

Experimental and conceptual approaches for testing the transformation of volatile chemicals on the basis of standard test guidelines

BORIS MEISTERJAHN¹; MICHAEL HÜBEN¹, HELENA TOMM¹, DIETER HENNECKE¹,

¹Fraunhofer IME, Division Applied Ecology, Auf dem Aberg 1, 57392 Schmallenberg, Germany, boris.meisterjahn@ime.fraunhofer.de

For the investigation of biodegradation and transformation processes of chemicals in matrices such as soils or aqueous environments (surface water, water/sediment) normally the OECD test guidelines 307 (soil), 308 (water/sediment) and 309 (surface water) are applied. These test systems were originally developed for pesticide regulation and were adopted 15 years ago.

Meanwhile regulation progressed and chemicals other than pesticides are regulated in different regulatory frameworks like e.g. REACH or the regulation for veterinary pharmaceuticals. The practical implementation of the regulations requires appropriate tools: the testing guidelines. In most cases the new regulations make use of existing guidelines where long-year experience is available. They often do not take into account that the substances regulated under the new frameworks might have significant different properties to those for which these guidelines were originally developed.

Currently in REACH authorities ask for studies according to the guidelines with substances which are clearly out of their application area. In the chapter “applicability of the test” each of the guidelines exclude the application of the test to “highly volatile compounds”. Only OECD 309 gives as a definition for “slightly volatile compounds” a Henry’s law constant $<100 \text{ Pa m}^3/\text{mol}$. However, that is not considered in REACH and thus laboratories currently face requests to test highly volatile substances according to OECD 307, 308 and 309 test guidelines.

This creates a challenge to the study setups. The use of the flow through or biometer type flasks standard set-up suggested in the guidelines often results in incomplete mass balances, which can be erroneously interpreted as degradation if no radiolabelled test compound is used. Furthermore, wrong degradation kinetics might result from the fact that major amounts of the tests substance stay in the gaseous head space, away from the matrix where it is supposed to be degraded.

A promising approach is the use of biometer-type flasks with adsorbent traps directly placed in the test vessel and a minimized head space volume. By directly placing the traps in the test vessel the risk of losses due to sorption to tubes and other surfaces is reduced.

The oxygen concentration in the closed incubation vessel can be measured by optical non-invasive methods. To keep the systems aerobic it can be aerated carefully. Volatilized compounds can be captured by an adsorption tube connected to the vessel. First experiments with such systems using radio-labelled substances have shown promising results in terms of mass balance but also indicated that there are further challenges with this kind of set-up. The permanent connection of adsorption tubes to the incubation vessel might provide an infinitive sink for the test compound which thus could escape from the test system. To keep aerobic conditions an oxygen supply like in the SaproMat respirator could be an option. First tests with limited head space volume indicate further challenges.