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Mathematical modelling of NSAIDs transport and degradation in an urban river using an advection–dispersion framework

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Abstract:

Pharmaceutical contamination in aquatic environments has emerged as a global environmental concern due to the persistence and ecotoxicological effects of active pharmaceutical ingredients, particularly non-steroidal anti-inflammatory drugs (NSAIDs) such as, ibuprofen, ketoprofen and diclofenac. This study develops and applies a one-dimensional advection–dispersion–degradation model to simulate the transport and transformation of these compounds in the Murray Burn, a small urban river in Scotland. Rhodamine WT experimental data from tracer experiments were used to calibrate water velocity and dispersion coefficients with the help of an optimization algorithm using multiple MATLAB optimization functions, with fminsearch demonstrating the most consistent performance. The degradation of NSAIDs was then integrated using literature-based first-order rate constants under different environmental scenarios (e.g., aerobic sediment, hyporheic exchange, and low light conditions). Simulation results highlight compound-specific behaviour: ibuprofen degraded rapidly under aerobic conditions, ketoprofen showed intermediate persistence, and diclofenac remained poorly biodegradable. This approach provides insights into how hydrodynamics and chemical degradation jointly affect pollutant fate and demonstrates the importance of compound-specific modelling for environmental risk assessment. The developed model framework will be further applied for the Someș River in Romania, and may be applied to other rivers as well, as it offers a valuable tool for supporting pharmaceutical pollution mitigation strategies under the EU Water Framework Directive.

Keywords:

Non-steroidal anti-inflammatory drugs (NSAID), river water quality, transport and transformations in rivers; advection-dispersion model, water quality modelling.

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