Ensuring compliance with REACH regulations

Example investigation of the degradation products of various organic peroxides under environmental conditions with combined ecotoxicity & physical chemical testing

Executive Summary

In the era of sustainable development, a big challenge for every chemical producer active in Europe is to comply with the REACH regulations. Achieving full compliance is a time consuming and costly procedure, especially for highly reactive chemistry with multiple degradation routes. Application of existing standard testing approaches for such materials is not always possible.

This paper highlights a multi-analytical approach combined with environmental testing that was used to address competent authority concerns for difficult to test organic peroxides.

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Key facts

>100	Analytical Techniques
>1000	Customer Requests per year
>10000	Samples Analyzed per year

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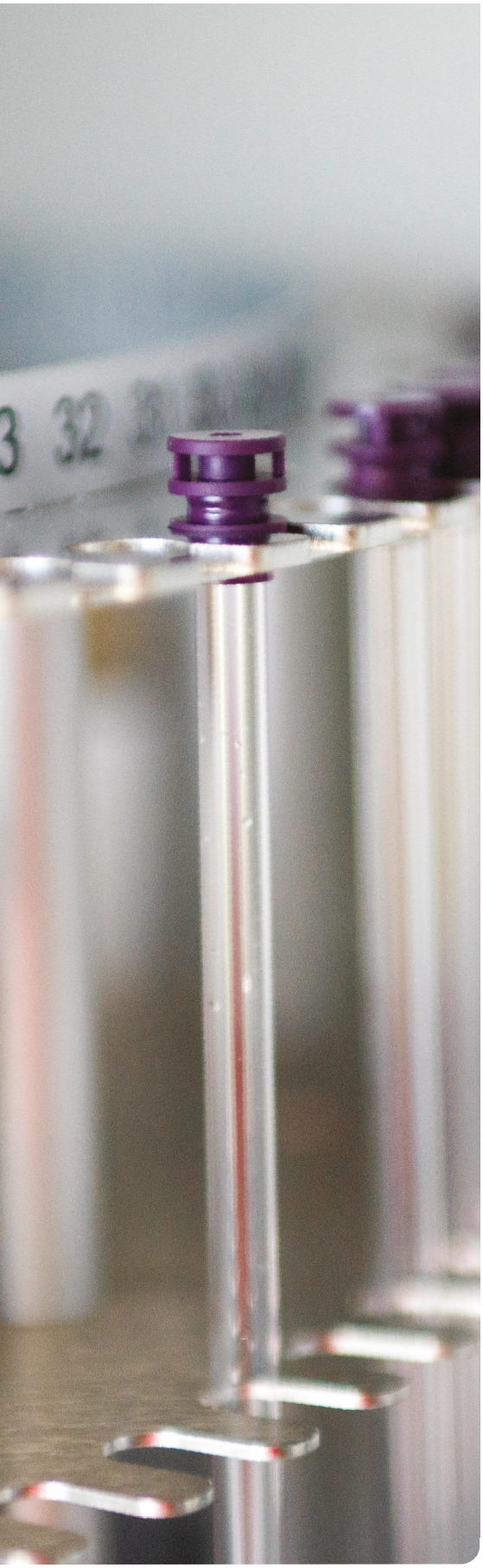

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Some chemical compounds such as organic peroxides are subject to hydrolytic, thermal and reactive decomposition mechanisms, as well as being degraded by biological routes. This makes it particularly difficult to provide the quantitative analytical data required to generate a valid eco-toxicity endpoint and subsequently provide an accurate risk assessment to the European authorities. Scientists at the ECCD in Deventer were able to implement a cross disciplinary approach combining Ecotoxicity and Biodegradation testing with state-of-the-art analytics to address the concerns of the authorities.

A case study substance was highlighted as a potential PBT/vPvB (Persistent, Bioaccumulative and Toxic / very Persistent and very Bioaccumulative) material with many chronic tests and higher tier studies being recommended by the reviewing authorities. The experts at ECCD Deventer were able to demonstrate exactly how the material degrades under various conditions using a number of analytical techniques. Subsequent biodegradation and ecotoxicity testing was used to demonstrate the true hazard of the material concerned. The material is no longer considered to be a potential PBT/vPvB.

How to develop a method to comply with REACH regulations?

Exploiting an in-depth knowledge of the products, together with expertise in regulatory Ecotoxicity and Biodegradation meant a successful evidence-based counter proposal was used to address previous shortcomings in existing data.

Hydrolytic decomposition investigation:

To identify the decomposition profile, the material concerned was decomposed under a variety of conditions and temperatures. It was observed that at higher temperatures, decomposition yielded different products to those generated at the average environmental temperature of 12 degrees used for risk assessment. Furthermore, abiotic decomposition continued in the presence of naturally occurring humic acids and suspended matter. Finally, the half-life of the parent material under these conditions was shown to be <12 hours. Assessment of the properties of the degradation products assumed greater relevance than initially thought.

NMR, LC/MS and SPE-uHPLC were among the techniques used to evaluate the parent molecule half-lives and to identify the chemical compounds that were produced from the decomposition of the test materials. The true picture of the environmental scenario could be demonstrated and subsequently confirmed in standard ecotoxicity tests employing a multi-analytical approach and adapted biodegradation tests.

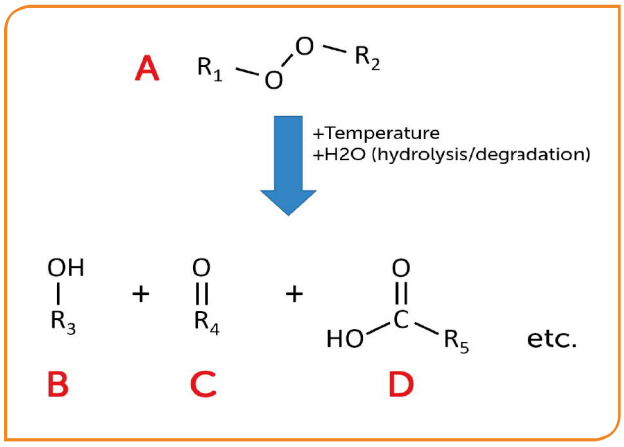

Figure 1: Test substance and the hydrolysis/degradation products.

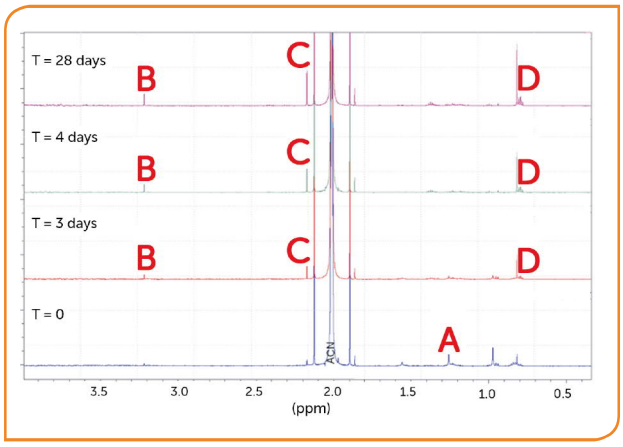

Figure 2: 1H-NMR hydrolysis at buffer pH=7 at different time intervals.

Closed bottle investigation (OECD301D)

A literature search of the degradation products identified at 12^{0}C showed that they were expected to be non-persistent, not bio-accumulating and of relatively low toxicity. This was confirmed for a mixture of the individual degradation products as well as for the test material itself after being subjected to a short (72 h) period of degradation at 12^{0}C . In both cases a ready biodegradable conclusion was reached.

Toxicity investigation (OECD 201)

Confirmation of the half-life of the substance as <12h indicated that both parent and degradation products needed to be considered during follow-up ecotoxicity testing. Using a standard OECD 201 test and a combined multi analytical approach the concerns raised by the regulatory authorities from the existing study could be further investigated and addressed. Illustrating a lack of toxicity of the parent material at its water solubility limit and demonstrating the products that are formed during the study and the effects of the mixture of parent material and degradation products had on the toxicity to the test organism. This additional data was provided to the authorities facilitating their positive conclusions on the material being registered.

Conclusion

Utilising in-depth knowledge of the chemical entities as well as experience in the standardized test methods used in the registration process helped the ECCD to deploy the best advanced analytical techniques to achieve an advantageous result for the client and deliver significant savings on the costs of higher tier testing.

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