

# pH-dependent Equilibrium Behaviors Between two Metabolites of a Fungicide



Ye Yuan, Erika Seidel, Bayer AG, Crop Science Division, Environmental Safety, 40789 Monheim am Rhein, Germany

## Introduction

Active substances of plant protection products are subject to a variety of degradation processes after application, including the potential formation of degradation products. The degradation may be the result of microbially-induced and/or abiotic-chemical processes. Knowledge and comparison of behaviors of two degradation products of a fungicide, Metabolite A and Metabolite B, in buffer solutions at different pH values (pH 4, 7 and 9) is necessary for the overall assessment of the fate in the environment.

## Objective

The objective of this study was to gain knowledge on comparison of the behaviors of Metabolite A and Metabolite B in buffer solutions at different pH values, which supports an overall assessment of the fate in the environment. Therefore, the rate of degradation and formation of Metabolite A and Metabolite B in buffer solutions at different pH value conditions was investigated in the dark in the laboratory.

The amounts of Metabolite A and Metabolite B were determined throughout the study. The rates of degradation and formation were calculated as DT<sub>50</sub> and DT<sub>90</sub> values for each buffer solution at different pH value.

## Test Conditions

The test was performed in glass crimp top vials with septa each containing 25 mL of test solution. Incubation was carried out at 20 ± 2 °C in a walk-in climatic chamber in the dark.

Duplicate samples were processed and analyzed 0, 2, 4, 7, 24, 48, 120, 195 and 336 hours after treatment. At each sampling interval, the amounts of test items in the test solutions were determined by HPLC-MS/MS analysis.

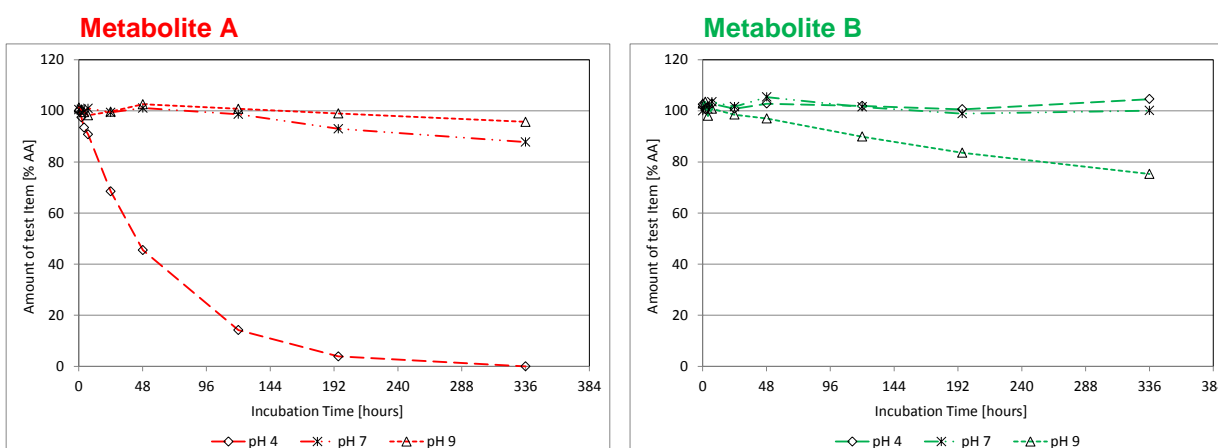
## Results & Conclusions

The degradation rate of Metabolite A and Metabolite B for all pH values was calculated using first order kinetics. The table below summarizes the results of the DT<sub>50</sub> and DT<sub>90</sub> calculations:

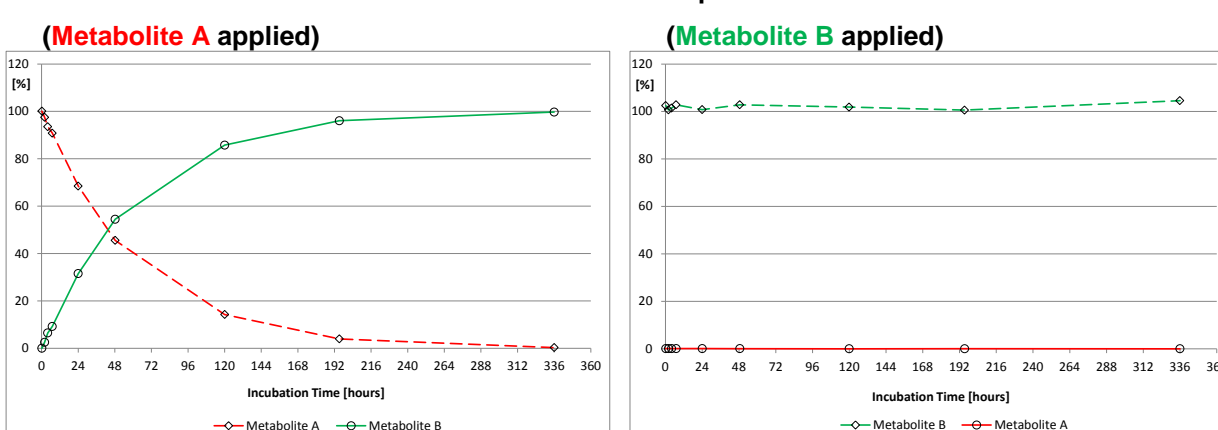
- The degradation of Metabolite A and Metabolite B in buffer was observed to be pH dependent.
- It was proven, that degradation of Metabolite A in buffer solution was caused by transformation into Metabolite B and vice versa as a function of the pH value.
- Metabolite A was degraded rapidly at pH 4, moderately at pH 7 and very slowly at pH 9. Metabolite B was degraded well at pH 9 and stable at pH 4 and pH 7.

Based on the results it is assumed that in aquatic systems an equilibrium between the two compounds occurs which is pH-dependent. At pH values ≤ 7 mainly Metabolite B occurs while in aquatic systems with pH values ≥ 9 mainly Metabolite A is expected.

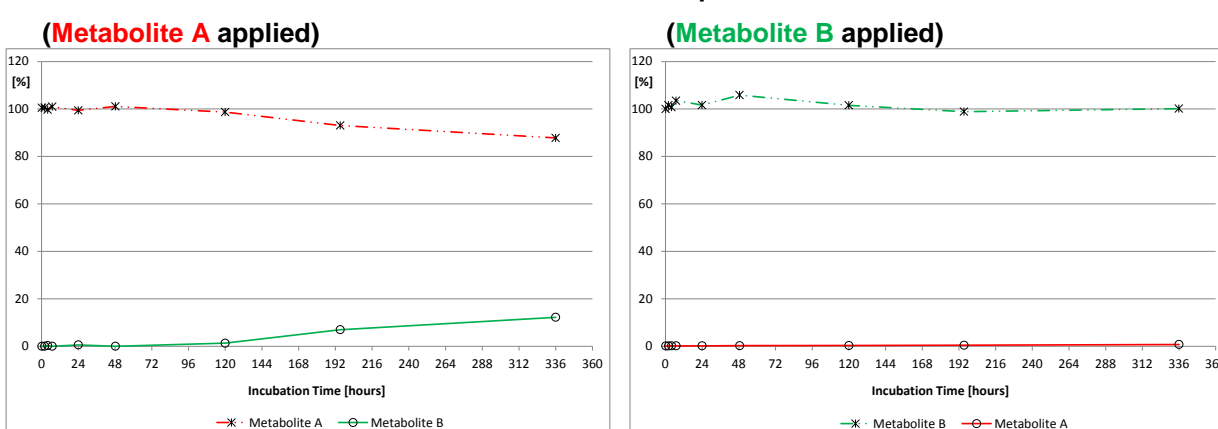
Degradation at different pH values



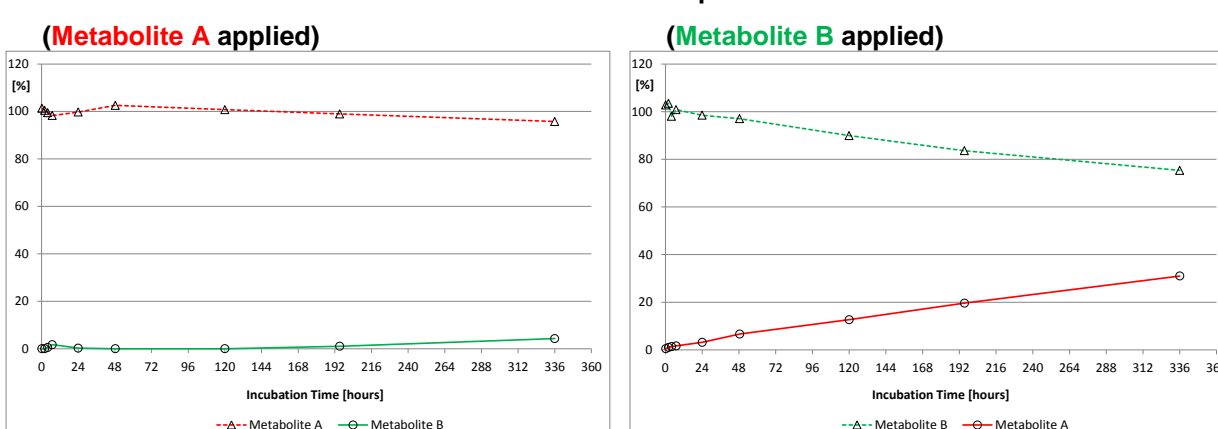
Buffer solution pH 4



Buffer solution pH 7



Buffer solution pH 9



The study was conducted in compliance with the OECD Principles of Good Laboratory Practice and the Principles of Good Laboratory Practice – German Chemical Law (ChemG), Annex 1.

Compound	pH	SFO		
		DT <sub>50</sub> [days]	DT <sub>90</sub> [days]	chi <sup>2</sup> Error [%]
Metabolite A	4	1.77	5.89	0.7
	7	73.2	243	0.9
	9	257	852	1.1
Metabolite B	4	> 1000	> 1000	1.0
	7	412	> 1000	1.4
	9	31.4	104	1.2