Tracking and Estimating Industrial Wastewater Transfers to Publicly Owned Treatment Works, Using an Integrative Plant-Wide Model

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The transfer of large volumes of industrial wastewater, containing both conventional and emerging contaminants, to Publicly Owned Treatment Works (POTWs) is end-of-life (EOL) management processes that present potential risks to environmental and human health. To address these challenges, this study introduces a hybrid data engineering framework that integrates top-down and bottom-up methodologies for tracking and estimating chemical transfers to POTWs. By combining information from public databases such as the Toxic Release Inventory (TRI), Discharge Monitoring Reports (DMR), and the CompTox Chemicals Dashboard, the framework supports chemical risk evaluations and regulatory compliance by capturing industrial-to-POTW transfers. The framework emphasizes integrating life cycle analysis (LCA) with risk assessments to better predict the fate and transport of contaminants within POTW systems.

The Chemical Tracker and Exposure Assessor in POTWs (ChemTEAPOTW) model simulates an integrated network of submodels for various treatment units, such as primary clarifiers, activated sludge reactors, anaerobic digesters, and sludge management systems, while also accounting for occupational exposure pathways. The ChemTEAPOTW model tracks chemical transfers and assesses the fate of contaminants during treatment, considering biodegradation, sorption, and mass transfer processes to supplement

existing data to address data gaps in chemical transfer reporting. This study demonstrates the effectiveness of using regulatory databases like TRI and DMR to provide chemical flows and treatment efficiency data as introductory data for the ChemTEAPOTW model. A case study focusing on n-hexane in the soybean industry illustrates the framework's ability to track chemical transfers, identify regulatory gaps, and enhance understanding of EoL chemical management.

The study underscores the importance of using top-down and bottom-up methodologies to ensure comprehensive chemical tracking while addressing location-specific data gaps. This hybrid approach offers a useful tool for practitioners to simulate and evaluate chemical behavior within POTWs, with applications in system retrofitting, process optimization, and compliance assessment. Ultimately, this work aligns with the EPA's mission to improve chemical lifecycle transparency and reduce human and environmental health risks.