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## The Role of Dissipation Processes in Plants for Modeling Bioaccumulation

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# ABSTRACT BOOK



**BUZZING WITH SCIENCE**  
Cross-Pollination for Environmental Progress

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of soil matrix. The different CW mesocosm were assessed in terms of contaminant mass removal. The bioaccumulation behavior of the several PPCPs and PFCs was assessed in the different mesocosms, including determination of uptake and elimination rate constants ( $k_u$ ,  $k_e$ ), bioconcentration factors (BCFs), translocation factors (TFs) and half-lives ( $t_{1/2}$ ) in plant roots and leaves. In general, the presence of plants enhanced the removal of PPCPs and PFCs, resulting in lower effluent concentrations compared to influent concentrations. The influence of mesocosm design and physical-chemical properties on bioaccumulation phytoremediation potential will be presented and discussed.

#### 84 The Role of Dissipation Processes in Plants for Modeling Bioaccumulation

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Plant bioaccumulation estimates used in exposure, risk and impact assessments; phytoremediation; and biomonitoring rely on a combination of experimental data and models. Dissipation processes, such as degradation, volatilization, and growth dilution, are known to be major contributors to plant bioaccumulation model uncertainty. Unfortunately, while overall dissipation half-lives are often determined in pesticide fate studies and models exist to predict overall dissipation, empirical data describing the individual dissipation processes, the necessary input for most mechanistic plant bioaccumulation models, are scarce. In particular, while degradation rates are thought to be the major dissipation mechanism in many cases, such data are extremely difficult to measure directly. In a case study using 42 pesticides we estimated the volatilization and growth dilution components of overall plant dissipation. From comparing our estimates with measured dissipation we calculated that degradation accounts for between 30% and 83% of the total dissipation from plants. Overall, our results suggest that degradation is the most important plant dissipation processes followed by growth dilution. These processes, critical input for designing and calibrating models, depend on a wide range of chemical, plant and environmental characteristics that are not often reported in current plant bioaccumulation testing studies. To address uncertainty in plant bioaccumulation knowledge and modeling we recommend harmonizing and updating current plant bioaccumulation testing guidelines to require the reporting of additional measured data related to plant characteristics (e.g., plant stage and leaf area), environmental field test conditions (e.g., soil organic carbon content, air temperature), and detailed application data (e.g., treated plant components, application dates and duration). We further recommend developing targeted models for an improved prediction of individual processes contributing to overall plant dissipation – most importantly biodegradation – as a function of chemical properties, plant species characteristics, application and environmental conditions.

#### 85 Fate and Metabolism of 2,4-Dinitroanisole in Willow Trees

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The environmental fate of 2,4-dinitroanisole (DNAN), a component of new insensitive munitions explosives (IMX), is an emerging global issue. The new IMX formulations are replacing old formulations at a rapid pace, but the environmental fate and ecosystem toxicity of IMX components remains largely unknown. DNAN and other nitroaromatics have been shown to cause harm to human health and ecosystems which makes widespread use of DNAN concerning. Full-scale remediation will be necessary for military testing sites and ammunitions manufacturing plants around the world as more countries adopt the new IMX formulations and the compounds are inevitably released. Therefore, knowledge regarding the fate of DNAN within natural systems is needed to characterize ecosystem risk and inform future phytoremediation efforts. The research presented is what we believe to be the first comprehensive

study of 2,4-dinitroanisole transformation in a plant system. Data will be shared on the fate of DNAN in willow trees, including bulk partitioning to roots, stems and leaves resulting from 14C-labeled DNAN studies. Furthermore, the metabolic fate of DNAN was examined using 13C-DNAN and 15N-DNAN stable isotope analysis. Suspected DNAN metabolites were identified and confirmed with liquid chromatography tandem mass spectrometry. Similar to other studies on biological systems, metabolites such as 2-amino-4-nitroanisole have been confirmed in willow and other metabolites are being confirmed. A full metabolic profile and suspected pathways will be presented. Implications for the environment and full-scale phytoremediation will be offered.

#### 86 Mixture Effects on Uptake of Pharmaceuticals and Personal Care Products by *Arabidopsis thaliana*

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Municipal wastewater treatment plant effluents typically contain a variety of pharmaceutical and personal care product ingredients (PPCPs). In arid and semi-arid areas worldwide, reclaimed wastewater (RWW) is often used to irrigate crops, resulting in exposure of the plants to PPCPs. Crops irrigated with RWW may take up PPCPs through their roots. However, the extent of their bioaccumulation in food crops is not well understood. Plants may respond to PPCPs in a concentration-dependent manner that affects their uptake, and some PPCPs may exert toxicity on plants. In the field, plants are exposed to complex mixtures of PPCPs, but to our knowledge, the effects of mixtures on PPCP uptake have not been evaluated. We exposed the model plant *Arabidopsis thaliana* to a mixture of 18 PPCPs commonly found in RWW and measured uptake into leaves and roots. *A. thaliana* was selected because it matures rapidly, its genome has been fully sequenced, and a variety of mutants are available. We found that all 18 compounds were taken up to some extent. However, the plants exposed to the PPCP mixture showed evidence of toxicity including lower leaf and root mass along with small amounts of wilting and leaf discoloration. Using root elongation assays, we determined the compounds in our mixture that have the largest phytotoxic effect on *A. thaliana*. We repeated the uptake experiments at two exposure concentrations and directly compared PPCP uptake into plants grown with and without exposure to the most toxic PPCPs. Results from these experiments will be presented.

#### 87 Tree Diameter and Rooting Morphology Impacts on Phytoscreening for Vapor Intrusion Potential

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Trees are masters of mass transfer, intimately interacting with surrounding soil, water, and vapor. Their inherent ability to collect spatially and temporally composited samples suggests trees are good surrogate candidates for vapor intrusion risk. Phytoforensics has been shown to be a cost- and time-effective tool in qualitatively delineating groundwater contaminant plumes as contaminants translocate into trees from groundwater the vapor phase in the vadose zone; however, little is known about how tree characteristics (such as tree species, size, and age) affect sampling results. Considerable unknowns include the subsurface volume sampled by plants and plant responsiveness to subsurface contaminant changes. To investigate how tree diameter affects tree contaminant concentrations, tree coring was used at a Superfund site contaminated primarily with perchloroethylene (PCE) in Missouri. As part of tree-core and soil sampling, over 300 tree-core samples and about 900 soil samples were collected over 7 and 35 days, respectively. Paired samples, which consist of tree cores from pairs of large- and small-diameter trees in close proximity, were collected from 18 tree pairs. Phytoforensics was about 5 times quicker than soil sampling, about an order of magnitude less expensive, and encompasses a larger environmental volume with