A Time-dependent Compartmental Model for PFAS Uptake and Tissue Distribution in Tomato Plants Across PFBA–PFUnA

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Abstract

Background & Objective: Understanding how per- and polyfluoroalkyl substances (PFAS) accumulate in different tissues of food crops is essential for evaluating food safety risks in the circular food system. However, quantitative models that capture time-dependent PFAS uptake remain limited. In addition, most studies often focus on the influence of compound properties, while the influence of the plant-related factors were underexplored. To address this, this study developed and evaluated a time-dependent, mass-balance-based compartmental model predicting uptake and distribution of PFCAs (PFBA-PFUnA) in tomato plants, with differentiation of root, stem, twig, leaf, and fruit concentrations. *Methods*: The model incorporates compound hydrophobicity, transpiration-driven transport, carrier-based active transport, and tissue-specific accumulation behaviors. Model predictions were evaluated against data from an experiment measuring the uptake of multiple PFAS in a hydroponic system. *Results & Conclusion*: Predicted PFAS concentrations across plant tissues ranged within one order of magnitude from the experimental data. The model successfully reproduced characteristic chain-length patterns, including higher mobility of short-chain PFAS and increased retention of long-chain PFAS in roots. However, concentrations in roots were underpredicted for long-chain PFAS (C9-C11). This study provides a mechanism-based yet tractable model, contributing to improved comprehensive exposure assessment and supports future risk evaluation for PFAS uptake in crops in circular food system.

Keywords

PFAS, Perfluoroalkyl Carboxylic Acids (PFCAs), Tomato Plants, Food Safety, Crop Uptake Modeling, Mass-Balance Model, Environmental Contaminants, Circular Food Systems