Polyethertrisiloxan-Tenside – Verhalten in der Umwelt und Spurenanalyse in Oberflächenwässern

Silicone surfactants are used in a broad range of products, from pesticides to cosmetics, polyurethane foams, textiles and fibers, paints and coatings or car care products. In spite of these numerous applications, the knowledge on their environmental occurrence and fate is scarce.

Trisiloxane surfactants, often referred to as superspreaders or superwetters, are added for instance to pesticides to enhance the activity and the rainfastness of the active substance by promoting a rapid spreading over hydrophobic surfaces. The objective of this work was to fill the lack of knowledge on the environmental occurrence and fate of a trisiloxane surfactant and to evaluate its potential to contaminate water resources.

As a first step, an analytical method for the trace analysis of the trisiloxane surfactant in the aqueous environment was developed and validated. The method, based on liquid-liquid extraction and HPLC-MS/MS, reaches limits of quantification in the ng L^{-1} range and allows an individual quantification of every homologue of the targeted trisiloxane surfactant. The newly developed analytical method was applied to analyze 40 river water samples. The trisiloxane surfactant was detected in 14 samples, between 1 ng L^{-1} and 100 ng L^{-1}. The results showed that the studied trisiloxane surfactant does not ubiquitously occur in the aquatic environment in measurable concentrations, but can reach surface waters on a local scale.

In order to assess the persistence of the trisiloxane surfactant in surface waters, its hydrolysis was studied in the lab, under various conditions (temperature, pH, and concentration). The half-lifes at pH 7 and 2 mg L^{-1} were found to be between 29 days and 55 days at 25 °C and between 151 days and 289 days at 12 °C. Taking only into account the hydrolysis, these results indicate that the trisiloxane surfactant could persist several weeks in surface waters. A degradation product of the trisiloxane surfactant was tentatively identified by high resolution mass spectrometry.

When used as agricultural adjuvants, trisiloxane surfactants may reach the soil compartment and might further leach to ground water. The behavior of the trisiloxane surfactant on soil was

investigated to assess its potential to reach ground water. With a sorption batch equilibrium method, distribution coefficients between water and soil (K_d, K_{oc}, and K_{clay}) were estimated for two soils (loam and sandy loam) and for every homologue of the trisiloxane surfactant. The obtained values for K_d were between 15 L kg^{-1} and 135 L kg^{-1}, indicating that the trisiloxane surfactant is only slightly mobile in soil. To further investigate the possibility of reaching ground water after application on agricultural fields, the leaching in soil was simulated in the lab in a soil column. The experimental settings were designed to simulate a worst case scenario where the application of the trisiloxane surfactant is done on quartz sand and is immediately followed by a heavy rainfall. Even under these conditions, less than 0.01 % of the initially applied trisiloxane surfactant leached through 20 cm of soil. Based on the K_d values and the results of the leaching in soil column, the studied trisiloxane surfactant is considered to be unlikely to leach to ground water after application as an agricultural adjuvant.

Future research should focus rather on the environmental properties of the polyether trisiloxane breakdown products than on the parent compounds. Another objective of further research would be to assess the influence of the trisiloxane surfactant on the mobility of other substances on soil, especially pesticides.

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Investigation of a polyether trisiloxane surfactant: Environmental fate and homologue specific trace analysis from surface water, Dissertation von Amandine Michel, Betreuer: Prof. Dr. Eckhard Worch, Institut für Wasserchemie der TU Dresden. Die experimentellen Arbeiten wurden am DVGW-Technologiezentrum Wasser (TZW), Karlsruhe, unter Leitung von Dr. Frank Thomas Lange und Prof. Dr. Heinz-Jürgen Brauch durchgeführt. Kostenloser Download: http://www.qucosa.de/fileadmin/data/qucosa/documents/19754/160213_Michel_thesis_A.pdf