# Identifying strategies that will provide greater confidence in estimating the degradation rates of organic chemicals in water, soil and sediment

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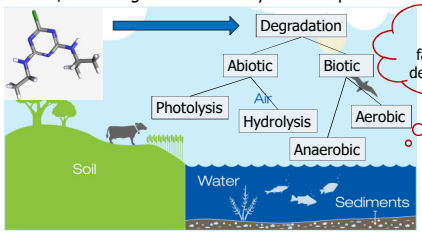
## Introduction

***chemical release into environment***

abiotic/biotic degradation are key removal processes

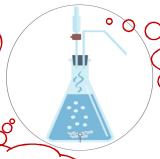



What key environmental factors influence degradation rates?

Are key environmental factors considered in testing strategies?

***persistence assessment***

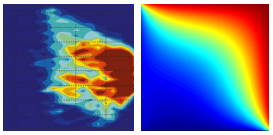
degradation rates estimated from simple screening assays



Are we confident using estimated degradation rates in highly spatially resolved exposure models?

***exposure modeling***

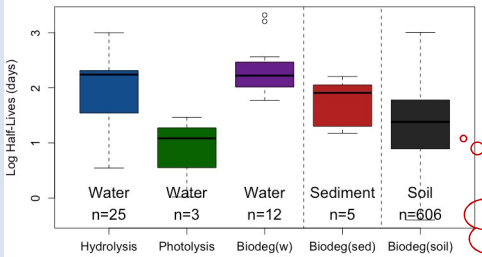
highly spatially resolved exposure models are becoming widely accessible



### Objectives of Project:

1. Review existing approaches for persistence and exposure assessment.
2. **Identify key environmental factors influencing degradation rates.**
3. Recommend experimental framework for considering variable degradation.

## Example Case Study - Atrazine degradation

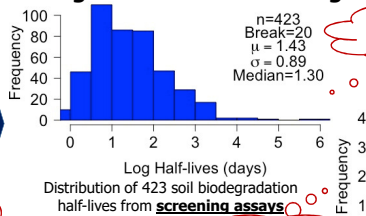



**Data Sources**

- Literature
- AMBIT
- ECHA eChemPortal
- USEPA pesticides
- NIH TOXNET
- Handbooks
- Other sources

Estimated atrazine biodegradation half-lives vary over three orders of magnitude

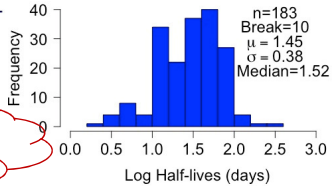
## Histogram of atrazine biodegradation half-lives in soil




What factors influence half-lives in screening assays versus field studies?

Distribution of 423 soil biodegradation half-lives from **screening assays**

Distribution of 183 soil biodegradation half-lives from **field studies**




The mean half-life is similar for screening assays and field studies, but the shape of the distribution is different

## General approach to identify key environmental factors

Build matrix of half-lives and experimental metadata

pH, organic carbon ($C_{org}$), temperature, sand, silt, clay, total nitrogen ($n_{tot}$), moisture (water), min sample depth ($d_{min}$), difference between min and max sample depth ($d_{diff}$), bulk density (BD), cation exchange capacity (cec), atrazine use history (atr.cond)

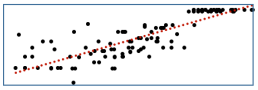
use multiple imputation to fill-in missing data

remove variables with too many missing values (80%)

GAM shows what kind of shape/function best describes the contribution of each environmental factor to the degradation rate.

construct generalized additive model (GAM)

use stepwise variable selection to identify key variables

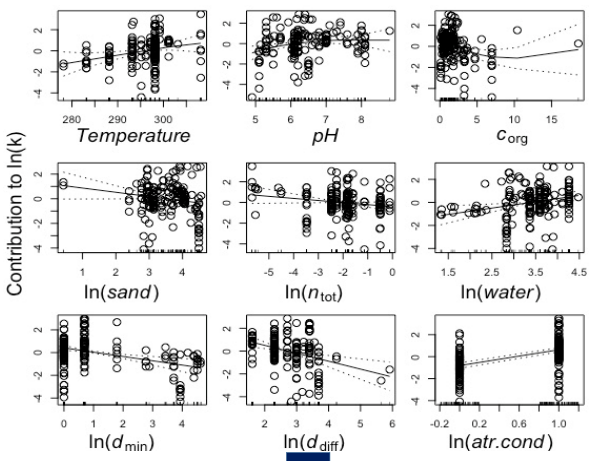


## Multivariate regression – GAM for atrazine screening assays

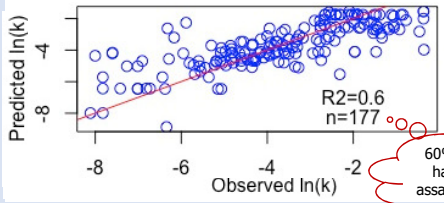
Based on literature review, we built a generic model for atrazine soil degradation rates:

$$\ln(k) = k_0' + f'(T) + g'(pH) + h'(c_{org}) + b_s \ln(sand) + b_n \ln(n_{tot}) + b_w \ln(water) + b_m \ln(d_{min}) + b_d (\ln(d_{diff}) + b_a atr.cond$$

We fit the ln(k) equation to the collected data from atrazine screening assays using nonparametric smoothers for functions $f(T), g(pH), h(c_{org})$ in the GAM.




### Stepwise variable selection

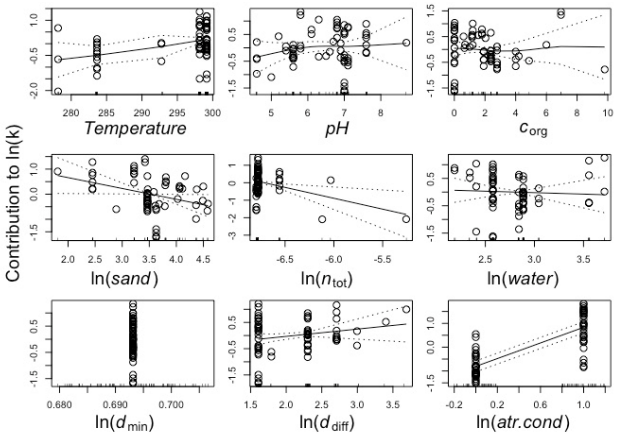



**Key factors (p-value)**

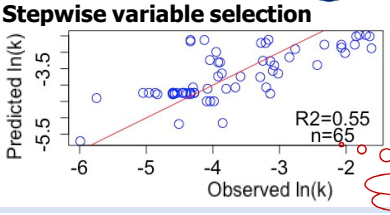
- Organic carbon (<0.001)
- pH (<0.001)
- History of atrazine use (<0.001)
- Temperature (0.001)
- Moisture (0.001)
- $D_{min}$ (0.001); $D_{diff}$ (0.01)

60% variability in atrazine half-lives from screening assays explained by 7 factors

## Multivariate regression – GAM for atrazine field data




### Stepwise variable selection




**Key factors (p-value)**

- History of atrazine use (<0.001)
- Total nitrogen (<0.001)
- Soil texture (sand) (0.001)
- Temperature (0.001)
- Organic carbon (0.05)

55% variability in atrazine half-lives from field studies explained by these 5 factors

## Conclusion

- Multivariate analysis indicates that history of atrazine use is a key factor influencing half-lives in screening assays and field studies.
- Organic carbon and pH are highly significant factors influencing half-lives in screening assays.
- Total nitrogen content is a highly significant factor influencing half-lives in field studies.

## Future work

- Apply GAM and stepwise variable selection procedure to broader set of chemical classes.
- Apply GAM and stepwise variable selection procedure to study other reaction types.

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