Executive summary of the report

"Does D5 meet PBT or vPvB Criteria? Regulation in the context of developments in science"

The purpose of this executive summary is to provide a short and easily read compilation of the findings of the report **"Does D5 meet PBT or vPvB Criteria? Regulation in the context of developments in science**". The aim of the report is to present a summary of the available evidence on the persistence (P), bioaccumulation (B) and toxicity (T) properties of the siloxane decamethylcyclopentasiloxane (CAS 541-02-6) "D5". The study was carried out following the indications of D5 and D4 as vPvB and PBT respectively, as expressed by the ECHA PBT expert group and in the ECHA Member States Committee opinion dated April 2015. .

A weight-of-evidence assessment of the available evidence of "P", "B" and "T" properties is indicated as a relevant and useful approach by the REACH regulation and guidance, and other expert sources.
This report provides a collection of the available evidence in terms of lines of inquiry and considers this evidence in the overall conclusion on each of the properties

Process

The driving force behind the work presented in this report is the view that the weight of evidence should allow a substance to be appraised as PBT in the light of all available lines of evidence. The criteria for "P", "T" and in particular the criterion for "B", as set out in REACH and associated guidance material, serve to identify substances that *could* require a precautionary approach. This approach is necessary where there is a limited evidence-base and swift regulatory action is required. However, where there is a substantial body of evidence, as in the case of D5, it is not enough to rely on indicative criteria only, real life behaviour should also be considered. The intention of the Regulation to restrict the use of hazardous substances should prevail. This should be done using robust scientific methods. The existing evidence comprises considerable amounts of data on D5, including that which has been used for the REACH registration dossier, summarised below.

Emerging consensus amongst environmental scientists worldwide is that current criteria alone do not allow for an accurate assessment of PBT characteristics of a substance. An international expert workshop in 2008 (Klecka et al., 2009) concluded that the existing regulatory framework for evaluating PBTs is not consistent with the latest scientific advancements. "P", "B" and "T" are considered to be different but inter-related properties and a conclusion regarding D5 therefore consider all three properties together. Of the three criteria, the properties of D5 in respect to the "B" criterion are subject to the most uncertainty because the "B" criterion is based on relative rather than absolute measures. It is therefore paramount that the evaluation of the "B" criterion in relation to D5 includes all available lines of evidence.

In the context of this review, it is necessary to first define the terms associated with "B":

- Bioconcentration is used to describe the concentration of a chemical in an organism derived from water uptake alone. The bioconcentration factor (BCF) is a point measure that is determined as the ratio of the chemical concentration in test organisms to the chemical concentration in water, at steady-state.
- Bioaccumulation describes the accumulation of contaminants in the tissue of organisms through water and food uptake. The bioaccumulation factor (BAF) is a point measure that is determined as the ratio of the chemical concentration in test organisms to that in water, at steady-state.
- The biomagnification factor (BMF) is the lipid-normalized ratio of the chemical concentration in the predator to the chemical concentration of the prey species. The BMF is a slope that describes the increase or decrease in concentrations of the chemical across a simple predator–prey relationship (i.e., predator and prey that are separated by a single trophic level step).
- The biota-sediment accumulation factor (BSAF) is a point measure that is determined as the ratio of the lipid-normalized biota concentration to the organic carbon-normalized sediment concentration.
- The trophic magnification factor (TMF) is similar to the BMF in in that it is a slope that expresses the average BMF across a food web. The TMF describes the increase or decrease in concentrations of the chemical in multiple organisms that occupy successively higher trophic levels or positions within a food web.

The available data with regard to the assessment of "B" for D5 comprise laboratory studies of the bioconcentration factor (BCF) and the biomagnification factor (BMF), laboratory and field studies for the biota-sediment accumulation factor (BSAF), and field studies of the trophic magnification factor (TMF).

The BCF, BAF and BSAF metrics are expressed in terms of ratios and their magnitudes therefore depend on the exposure concentrations in the tested organisms. This increases the level of variability, especially for highly lipophilic and adsorbing substances such as D5, because the outcome is dependent on the quantity of the substance in the test system. It has been shown that dual exposure (from water and diet) may have occurred in the BCF and BMF studies which may confuse the understanding of the actual exposure route (Qiao et al., 2000; Thomann, 1989).

Laboratory BCF ratios can only to a limited extent be applied to predict the ability of a highly lipophilic and adsorbing substance such as D5 (log K_{OW} >8) to biomagnify in the environment. Dietary biomagnification appears to be the main route of uptake for bioaccumulation of highly lipophilic substances, as research indicates that at naturally-occurring food/water concentration ratios, uptake of highly lipophilic chemicals (i.e., log K_{OW} >6) from water into biota is low compared to uptake via consumption of contaminated foodstuffs, with the importance of dietary uptake increasing with increasing lipophilicity (Thomann, 1989; Qiao et al., 2000). Uptake via water may be an important exposure route in aquatic ecosystems for lower trophic level species, but uptake from food becomes increasingly more significant as trophic position increases. Other data demonstrates that fish are able to significantly eliminate and metabolize the D5 from their tissues, which supports the field data demonstrating limited evidence of food web biomagnification of D5 (Domoradzki et al., 2015, a, b, c).

It is difficult to clearly interpret a BCF ratio in order to understand biomagnification in the environment of highly lipophilic substances. Because of this the depuration (elimination) and metabolism rates from laboratory studies (in particular, metabolism interpreted from dietary exposures) can be assessed to better predict the behaviour of D5 in the environment. Depuration rates show that elimination of D5 from fish (representative of predators in the aquatic food chain) is moderately fast (Huggett, 2015, a, b). Depuration rates from sediment organisms may be faster still (Krueger et al., 2010; Selck, 2014). Indeed, based on the collective reliable depuration rates available for D5, the use of elimination half-life as a metric for the bioaccumulation potential of chemicals, as proposed by Goss *et al.* (2013), indicates that D5 is not likely to bioaccumulate. There is also clear evidence of metabolism of D5 in aquatic organisms; a constant metabolism rate (k_M) in mature fish of >0.01 d^{-1} (equivalent to a half-life of <70 days). These findings further support the lack of biomagnification potential of D5 in the aquatic environment.

Abundant field data on D5 is demonstrating biodilution (TMF <1) of D5 in benthic-pelagic systems, both marine and freshwater (Powell et al., 2010; Powell et al, 2009; McGoldrick et al., 2014). In heterogeneous, pelagic systems however, measured TMF >1 may suggest food web biomagnification.

The interpretation of field TMF data available for D5 is complicated by concentration gradients and other factors such as the sediment-water fugacity ratio (Fsw), and metabolism within the ecosystem studied.
In complex ecosystems, TMF calculations must mathematically integrate the impact of concentration gradients and other factors such as the sediment-water fugacity ratio (Fsw), species migration, and metabolism.

A strict comparison of data with the "B" criterion as set out in Section 1 of REACH Annex XIII (using BCF data), allows for the conclusion, on the basis of BCF data alone, that D4 is vB.). However, based on a review of all the lines of evidence above, BCF alone is not a reliable indicator of whether the substance in reality poses a risk to the environment that could not otherwise be controlled by conventional risk assessment. If all influencing factors are considered in the assessment (such as concentration gradients, migration, and sediment/water fugacity ratios), there is a clear indication that D5 will not biomagnify but will instead biodilute in the environment, and therefore D5 should not be considered a potential B or vB substance.

We have considered all lines of evidence in the current regulatory context and the potential concerns for bioaccumulation. Concerns are higher for lower trophic level species, but uptake from food becomes increasingly more significant as trophic position increases.

- Some compounds possess a high bioconcentration factor without trophic transfer. Although water is an exposure route for lower trophic level organisms, a concern for bioaccumulation would require presence in water, high persistence in water, low potential for elimination from biota at the lower trophic levels and the potential for toxicity to these organisms. This is not the case for D5, because the substance is volatile, poorly soluble and not very persistent in the majority of natural waters. Its presence in surface water is low to non-existent (Knoerr, 2014), the rate of elimination from biota is moderately high and there is no demonstrated toxicity in aquatic species.
- The substance is very persistent in sediment, but sediment does not give an elevated potential for uptake of the strongly-adsorbed D5 into biota. In addition to this, benthic organisms are capable of metabolism (Selck, 2014), and there is no demonstrated toxicity to these organisms (Woodburn and Powell, 2014).

With regard to the "T" criterion, there are no known toxic mechanisms that would be manifested at low concentrations over long periods that could cause potential harm not already captured by what is known about the toxicity profile. A probabilistic risk assessment with benthic organisms indicates that current field concentrations of D5, even at highly improbable distribution levels (i.e., 95th centile), indicates no overlap of D5 sediment exposures with benthic species chronic NOEC levels (Woodburn and Powell, 2014).

The overall conclusions on the individual parameters based on the above lines of evidence are:

Persistence

- The persistence criteria (vP) in water and sediment according to Annex XIII are met, although the overall persistence (balanced across all compartments) is low.

Bioaccumulation

- The substance does not biomagnify in aquatic food chains.
- The substance does not biomagnify in terrestrial food chains.

Toxicity

- The substance does not fulfil the T criterion.

The overall conclusion is that D5 should not be considered vPvB when taking into account all lines of evidence from the robust data available.

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