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Building Knowledge from Available Degradation Simulation Studies.

ABSTRACT / BACKGROUND

Higher tier degradation simulation tests may be required for substances registered under the REACH Regulation ((EC) No. 1907/2006) at tonnages greater than 100 tonnes/year. For lower tonnage substances, these tests may also be requested if there is a PBT/vPvB concern. Since 2020, a total of 315 new biodegradation simulation tests (OECD TG 307, 308 or 309) have been requested as part of the REACH regulatory process of Dossier Evaluation. Such simulation studies are complex, costly and can be technically challenging for a broad range of chemicals (e.g. [1], [2]). This project aims to gain insights to increase our understanding of these tests and improve their interpretation for regulatory decision-making.

Scope of work: In this project, we compiled a database consisting of relevant information from simulation studies and corresponding screening studies, in order to investigate influential factors that can drive the outcome of the simulation tests. The initial focus was on OECD TG 309 simulation studies, but the approach could potentially be extended to other simulation test methods. The factors considered included substance properties, inoculum information and test conditions. The goal was to identify predictors of chemical biodegradation in surface water (i.e., factors influencing biodegradation removal, half-lives, etc.), but also potential limitations and drawbacks of the current test guideline study setup to potentially provide guidance to design better studies, that can be applied to substances covering a broad range of physico-chemical properties. Opportunities to apply grouping approaches for degradation assessment will also be explored.

METHODS

Results and relevant metadata were collected from OECD TG 309 degradation simulation studies into a database. Data were obtained from multiple sources. REACH registered substances data were collected from the ECHA dossier dissemination portal. Data on plant protection products (PPP) were extracted from draft assessment reports available on the EFSA website. Data on 12 substances were also available from KWR Water Research Institute reports. Company owned R&D data were also collected. Test substance data included ECOSAR classes, BioWin fragments and a range of physico-chemical property information such as Henry's Law constant. Study data information included test duration, test substance concentration, temperature during test, information related to inoculum source and storage. Test validity information was also collated, such as reference substance degradation and mass balance criteria. Study results were also collected, including substance degradation half-life and presence/absence of metabolites. After metadata collection was completed, the quality of the database was assessed.

PRELIMINARY RESULTS

Data source	# substances	# of datapoints
REACh	128	257
PPP	82	259
Other	22	39

Table 1: Overview of substances in database

Test substance information	
Water solubility	2E-3 – 1E+6 mg/L
Henry's Law constant	5E-19 – 2E+5 Pa m3/mol
Log Kow	-4.9 – 7

Table 2: Overview of test substance information (subset - not yet including REACH registrations)

Test system parameters	
Test substance concentration	0.01-1300 µg/L
Agitated ; stagnant system	67% ; 3%
closed ; open system	27% ; 44%
Water temperature at sampling	4 – 24 °C
Studies with biomass meas.	12%
Aq oxygen concentration at end	4.8 – 9.8 mg/L
Reference sub condition not met	3% of studies
Mass balance condition not met	3% of studies

Table 3: Overview of meta data collected (subset - not yet including REACH registrations)

NEXT STEPS

The metadata availability will drive the statistical analysis that can be performed. From our preliminary assessment of the database, it is already clear that not all hypotheses can be tested due to limited data availability. For example, most studies were performed in the dark and at a temperature of ~ 20 °C, meaning that there may not be enough variability in the dataset to conduct a statistical analysis on these parameters. Nevertheless, sufficient data are available to evaluate other potential influencing parameters. BioWin fragments and physico-chemical property information are also available for investigation.

A preliminary principal component analysis (PCA) will be performed. More targeted hypothesis testing will then be based on suspected influencing factors identified in the literature. Additional statistical evaluations will be carried out, however, exact methods that will be applied are still being evaluated.

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