
Preface

Following release to the environment, synthetic chemicals may be degraded by biotic and abiotic processes. The degradation of the chemical can follow a plethora of pathways and a range of other substances can be formed via these different pathways (e.g. [1]). A number of terms have been used for these substances including metabolites, degradates and transformation products – in this book we use the term transformation products. While we often know a lot about the environmental properties and effects of the parent synthetic chemical, we know much less about the transformation products.

Transformation products can behave very differently from the parent compound (e.g. [2]). For example, selected transformation products are much more persistent than their associated parent compound in soils, waters and sediments and some may be transported around the local, regional and global environments to a different extent than the parent compound. Transformation products can also have very different toxicities than the parent compound (e.g. [3]) and in some cases transformation products can be orders of magnitude more toxic than their parent compound; although this situation is rare. The environmental risks of transformation products can therefore be very different than the risks of the parent compound.

The potential environmental impacts of transformation products are recognised by many regulatory assessment schemes. For example, in the EU, pesticide producers are not only required to assess the fate and effects of the parent pesticide but are also required to assess the potential adverse effects of major metabolites and minor metabolites that are deemed to be of concern [4]. Similar requirements also exist for new human and veterinary pharmaceuticals and biocides (e.g. [5]). However, for many older substances and many other substance classes (e.g. industrial chemicals), data on the environmental risks of transformation products can be limited or non-existent.

The assessment of the environmental risks of transformation products can however be challenging. Perhaps the biggest challenge is that there are a vast number of synthetic chemicals in use today which can each degrade into a number of transformation products; we don't have the resources to test the fate and environmental effects of the parent compounds let alone the transformation products. The identification and characterisation of transformation products arising from a particular parent substance in a particular system can

also be extremely difficult due to problems of extraction, detection at environmentally relevant levels, and quantification in the absence of standards; although the arrival of new analytical methodologies (e.g. time-of-flight mass spectrometry) and the availability of expert systems for predicting transformation pathways is now making this task less daunting. The modelling of transformation product exposure and effects can also be challenging as we are faced with a dynamic system involving a complex mixture of substances where parent compounds are being degraded to transformation products which are then degraded to other transformation products. Finally, while treatment methodologies that are used to control human and environmental exposure are able to remove transformation products, they can also act as a mechanism of transformation product formation and selected treatment processes (e.g. advanced oxidation processes for drinking water treatment) may even produce transformation products more hazardous than the substance that has been treated.

While, there are a number of scientific challenges and large knowledge gaps, a significant amount of information is available on the routes of formation, detection, exposure, effects and modelling approaches for transformation products of some classes of substances. If we can bring this information together, we should be able to assess transformation products in a much more pragmatic way. This will allow resources to be focused on transformation products of most concern while maintaining the health of the natural environment.

Therefore in this book, we have brought together contributions from leading experts in this field to provide an overview of the current knowledge on the formation, detection, occurrence, effects and treatability of transformation products in the environment. Many of the chapters introduce methods for assessing the different components required to determine the risks of transformation products to natural systems. In the chapter *Mechanisms of degradation of synthetic chemicals*, Wackett et al. (this volume) discuss the mechanisms by which transformation products are formed and describe how this information can be used to predict the structures of transformation products. Howard discusses a wider range of methods for predicting degradation rates and degradation pathways in the chapter *Predicting the persistence of organic compounds*. The chapter *Analysing transformation products of synthetic chemicals* by Perez et al. describes the challenges for analysing transformation products and discusses the application of some of the new analytical methods for identification and quantification of transformation products in environmental systems. In *Occurrence of Transformation Products in the Environment*, Kolpin describes the results of a series of monitoring studies into the occurrence of selected transformation in US water bodies. Hu et al. (*Fate of Transformation Products of Synthetic Chemicals*) discuss experimental data on the persistence and mobility of transformation products in environmental systems and in the chapter *Modeling environmental exposure to transformation products of organic chemicals*, Fenner et al. describe modelling approaches for assessing exposure levels for transformation products in a range of environmental systems. The chapters

Ecotoxicity of Transformation Products (Sinclair and Boxall) and *Predicting the Ecotoxicological Effects of Transformation Products* (Escher et al.) describe the ecotoxicological effects of transformation products and discuss approaches that could be employed for estimating ecotoxicity based on transformation product structure and information on the associated parent chemicals. Finally, in *Treatment of Transformation Products*, Adams et al. discuss how transformation products can be removed in treatment processes but also discuss how treatment processes can act as routes of transformation product formation.

It is clear from each of the chapters that while we are now well placed to better assess transformation product risk, there is still much that needs to be done. Areas where we need further development include:

- Expert systems for predicting the nature of transformation products – Work should focus on the development of methods to identify the most probable transformation pathway in a particular environmental system. The approaches need to be evaluated against high-quality experimental data on degradation pathways in different media. New expert systems need to be developed for systems where they are not yet available, e.g. drinking water treatment processes.
- Analytical methods – We need to develop high-quality methods that are able to extract and identify all transformation products of potential concern in a range of environmental systems. We should explore how we can quantify (or semi-quantify) transformation product concentrations in the absence of standards.
- Monitoring studies for transformation products – A number of monitoring studies have explored the occurrence of transformation products in the environment. These studies have tended to focus on transformation products arising from the use of only a few pesticide active ingredients. It would be useful to prioritise transformation products in terms of their potential risk to a particular system (e.g. using approaches similar to that described by Sinclair et al. [6]) and extend these monitoring studies to a much wider range of substances. Where possible, monitoring studies should not just look at occurrence but should also aim to understand the underlying mechanisms determining the transport of transformation products around the environment.
- Exposure models – Models are available for estimating exposure of transformation products at a range of scales. These models need evaluation and may need further development as our knowledge expands.
- Ecotoxicological effects – Most experimental data is on the acute toxicity of transformation products to aquatic organisms so it would be valuable to generate an understanding of the potential chronic effects as well as an understanding of the impacts on terrestrial organisms. Predictive approaches for estimating the ecotoxicity of transformation products show some promise, however these need further development and validation. It

is also important to recognise that a transformation product will not occur in the environment on its own but will co-occur with its parent compound, other parent compounds and other transformation products, the further development of approaches for assessing the risk of mixtures is therefore critical. As the system is a dynamic system (i.e. concentrations of parent compounds and transformation products will be changing at different rates), in the future mixture assessment models that can deal with changing exposure concentrations may be required.

- Human health implications of transformation products – Most work to date has focused on the assessment and prediction of the ecotoxicity of transformation products. We need to begin to assess the potential human health implications of the presence of transformation products in the environment and develop approaches for identifying transformation products of most concern to human health. Expert systems for predicting mammalian toxicity endpoint may play a role here.

To address these issues will require input from a wide range of disciplines including ecotoxicologists, exposure modellers, analytical chemists, toxicologists, treatment scientists and biochemists. Hopefully this book will encourage researchers, students and regulators from these different fields to begin, or continue, to work to develop approaches and knowledge so that in the future we have a much better understanding of the risks of transformation products and of how to control these risks.

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