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# Measuring partitioning behavior of environmental chemicals

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There is a great variability in polarity, size and functional groups of organic agrochemicals. Therefore this presentation focuses on the properties of chemicals.

The fate of a chemical in the soil is subject to partitioning processes. A mechanistic approach to quantify molecular interactions that govern partitioning processes is provided by polyparametric linear free-energy relationships (pp-LFERs). They allow the calculation of the equilibrium partitioning of a neutral chemical in any given two-phase system using one single equation.

Today, one of the most widely applied pp-LFER is the Abraham equation:

log k= eE + sS + aA + bB + vV, where log k is the equilibrium partitioning constant and the five parameter pairs quantify the molecular interactions between any given two phase-system and the chemical.

These parameters can be used as a precise physico-chemical characterization in order to model and predict the transport and fate of chemicals in the environment.

However, for complex environmental chemicals, e.g. pesticides, there is still a lack of substance parameters and the calculation of those using group-contribution approaches like Absolv is inaccurate to date. Therefore a liquid chromatography method for determining substance parameters for environmental chemicals is being developed and validated and will be presented. Results will be compared to predictions from a group-contribution approach.