Cleaning up the data: Concawe's first environmental update to the REACH dossiers since 2010

This article presents a brief overview of the work involved in Concawe's most significant update to the Other Gas Oil REACH registration dossier since 2010. This update will serve as a template for updating the dossiers for the remaining petroleum categories, ahead of the ECHA-mandated 2030 deadline for updating all Concawe REACH dossiers.

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Is it safe? A brief background on chemical regulations

Imagine that you are on a riverside holiday, hoping to catch a fish for dinner. You spot a nearby farm where something is being sprayed on the crops. You glance back at the river—its water looks clear, but some of the fish look ... off. You start to wonder: 'Is it safe to eat the fish? Are there harmful chemicals in the water?'

Figure 1: The value of chemical regulations—would you eat this fish?

Source: AI generated

These are exactly the kinds of questions that chemical risk assessments are designed to answer. A chemical risk assessment combines two key pieces of information: how hazardous a chemical is; and how much of it is actually present in the environment. Toxicology is the science that studies the harmful effects of chemicals. Ecotoxicology, more specifically, focuses on those effects in the environment.

So, in our riverside scenario, you would first identify what chemicals are being used on the farm (chemical identification), find out how much of those chemicals it takes to harm fish (ecotoxicology), and measure or estimate how much of it is in the river (exposure assessment), and then decide whether it is enough to cause concern—or whether it is time to find a seafood restaurant instead.

Many countries have rules that require companies to prove that a chemical is safe before they can promote it or put it on the market. In the European Union, that rulebook is called REACH, which stands for Registration, Evaluation, Authorisation and Restriction of Chemicals.[1] It is overseen by the European Chemicals Agency (ECHA). REACH came into force in 2007.[2] By 2010, companies had to submit information about all chemicals produced in, and imported into, the EU in large volumes—more than 1,000 tonnes per year—and all produced and imported chemicals known to cause cancer (carcinogenic), genetic damage (mutagenic) or reproductive issues (reprotoxic). These submissions are called registration dossiers, and they contain detailed information about each chemical.

For petroleum-based substances, the task of compiling this information was led by Concawe, a scientific organisation representing European oil refiners. Since these companies were all registering similar types of substances, Concawe helped coordinate the effort by forming a Substance Information Exchange Forum (SIEF). This made it possible to share confidential data and build consistent dossiers.

1 'Understanding REACH' (European Chemicals agency website)

2 'REACH' (European Commission website)

A dossier includes several types of information about the substance, depending on how much of it is produced or imported. This includes:

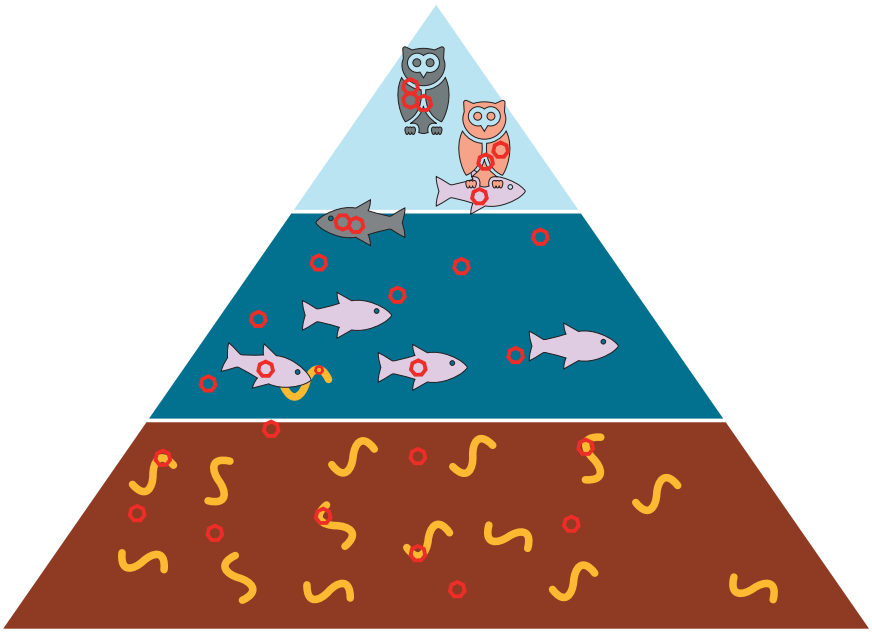
- physical and chemical properties (e.g. is it a solid, liquid or gas; does it dissolve easily in water?)
- human health data (e.g. is it toxic to people?)
- environmental data (e.g. does it break down in nature, or stick around and build up concentrations?)
- descriptions of how it is used and released, to calculate an exposure assessment.

Environmental information is especially important for identifying substances that are persistent, bioaccumulative and toxic (PBT) or very persistent and very bioaccumulative (vPvB) (Figure 2). These are chemicals that:

- remain in the environment long after they have been released
- build up concentrations in animals and plants over time
- cause harm at low concentrations.

These types of chemicals are the most worrying, because they are more likely to stay in environmental systems after emissions have stopped, and can build up concentrations in organisms upwards through the food chain, with relatively low concentrations leading to toxic or other unpredictable effects. A more thorough explanation of these hazards is given in the article on pages 21–31 of this *Review*.

Figure 2: A PBT/vPvB chemical (red shape), even at low concentrations, can stay in the environment, increase in concentrations in organisms, and be toxic. Would you eat this fish?



Population of the environmental sections of Concawe-supported REACH dossiers since 2007

Between 2007 (entry into force of REACH) and 2010 (the first pre-registration deadline for the highest-volume chemicals), Concawe was responsible for helping to register a large number of petroleum substances. To make the job more manageable, these substances were grouped into categories based on how they were made and what they were used for. For each substance, companies had to provide information on various ecotoxicological data—called Standard Information Requirements (SIRs)—to show that the substances could be used safely. To fulfil a SIR for a REACH dossier, a registrant would either need to provide test data, provide an estimation of the data, typically using a computer model, or have a waiver for that data point because it was not environmentally relevant for the substance or because it was not possible to perform such a test on the chemical. But there was a catch: the SIRs were developed with single, water-soluble chemicals in mind. Petroleum products do not fit well in this paradigm.

Petroleum substances are what's known as UVCBs—chemicals of Unknown or Variable composition, Complex reaction products, or Biological materials. This means that each petroleum substance can contain hundreds to more than millions of different hydrocarbon molecules, with a wide range of carbon chain lengths and types of hydrocarbon molecules. Some of those molecules do not mix well with water (hydrophobic), some evaporate easily (volatile), and others stick to soil or sediment (sorptive).

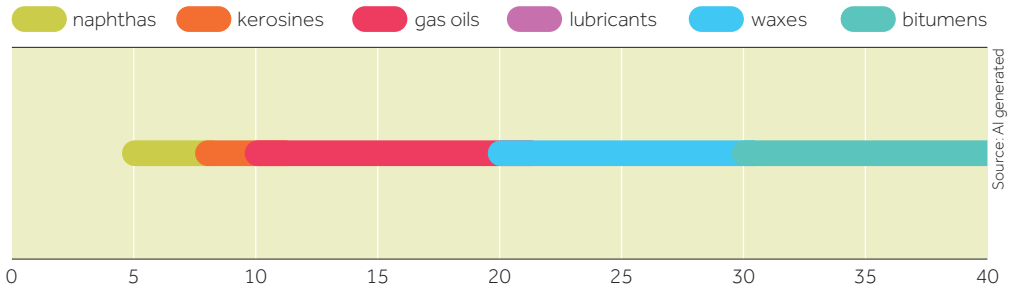
When millions of these molecules are present in one UVCB substance, it becomes very challenging to assess them all together. For evaluating aquatic toxicity, it is not possible to suspend all of the UVCB substances in water (think of oil floating on top of water). It is therefore necessary to utilise an alternative dosing approach, in this case by dosing the water-accommodated fraction (WAF)[1] of the substance, which contains only the water-soluble fraction of the UVCB. Adaptations to the standard test protocols have to be made for the other environmental data as well. When test data were not available, two different approaches—read-across and predictive models—were used to fulfil specific information requirements. These are described in more detail below.

Read-across

Since petroleum substances are, put simply, different fractions of crude oil, the composition of the different substances supported by Concawe overlap and can be treated as a continuum (see Figure 3 on page 7). If one can demonstrate that two substances are similar enough in composition, it is possible to 'read across' ecotoxicological properties from one substance to the other. Concawe made extensive use of read-across in its REACH dossiers, as test data were not available for every substance. This allowed for a more efficient approach to fill in the environmental data needed for regulatory compliance.

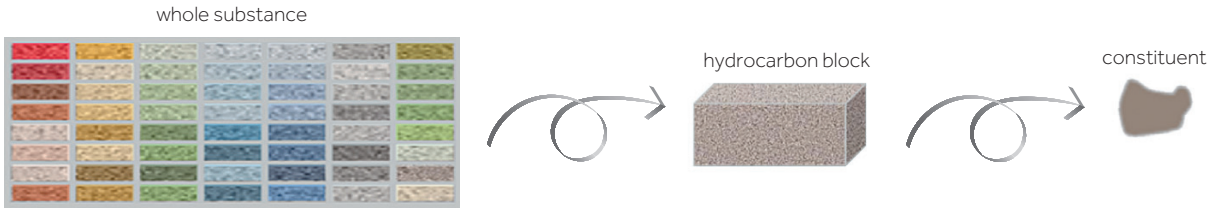
Sometimes, even read-across is not enough—especially when no acceptable test data are available for similar substances. That is where predictive computer models come in. To enable and simplify the assessment of complex petroleum substances, scientists developed the hydrocarbon block approach (see Figure 4 on page 7).[2]

Figure 3: Carbon number ranges and overlap between petroleum substances (up to C40)



Petroleum substances overlap in a continuum of carbon range.

Figure 4: A 'hydrocarbon block' is a hypothetical UVCB fraction that encompasses the constituents that belong to the same chemical class (e.g. isoparaffins) and have an identical carbon number or similar boiling point.



This method simplifies the composition of petroleum substances by grouping potential constituents that are assumed to have similar environmental properties into 'hydrocarbon blocks' (HCBs) based on their molecular size (carbon number or boiling point) and chemical structure, and then selecting one or a few constituents to represent the HCB for further analysis.

The hydrocarbon block approach has been used in the PetroTox model to estimate the aquatic toxicity of petroleum substances.[3] The relative amounts of each HCB in water are based on the compositional data for the petroleum substance and the solubility of each block. PetroTox then uses a concept called the Target Lipid Model (TLM), which assumes that chemicals cause harm when they build up in an organism's fatty tissues beyond a certain concentration limit. The model uses the chemical's octanol-water partition coefficient (Log Kow) to predict how easily it partitions to fat, and compares that to toxicity thresholds. The PetroTox model has been extensively validated using acute and chronic toxicity data for fish, invertebrates and algae for a wide range of petroleum substances. This approach is powerful because it allows scientists to estimate toxicity without having to perform physical tests on every variant of a substance.

PBT assessment

A PBT/vPvB assessment of the registered substance is needed under REACH, and this has been historically one of the more challenging requirements for Concawe substances. PBT/vPvB assessments are performed on a constituent basis, meaning that, in the case of a petroleum substance, a UVCB can be assessed as PBT/vPvB if one of its constituents is persistent (P), bioaccumulative (B) and toxic (T), or very persistent (vP) and very bioaccumulative (vB), assuming that the consitutent is present above a threshold concentration.

Because PBT/vPvB assessments are so complex and important, they are reviewed by a special panel called the PBT Expert Group. This group includes experts from ECHA, EU member state competent authorities, and accredited stakeholders like Concawe. They work together to evaluate difficult cases and provide scientific guidance. Since the Concawe substances are UVCBs, it would be necessary to evaluate millions of constituents that could be in petroleum substances. For a more rational approach, Concawe reverted to the hydrocarbon block approach again: a few representative hydrocarbons were selected from each HCB to perform the PBT assessment. While limited experimental data were available, much of the required biodegradation (persistence) data was generated using predictive models, namely BioHCWin, which was partly developed by Concawe.[4] Bioaccumulation was assessed using limited data and mostly predictive modelling. Toxicity was only addressed for constituents that were P and T, mainly using another predictive model. Concawe's PBT report was evaluated by the PBT Expert Group, with many suggestions being made for improvement.

PetCo

In 2015, the Petroleum and Coal stream Substances (PetCo) Working Group was established at ECHA, with the goal of prioritising PetCo substances for meeting the requirements of the SVHC (Substance of Very High Concern) Roadmap to 2020 (the roadmap prioritises SVHCs). Within PetCo, member state competent authorities, the European Commission, ECHA and industry stakeholders worked together to develop approaches to evaluate the hazards and uses of PetCo substances, as it was recognised early on that these complex substances would be challenging to assess and regulate. In 2022, ECHA announced at PetCo that all PetCo substance dossiers had to be updated by 2030, triggering a more concentrated programme in Concawe.

Present day: updating the environmental sections of Concawe dossiers

While Concawe had already been revising the human health data in its REACH dossiers, real momentum on the environmental sections began in 2021. Discussions with ECHA—particularly through the PetCo group—revealed that more updates were needed to meet current regulatory expectations. Although some minor tweaks had been made over the years, it became clear that a more comprehensive update was necessary. ECHA emphasised the importance of:

- avoiding the use of read-across from unrelated categories
- adding more actual test data where possible
- providing detailed justification documents to support all decisions made in the dossier.

To start this process, Concawe and ECHA agreed to focus initially on a relatively small and manageable category—OGO). The idea was that this update could serve as a template for how to handle the rest of the categories in future updates.

Reviewing and improving the existing data in the dossier

Concawe, with the support of a contractor (wca environment), met with ECHA to review the contents of the OGO dossier and discuss improvements. Some sections required major changes—especially where older information relied on read-across, modelling alone or testing waivers (see summary in Table 1). In cases where no experimental data existed, new testing proposals were submitted by Concawe, and several previously waived data requirements were now fulfilled using model predictions. A few highlights of the updated data requirements include:

- Aquatic toxicity: testing was proposed or conducted where there had previously only been modelling or read-across.
- Soil and sediment toxicity: new testing proposals were submitted where no data existed before.
- Biodegradability: an overhaul of the persistence assessments was undertaken.

All of these updates were aimed at creating a more robust and transparent scientific basis for the dossier—and reducing the risk of failing future ECHA compliance checks.

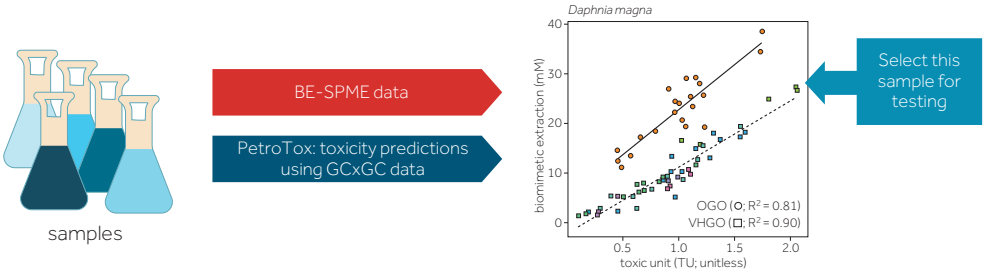
Table 1: Selected environmental data requirements that were significantly changed in the OGO dossier update

Data required	Previous data	Issue	New data
5.2.1 Ready biodegradability	Read-across from another category	Ready biodegradation test not applicable for UVCB	Modelled prediction on constituents
5.2.2 Biodegradation in water: simulation	Modelled prediction		Biodegradation testing proposal on constituent
6.1.1 Short-term toxicity testing fish	Read-across from another category and modelled prediction	No experimental data	Add test data and modelled prediction
6.1.2 Long-term toxicity testing fish	Modelled prediction	No experimental data	Testing proposal
6.1.4 Long-term toxicity testing on aquatic invertebrates	Read-across from another category and modelled prediction	No experimental data	Testing proposal
6.1.5 Toxicity to aquatic algae and cyanobacteria	Read-across from another category	Additional studies available but no detailed analytical data	Conduct testing
6.1.7 Toxicity to microorganisms	Modelled prediction	No experimental data	Conduct testing
6.2 Sediment toxicity	Waiver—testing not needed	No experimental data	Testing proposal
6.3.1 Toxicity to soil macro-organisms except arthropods	Waiver—testing not needed	No experimental data	Testing proposal
6.3.2 Toxicity to terrestrial arthropods	Waiver—testing not needed	No experimental data	Modelled prediction
6.3.3 Toxicity to terrestrial plants	Waiver—testing not needed	No experimental data	Modelled prediction

Choosing the right test sample: finding the worst-case scenario

Once it was decided that testing was needed for an environmental data point, Concawe had to select the appropriate sample to be tested. OGO, like many of the Concawe substance categories, has a large variation in sample compositions and therefore also in expected toxicities. Based on discussions with ECHA, it was decided to select the most conservative (toxic) but still compositionally representative sample for the whole OGO category, which would then only require one test per data point for the category. To identify the most conservative representative sample, available OGO two-dimensional gas chromatography (GCxGC) analytical data were evaluated using two methods: PetroTox predictions and laboratory biomimetic extraction-solid phase microextraction (BE-SPME) (Figure 5). BE-SPME uses silicone fibres that simulate an organism's fat (lipid) content to assess whether the hydrocarbon constituents in the petroleum UVCB will partition to the organism.[5] The more a hydrocarbon partitions into lipid, the more toxic it is expected to be. The composition of the potentially most toxic sample was compared to the compositions of all the other OGO samples to ensure that it was still representative of the category.

Figure 5: Test sample selection using two methods to identify the most potentially toxic sample



New biodegradation conclusions and evaluation approaches

One major shift in the dossier review process resulted from a clarification by ECHA: ready biodegradability (screening) tests are not appropriate for complex UVCBs like OGOs. These screening tests are designed to rapidly identify substances that break down very quickly in the environment (not persistent). But UVCBs contain many constituents of which some may degrade easily, while others may persist. Unless every single constituent can be shown to degrade quickly, the whole substance cannot be considered readily biodegradable. As a result, OGOs are no longer considered readily biodegradable, which affects how the toxicity of the OGOs is being concluded according to the classification, labelling and packaging (CLP) regulation: because there are OGO samples with a modelled chronic aquatic toxicity concentration value below the 0.1 mg/litre threshold, the OGO CLP classification changes from Chronic Aquatic Category 2 (H411) to Chronic Aquatic Category 1 (H410), or from 'toxic' to 'very toxic to aquatic life with long-lasting effects'.

As ready biodegradability data could no longer be used, Concawe had to propose more elaborate simulation biodegradation testing on one or more individual constituents suspected of being persistent. The discussions with ECHA in PetCo and also with the PBT Expert Group took more than a year, during which time Concawe performed an interim update of the PBT report to support the justification and selection of constituents that could be tested. The constituents were selected based on available experimental biodegradation data and data predicted with HC-BioSIM,[6] a new tool developed with the support of Concawe.

The OGO dossier update in numbers

In January 2025, the updated OGO dossier was released to all registrants. This marked the first major update to the environmental sections of Concawe's REACH dossiers—and it sets the stage for how future environmental dossier updates will be handled. Here's what went into it:

- ~ €600,000 in planned testing costs.
- More than 500 pages of supporting documentation, including scientific justifications for every model, read-across decision, and laboratory test.
- Two new aquatic toxicity studies completed and included in the dossier.

Fortunately, many of these materials—especially the justification documents—can be reused or adapted for the dossier updates of other substance categories, helping to reduce future workload and cost.

What's next? A roadmap for the coming years

Over the next five years, Concawe is planning to update all of the remaining dossiers' environmental information requirements, some with testing proposals where necessary. The time frame to accomplish all of the proposed testing will go beyond the 2030 deadline. Some categories, such as lubricant base oils (LBO) and bitumen, are even more complex. These substances are extremely water-insoluble, which makes traditional toxicity testing even more difficult (if not impossible). Concawe will continue to work closely with ECHA to find practical, scientifically valid ways to assess these substances.

In addition, there are new hazard standard information requirements which are being incorporated into REACH and CLP, such as endocrine disruption (ED) and constituents that are persistent, mobile and toxic (PMT), and very persistent and very mobile (vPvM). For more detail on the new hazard classes please see the article on pages 21–31 in this issue of the Concawe *Review*.

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