

## ABSTRACT

The pervasive presence of pharmaceutical and personal care products (PPCPs) in the environment has raised significant concerns due to their potential adverse effects on ecosystems and human health. Even at trace concentrations, these emerging contaminants can persist in subsurface environments and threaten drinking water sources. This study focuses on two PPCPs, metformin (MTN) and erythromycin (ETM), and explores their fate and transport in subsurface environments, particularly in sediments and compacted subsurface soils. Notably, research on the migration of PPCPs at environmentally relevant concentrations in sediments and subsurface soil core samples is limited. The study begins by examining the migration of MTN and ETM in a saturated sandy soil column using temporal moment analysis. The results reveal that MTN, a highly mobile contaminant, is eliminated in approximately 40 days, while ETM, with substantial adsorption due to its hydrophobicity, migrates more slowly through the porous media. The study emphasizes the critical roles of Darcy velocity and adsorption coefficients in controlling the transport of PPCPs, as seen in variations in solute mass recovery at the column outlet.

Further, the study investigates the adsorption behaviour of MTN and ETM in sediments and subsurface soils with varying organic matter and particle composition, analysing sorption kinetics, isotherms, and the effects of pH, temperature and moisture content at relevant concentrations. High adsorption coefficients for both MTN (6.14 L.Kg<sup>-1</sup> in sand and 245.70 L.Kg<sup>-1</sup> in silty loam) and ETM (8.28 L.Kg<sup>-1</sup> in sand and 488.13 L.Kg<sup>-1</sup> in silty loam) indicate a strong affinity for soil, with thermodynamic analysis confirming the feasibility and exothermic nature of adsorption. Additionally, reduced soil moisture content was found to enhance adsorption, improving the understanding of these contaminants' mobility and aiding in formulating management strategies.

The study also employed a sandy soil column to investigate PPCP migration, finding that MTN showed higher mobility, with a recovery rate exceeding 90%, while ETM exhibited slower migration with a recovery rate of less than 15%. Fate and transport parameters determined using breakthrough curves and inverse optimization in HYDRUS 1D indicated a dispersivity of 0.4 cm and a saturated hydraulic conductivity of 0.75 cm.h<sup>-1</sup>. The findings highlight concerns about groundwater contamination due to MTN's higher mobility and lower adsorption compared to ETM.

Additionally, 2D soil cores from the Micromodel Lab at IIT Delhi were used to study PPCP migration, revealing limited horizontal and vertical movement, particularly for ETM, due to its strong sorption. These findings enhance the understanding of PPCP behaviour in subsurface systems, supporting the development of more effective environmental management strategies. Future research should aim to validate numerical models with larger-scale field experiments and broaden the scope to include additional contaminants.