

# Systematic Handling of Environmental Fate Data for Model Development—Illustrated for the Case of Biodegradation Half-Life Data

Jasmin Hafner,<sup>#</sup> Kathrin Fenner, and Andreas Scheidegger



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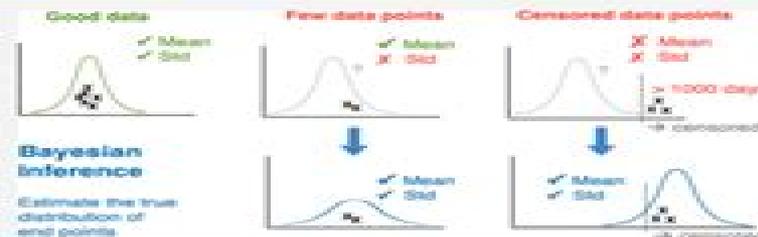
**ABSTRACT:** The assessment of environmental hazard indicators such as persistence, mobility, toxicity, or bioaccumulation of chemicals often results in highly variable experimental outcomes. Persistence is particularly affected due to a multitude of influencing environmental factors, with biodegradation experiments resulting in half-lives spanning several orders of magnitude. Also, half-lives may lie beyond the limits of reliable half-life quantification, and the number of available data points per substance may vary considerably, requiring a statistically robust approach for the characterization of data. Here, we apply Bayesian inference to address these challenges and characterize the distributions of reported soil half-lives. Our model estimates the mean, standard deviation, and corresponding uncertainties from a set of reported half-lives experimentally obtained for a single substance. We transform data with experimental soil half-lives of varying data quantity and quality, and we infer the half-life distribution for each compound. By estimating average half-lives, their experimental variability, and the uncertainty of the estimations, we provide a reliable data source for building predictive models, which are urgently needed by regulatory authorities to manage existing chemicals and by industry to design benign, nonpersistent chemicals. Our approach can be readily adapted for other environmental hazard indicators.

**KEYWORDS:** environmental fate data, biodegradation half-lives, soil, censored data, uncertainty, Bayesian inference

## INTRODUCTION

In the EU, different chemical regulations require different levels of hazard and risk assessment, partially depending on the amounts of substances used and produced.<sup>1–3</sup> The recently amended regulation for chemicals, labeling, and packaging (CLP) in Europe now requires hazard assessment covering toxicity, bioaccumulation, persistence, and mobility for substances and mixtures introduced into the EU market, to prioritize those with great potential for negative environmental impacts.<sup>4</sup> Experimental determination of these hazard indicators is costly and time-consuming, and the necessary data for a confident hazard assessment are missing for many substances on the market.<sup>5</sup> Computational models that predict environmental hazard indicators are necessary to fill data gaps for existing chemicals and to screen for environmentally safe chemicals during the industrial research and development of new chemicals,<sup>6</sup> ultimately supporting the phase-out of harmful chemicals on the market. However, model training requires reliable and abundant experimental data of sufficient quality, which is scarce, in particular for biodegradation end points.

In addition to the scarcity of data, the main issue is the high variability of environmental hazard indicator data. For example,



We apply our inference model to 893 pesticides and pesticide transformation products with experimental soil half-lives of varying data quantity and quality, and we infer the half-life distribution for each compound. By estimating average half-lives, their experimental variability, and the uncertainty of the estimations, we provide a reliable data source for building predictive models, which are urgently needed by regulatory authorities to manage existing chemicals and by industry to design benign, nonpersistent chemicals. Our approach can be readily adapted for other environmental hazard indicators.

OECD 307 studies require experimental determination of biotransformation half-lives of a substance in three different types of soil.<sup>7</sup> While testing in diverse soils is considered necessary to draw general conclusions about the persistence of a chemical in the environment, this will lead to variability in the determined end point data. In the case of soil biodegradation, sources of variability include physicochemical parameters (e.g., temperature and acidity), soil characteristics (e.g., soil texture, cation exchange capacity, biomass content, and organic carbon content), and the composition, activity, and enzymatic potential of the microbial community. Other factors that contribute to the variability of biodegradation data include low but environmentally relevant concentrations of spiked chemicals entailing larger analytical errors and the

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