



Why Science Matters?

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Robin Nelson

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Why Science Matters

Managing the uncertainties of Petroleum Substances (PS) in REACH

- How can we assure society we understand the hazards associated with our products and effectively manage the risk?
- How to understand the variability in composition and the impact of such variability in Environmental and Human Health risk assessments?
- This discussion focuses on the Chemistry of Petroleum Substances, Environmental Hazard and Risk Assessment, with Hans picking up the discussion in relation to human health assessment.

Fractionation and Processing of Crude Oil into Petroleum Substances



Distillation
Approximate cut points indicated

Conversion / upgrading processes
Subsequent distillation steps combined
Hydrodesulfurization / others omitted

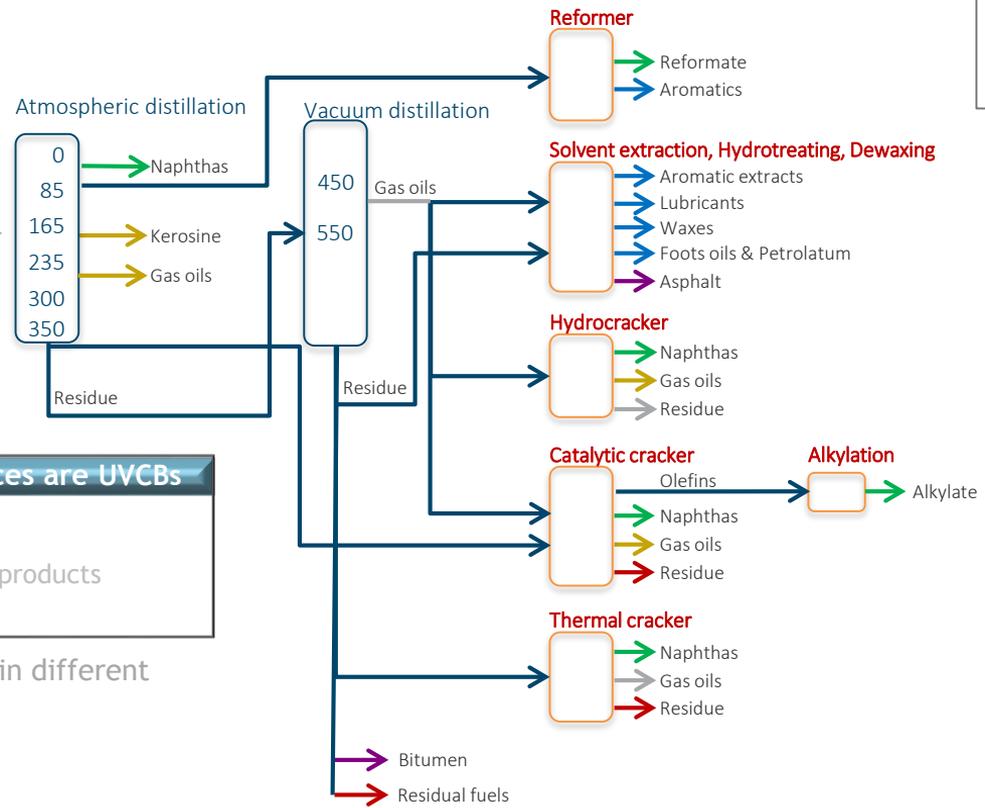
Petroleum Substances are UVCBs

- Unknown
- Variable
- Complex reaction products
- Biological origin

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Variability inherent in different crude feedstocks



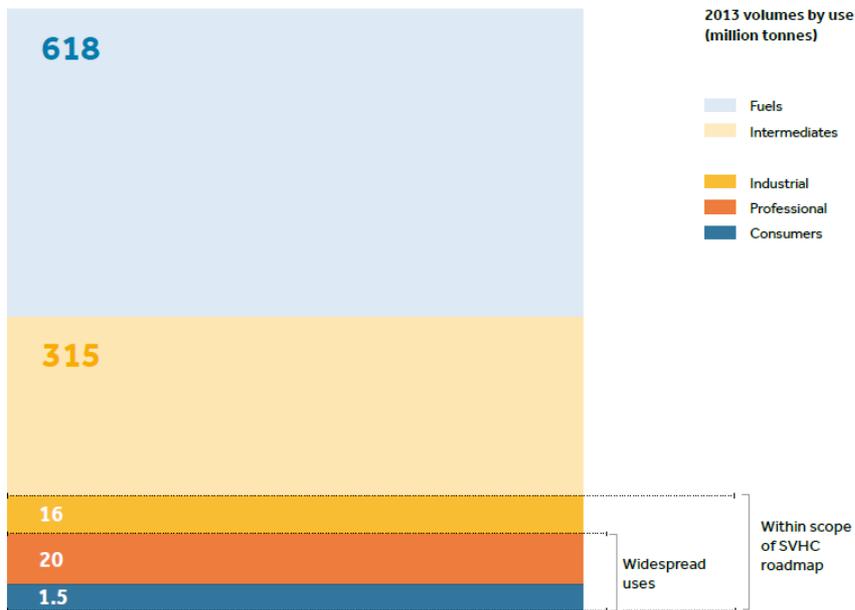
Main product types
(usually covering more than one EC number)

- Gasoline
- Distillate fuels
- Residual fuels
- Bitumen
- Others

Petroleum Substance uses in the EU

Fuel and non-Fuel uses of Petroleum Substances

- Petroleum substances have been in global commercial use for more than a century
- Fuels are intentionally combusted. CO2 is the main (but not the only) societal issue in using petroleum substances
- Petroleum Substances are also used in products not intended for combustion and which may end up in the environment e.g. solvents and lube base oils
- ECHA & Member States in the PetCo Working Group have prioritised substances with non-fuel, widespread uses



Some aspects of PS to keep in mind...

Petroleum Substances are UVCBs

- Unknown or
- Variable composition,
- Complex reaction products,
- Biological materials

- The chemical composition of petroleum UVCBs can never be fully characterized analytically

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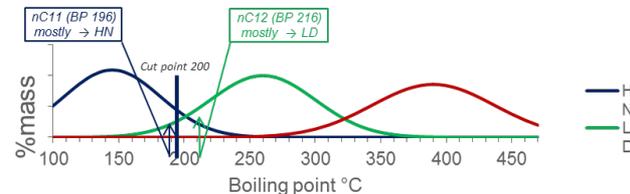
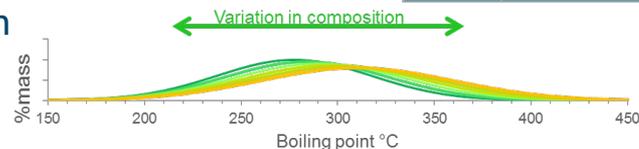
- Variability is limited by distillation and further treatment to meet product specifications

Petroleum Substances are UVCBs

- Unknown or
- Variable composition,
- Complex reaction products,
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- Neighbouring streams overlap: there is a “continuum of PS”

C number	Boiling point °C (n-alkanes) (*)	Number of isomers (alkanes only!)
3	-42	1
4	-1	2
5	36	3
6	69	5
7	98	9
8	126	18
10	174	75
15	269	4 347
20	343	366 231
25	402	36 777 419
30	450	4 108 221 447
35	490	493 054 243 760
40	525	62 353 826 654 563



Substance Information Exchange Forum

- REACH requires registrants from the same substance to share existing data or to generate new data, solely for the purpose of REACH compliance.
- Important to know that registrants are all working with the same substance.
 - What is the variability, both within a substance and across different substances from the same category?
- How does this variability inform the hazard characterisation?
 - Assess sample and substance variability within each petroleum substance category
 - *Are substances, with different EC numbers within the same category, chemically distinct?*
 - *Use this to inform the human health and environmental testing strategy*
 - *Reduce overall cost, time and animal use, whilst assuring compliance with REACH Regulation*

Lubricant base oil sample and substance variability

EC & CAS

265-091-3	64741-89-5
276-737-9	72623-86-0
265-156-6	64742-53-6
265-158-7	64742-55-8
265-159-2	64742-56-9
265-176-5	64742-71-8
265-077-7	64741-76-0
265-097-6	64741-96-4
265-155-0	64742-52-5
278-012-2	74869-22-0
265-157-1	64742-54-7
265-169-7	64742-65-0
265-090-8	64741-88-4
265-174-4	64742-70-7
276-738-4	72623-87-1
309-877-7	101316-72-7
276-736-3	72623-85-9
309-874-0	101316-69-2
265-096-0	64741-95-3
265-101-6	64742-01-4
265-160-8	64742-57-0
265-166-0	64742-62-7



Initial visual comparison of basic analytical data from registrants as submitted to ECHA using Lube Base Oils as an example

Multiple samples per EC number

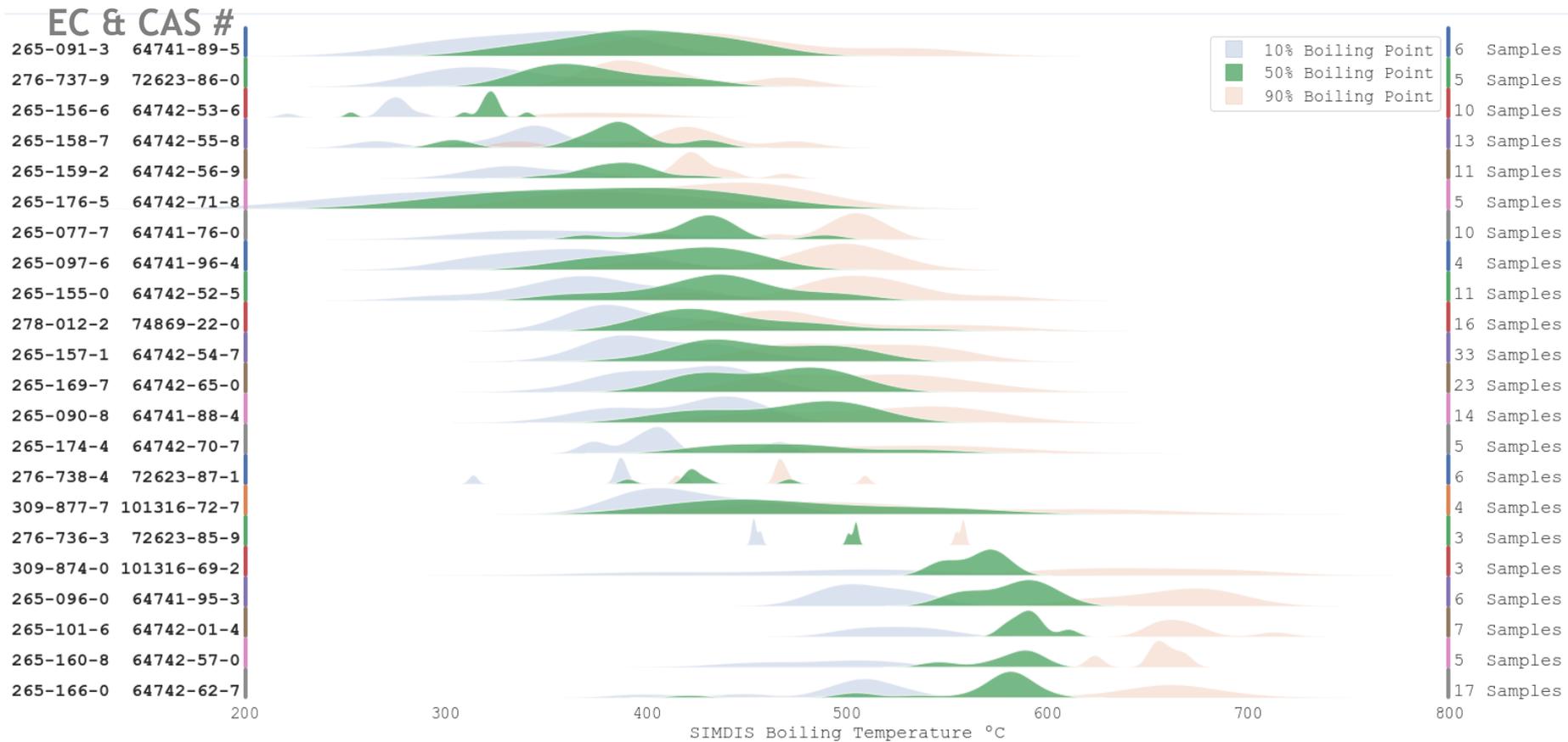


Single parameter (boiling point distribution) to start

6	Samples
5	Samples
10	Samples
13	Samples
11	Samples
5	Samples
10	Samples
4	Samples
11	Samples
16	Samples
33	Samples
23	Samples
14	Samples
5	Samples
6	Samples
4	Samples
3	Samples
3	Samples
6	Samples
7	Samples
5	Samples
17	Samples

Lubricant base oil sample and substance variability

Boiling point range distribution of sample components - kernel density



Sample and Substance variability

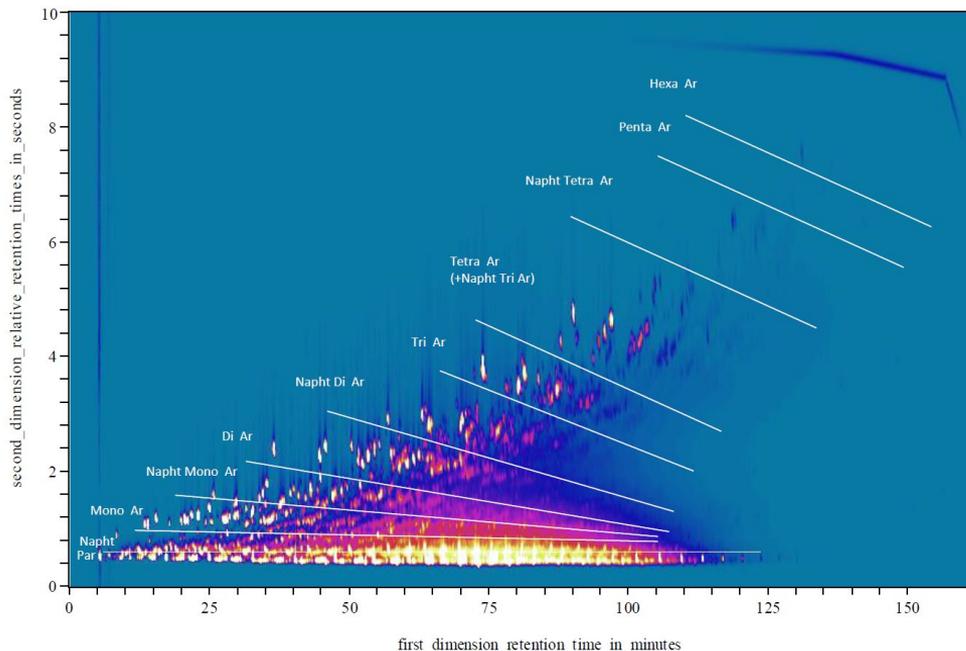
Work in progress

- Initial analysis indicates grouping is consistent with the substance descriptions for the LBO category
- Extend analysis to multiple parameters (basic analytical data from registrants and formal Concawe analytical programmes)
- Prioritise analysis of petroleum substance categories, in line with Petco priorities (substances with widely dispersive use)
- Complement visual comparison with statistical evidence for confidence levels to test hypothesis that sample data represent the same substance

Environmental assessments under REACH

The challenge

- Many PS contain millions of possible constituents with their own properties (see chromatogram)
- These properties dictate how these constituents behave in the environment,



- To what extent will they volatilise into the atmosphere, dissolve in water, deposit to land or sediments (compartments)?
- How fast will they degrade and be removed from these compartments?
- To what extent will they accumulate in organisms and magnify in the food chain?
- How toxic are they?

Environmental assessments under REACH

Some of the solutions industry has developed

Substance identity and chemical space

- GCxGC analysis
- Constituent library development
- Hydrocarbon block method

Hazard and PBT assessment

- Computational/predictive approaches (toxicity, bioaccumulation and persistence)
- New experimental methods (greater quality and quantity of data)
- Advances in science of toxicity, bioaccumulation and persistence assessment - more robust prioritisation and regulation of chemicals

Exposure assessment and risk characterisation

- Petrorisk

REACH regulation creates new challenges that only science can address

- Many Petroleum substances contain millions of constituents,
 - Only a limited number can be isolated and tested - there is a need for alternative approaches and pragmatic thinking!
 - Need to adapt testing and assessment approaches developed for single (mono-constituent) substances.
 - Even then it is not feasible to apply standard REACH approaches to test every constituent of a PS
 - Whilst we should develop the scientific understanding to reduce the uncertainty we cannot eliminate all uncertainty
 - *Uncertainty drives the precautionary principle*
- Scientific collaboration between industry and regulatory bodies is vital for progress

What it means to be PBT/vPvB

According to REACH PBT substances

- Cannot be assessed reliably by conventional hazard and risk assessment methods
- Accumulate in the environment and biota to an extent that may lead to toxic effects that are difficult to predict
- Once released into the environment, exposure is difficult to reverse
- Have the potential to contaminate remote and pristine environments
- A “safe” concentration in the environment cannot be established

PBT = Persistent, Bioaccumulative and Toxic
vPvB = very Persistent and very Bioaccumulative



Considerations of PBT/vPvB status

Standard approaches to PBT assessment are not well suited to hydrocarbon UVCBs, leading to different interpretations

- Some PAHs (constituents in Petroleum Substances) are considered to be PBT or vPvB and added have been to the SVHC list.
 - Concawe challenged this decision and is doing further work to support this challenge
 - We need to agree a clear, accepted methodology for persistence and bioaccumulation assessment
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- If a Petroleum Substance is designated as PBT/vPvB we will need to
 - update REACH dossier and SDS to indicate PBT/vPvB status
 - minimise environmental releases
 - PBT substances are given high priority for authorisation under REACH
 - Fuel uses are exempt from authorisation
 - substances with widespread dispersive uses (WDU) prioritised for assessment
 - Additional requirements for suppliers of articles

This is why Science Matters!



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**Thank you for
your attention**

Robin Nelson
robin.nelson@concawe.eu