention

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