Near-Infrared Spectroscopy as a Tool for Generating Sorption Input Parameters for Pesticide Fate Modeling

Sorption parameters (such as Kd values) are among the most sensitive input parameters in pesticide fate models. This study demonstrates that near-infrared spectroscopy (NIRS), in combination with batch equilibrium techniques, can be used to estimate Kd values, thereby increasing throughput of the many samples required to characterize spatial variability of pesticide sorption within fields. The Pesticide Root Zone Model version 3.12.2 (PRZM- 3) was used to compare scenarios that used NIRS spectral data, pedotransfer functions, and batch equilibrium methods as inputs for the calculation of 2,4-dichlorophenoxyacetic acid (2,4-D) and atrazine leaching in 591 soil horizons. Based on the 3564 simulation runs conducted, we concluded that the added benefit of NIRS is most useful when the pesticides under study have small sorption potentials and short half-lives in soil. The 2,4-D and atrazine sorption by soil was highly correlated to soil organic C (SOC) content in the fields under study. The feasibility of using NIRS to predict pesticide Kd values largely relies on the sorption of the pesticide being significantly correlated to SOC. In addition, successful regional approaches to predicting Kd values from NIRS spectral data can also be developed when the calibration model is derived by combining a set of fields where each has a similar statistical population characteristic in Kd