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Comparing the European Union System for the Evaluation of Substances (EUSES) environmental exposure calculations with monitoring data for alkyl sulphate surfactants

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Abstract

Background: The European surfactant and detergent industry initiated a project to conduct an EUSES-based environmental exposure assessment for the total volume of alkyl sulfate (AS) surfactants, and to verify if the EUSES assessment leads to a realistic prediction of the environmental exposure or to an over- respectively under-estimation of the environmental concentrations of the surfactants. Verification of the EUSES environmental concentration prediction ($C_{local,effluent}$) was carried out by benchmarking them against environmental monitoring data. Recently published data from the United States of America adjusted to the European Union (EU) frame conditions were used for the assessment, as for the EU only historical data from the mid-1990s are available. In addition to the standard (default) EUSES assessment, a higher tier assessment using substance-specific properties, particularly increased biodegradation rates (192 per day instead of the default of 24 per day for WWTP), was conducted.

Results: A figure of 178,400 tonnes of AS was established as the total maximum volume (2016) handled annually in Europe. This total volume includes the volumes from all EU manufacturers and all registered AS > 100 t/a, as well as the amount of AS contained in EU REACH registered alkyl ether sulfates (AES). The total tonnage was split and assigned to the different uses as reported to ECHA in the C12 AS, Na (151-21-3) registration dossier in 2010. The EUSES calculation was limited to widespread (professional and consumer) uses, covering in total 97,889 t of AS homologues. The EUSES calculation gave a $C_{local,effluent}$ of 335 µg/L for the SimpleTreat "readily" biodegradation rate default and a $C_{local,effluent}$ of 44.6 µg/L for the AS-specific degradation rates. Recent US monitoring data showed a mean effluent concentration of 4.24 µg alkyl sulfates/L (Σ C12 + C14 + C16 homologues). Taking into account the different annual per capita AS use (including AS from AES) in the US (295 g) and the EU (348 g), the daily per capita water use (EU 200 L, US 408 L), and the WWTP efficiency in the EU and the US (comparable), an US to EU adjustment factor of 2.4 was established. Application of the adjustment factor to the US monitoring data resulted in a calculated EU mean effluent concentration = 10.18 µg alkyl sulfates/L (Σ C12, C14, C16 homologues). This value was used as an independent benchmark for the EUSES calculations.

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Conclusions: Comparing the predicted $C_{local,effluent} = 335 \mu\text{g alkyl sulfates/L}$ (SimpleTreat default) and a $C_{local,effluent} = 44.6 \mu\text{g Alkyl Sulfates/L}$ (AS-specific degradation rates) with the $10.18 \mu\text{g alkyl sulfates/L}$ from the adjusted monitoring data it is evident, that the EUSES calculation overestimates the AS environmental exposure by factors of > 32 and > 4 , respectively. Taking into consideration, that only widespread uses (covering only 50% of the total AS volume) were included in the EUSES calculation, the overestimation of the default exposure by a factor of 4 is still conservative, despite the fact, that eightfold higher, substance-specific biodegradation rates were used. In conclusion, using the 2010 C12-AS REACH dossier (CAS-No. 151-21-3) as an example, it has been shown, that EUSES model exposure calculations using default biodegradation rates significantly overestimate effluent concentrations.

Keywords: Surfactants, Effluent concentrations, Predicted environmental concentration (PEC), REACH, EasyTRA, Environmental monitoring, Exposure assessment, $C_{local,effluent}$