Executive Summary

Abstract. The main goal of LRI-ECO31.2 was to identify key factors contributing to the range of degradation rates reported in water, water-sediment, and activated sludge systems. We collected literature- or database-reported degradation data for various types of environmentally relevant chemicals in water, water-sediment, and activated sludge systems and evaluated different approaches to assess chemical persistence. We report a multivariable framework that was used to discover key determinants of chemical removal in activated sludge systems and the application of chemical benchmarking as a tool to assess chemical persistence within a specific environmental compartment.

The goal of LRI-ECO31.1 was to develop a multivariable framework to evaluate the key environmental parameters that drive aerobic biodegradation rates in soil. For LRI-ECO31.2, we hypothesized that the multivariable approach that we developed in LRI-ECO31.1 can be applied to uncover key environmental factors that determine the range of degradation rate constants in water, water-sediment, and activated sludge systems. However, data limitations were expected to be an important challenge that would need to be overcome for multivariable modelling to be applied in a robust way.

Data limitations were an insurmountable challenge for the development of multivariable models for water and water-sediment systems, though we report on the data sources that we explored and analyses of the data collected for those compartments. Data limitations were not a problem for activated sludge systems, and we collected data on the degradation of chemicals in full-scale wastewater treatment plants and in laboratory-studies that simulate the activated sludge process. We manually curated the data from the full-scale wastewater treatment plants to generate a final dataset that consisted of 529 independent observations for 84 chemicals along with a set of associated activated sludge process parameters. We used the Eawag Pathway Prediction System to predict initial biotransformations for each of the 84 chemicals and hierarchical clustering to group chemicals based on similarities in their predicted initial sets of biotransformations. We then applied stability selection to generate well-performing models that can be interpreted to uncover the key factors contributing to the range of removal efficiencies calculated for each cluster of chemicals. The sludge-water partitioning coefficient, molecular weight, solids retention time, influent chemical concentration, and dissolved oxygen levels were consistently identified as key factors of chemical removal for clusters of chemicals that undergo certain types of initial biotransformations. Our findings highlight the importance of considering initial biotransformations when evaluating chemical removal and identify important process parameters that determine the fate of chemicals during activated sludge treatment.

Although multivariable modelling can lead to insights on the key parameters that determine the fate of chemicals in a particular environmental compartment, this approach requires significant amounts of degradation data and associated metadata that describe the conditions under which the data were collected. As an alternative to multivariable modelling, chemical benchmarking could allow for comprehensive persistence assessments without the need for extensive sets of associated metadata. Chemical benchmarking is an emerging approach for persistence assessments that compares the behaviour of a chemical of interest with the behaviour of a benchmark chemical for which its degradation or persistence behaviour has already been determined. We explored chemical benchmarking to assess

chemical persistence in activated sludge systems. We first examined case studies to identify benchmarking chemicals that can explain the variable removal of chemicals in activated sludge systems. We then assessed the persistence of chemicals across a diverse group of activated sludge systems and proposed an approach to calculate overall average persistence ratios for classifying the persistence behaviour of chemicals. Our results demonstrate the utility of chemical benchmarking for evaluating chemical persistence and suggest that benchmarking could be used as part of a tiered approach for chemical risk assessment.

The results of this research are presented in this report as follows:

- Chapter 1 summarises our approach to data collection;
- Chapter 2 details our approach to data processing to generate analytical datasets;
- Chapter 3 presents the results and discussion of our statistical analyses and models;
- Chapter 4 presents the results and discussion of our application of chemical benchmarking.

Major conclusions and recommendations resulting from this work include:

- Our results suggest that clustering chemicals based on their initial biotransformations can lead to improved prediction of chemical removal during activated sludge treatment;
- Our approach of clustering chemicals based on their predicted initial biotransformations should also have broad utility in exploring the drivers of chemical biotransformations in other environmental systems;
- The results of our stability selection approach provide novel insights on the types of biotransformations performed by wastewater microbial communities and the factors that influence those biotransformations;
- The ways in which the most significant parameters contribute to variable degradation is different among chemical clusters; therefore, process modifications that target the enhanced removal of certain chemicals might further inhibit the removal of others;
- Despite the large amount of available data on chemical biotransformations in wastewater treatment plants, reports on relevant process parameters is variable and sparse;
- Chemical benchmarking can be implemented without the need for experimental or environmental metadata that is often not reported for any environmental compartment;
- Overall average persistence ratios can be used to rank the persistence of chemicals in a particular environmental compartment; this metric can be used as part of a tiered approach for chemical risk assessment.

Perspectives on the future of assessing variable degradation of chemicals:

- It is challenging to work with database- or literature-reported data for a number of reasons including: poor reporting of associated metadata; lack of consistency among sources; poorly designed experiments or sampling campaigns; etc.
- Future studies aimed at improving our understanding of variable degradation of chemicals across environments would benefit from self-consistent datasets derived from experiments or sampling campaigns explicitly designed to generate data to that end.
- A key theme that connects the findings from our studies is the need to examine variable degradation from the perspective of initial biotransformations. Future studies should consider this carefully and perhaps be designed to explicitly address this paradigm.
- The full potential of chemical benchmarking is still largely unexplored, but our analyses demonstrate that chemical benchmarking can be applied in different ways and could be an effective way of prioritizing chemicals in a tiered approach for chemical risk assessment.