Coupling of water quality and toxicokinetic models to evaluate the exposure dynamics of wastewater-derived compounds

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INTRODUCTION

The use of modeling techniques in exposure science is increasingly recommended for predictive assessments and to supplement costly chemical and bioanalytical studies. Recently, there has been a strong push in predicting exposure that quantifies the contaminant concentrations in the receiving environment and also predicts the dynamics in exposed organisms [1].

STUDY OBJECTIVE

To demonstrate the utility of the coupled environmental compartment and toxicokinetic models in describing the temporal dynamics of contaminant exposure at sites previously determined to be heavily impacted by wastewater-derived compounds (pesticides and pharmaceuticals) [2].

MODELLING APPROACH

1. FORMULATE RIVER MODEL

Represent the river system as a single-compartment, 1st order ordinary differential equation (ODE, Eqn. 1). Test if the steady-state simplification is appropriate (i.e., dilution model, Eqn. 2).

**Wastewater Effluent**

\[ \frac{dC}{dt} = Q_e C_e - Q_w C_w \]

**RECIVING ENVIRONMENT**

\[ \frac{dC}{dt} = Q_l C_l + Q_r C_r - \alpha C \]

\( C_e \): downstream river concentration
\( C_w \): wastewater effluent concentration
\( C_u \): upstream river concentration
\( Q_e \): volume of the compartment
\( Q_l \): upstream river flow
\( Q_w \): wastewater outflow
\( Q_r \): instream river flow
\( \alpha \): degradation constant

2. FORMULATE TK MODEL

Since there were no daily effluent concentration, Monte Carlo Simulation was employed to approximate the concentrations at the effluent.

**Monte Carlo Simulation Results**

Forty-five compounds were modelled using the TK model (1st order ODE, Eqn. 3). Use gammadins as model species.

**Preparatory Work**

- All parts were coded in SAGE (Python based programming software).
- 36 of the 57 priority pollutants were modelled, see [2].
- 8 of 10 sites previously investigated in [3] were modelled.

3. FORMULATE CONCLUSIONS

This modeling work coherently describes the chemical exposure dynamics from the source to non-target organisms. We have obtained satisfactory results which demonstrates the utility of models when assessing the exposure of aquatic invertebrates to wastewater-derived chemicals. Model limitations exist (input data availability) which greatly influences the model outcomes.

**REFERENCES**