SPATIALLY EXPLICIT RIVER CATCHMENT MODELLING OF DECAMETHYLCYCLOPENTASILOXANE

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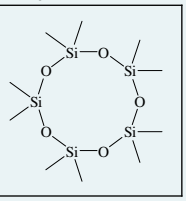
INTRODUCTION

• Decamethylcyclopentasiloxane (D_5) belongs to a group of chemicals known as cyclic volatile methyl siloxanes (cVMS).

• It is used in a wide range of applications including personal care products, such as skin creams, antiperspirants and hair care products.

Table 1: Summary of physico-chemical properties of D_5

Log K_{OW}	8.03
Log K_{OA}	5.06
Hydrolysis half-life (days at 9°C)	64 d (pH 8) 449 d (pH 7)
Log K_{OC}	4.4 to 6.6
Water Solubility (µg L^{-1} at 23°C)	17
Vapour Pressure (Pa at 25°C)	33.2



• Properties of D_5 suggest it is both highly volatile, hydrophobic and persistent in water/sediment environments.

• Regulatory assessments using EUSES indicate concentrations in surface waters (PEC_{local} = 330 ng L^{-1}; $PEC_{regional}$ = 100 ng L^{-1}) that exceed measured concentrations in surface water (30 ng L^{-1}) and Sewage Treatment Plant (STP) effluent (30 to 400 ng L^{-1}).

• The discrepancy between modelling and measured concentrations of D_5 in two river catchments (Great Ouse and Nene) in the UK is further investigated using LF2000-WQX, a GIS water quality model.

MATERIALS & METHODS

• LF2000-WQX provides spatial and temporal variations in chemical concentrations of down-the-drain chemicals.

• It combines a GIS hydrological model with information on STP locations, populations feeding STPs, dry weather flow.

• Distributions describing chemical usage (*PCC*), removal efficiency in STP (*F*) are combined to estimate concentration of chemical in STP effluent (C_{eff}).

• The concentration in the river (C_{sim}) are calculated as C_{eff} diluted by volume of river.

• Concentrations downstream of discharges are calculated assuming a single first order (SFO) dissipation rate.

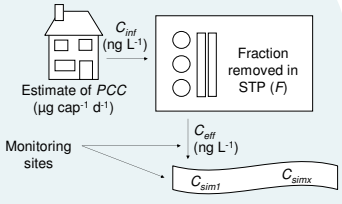


Figure 1: Schematic of chemical entry

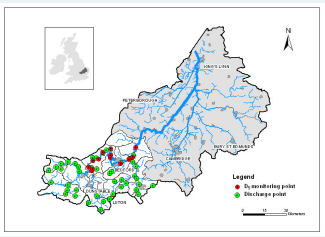


Figure 2: Great Ouse simulated region

• Estimates of *PCC* for D_5 based on the assumption that 10% of total tonnage used in personal care products enters wastewater (11.6 mg $capita^{-1}$ day^{-1}).

• STP removal fraction predicted to be 0.952 using SimpleTreat; three rates used in this study (0.92, 0.95 and 0.98).

• Estimated volatilisation rate (0.41 d^{-1}), sedimentation rate (0.0067 d^{-1}) and hydrolysis rate (0.0015 d^{-1}) were used to guide the selection of five SFO dissipation rates (0.1, 0.2, 0.4, 0.6 and 0.8) for use in LF2000-WQX simulations.

RESULTS & DISCUSSION

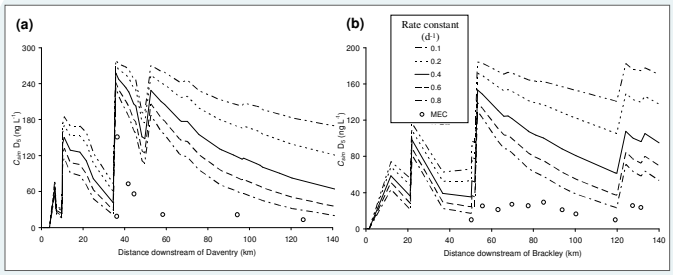


Figure 3: Concentrations of D_5 in (a) the river Nene and (b) the river Great Ouse assuming 98% removal in STP

• LF2000-WQX simulations conducted using estimates of C_{eff} (based on *PCC* and *F*) resulted in average C_{sim} values an order of magnitude greater than measured concentrations.

• LF2000-WQX simulations assuming 0.98 removal and using average river flow volumes resulted in C_{sim} values downstream of STPs that over predicted in-river concentrations, but were similar to EUSES predictions (Figure 3).

• LF2000-WQX simulations using measured effluent concentrations resulted in more accurate estimates of C_{sim} (Figure 4).

• Slower dissipation rates for D_5 fit the observed data better in the Great Ouse, however the dissipation of D_5 is more rapid in the river Nene.

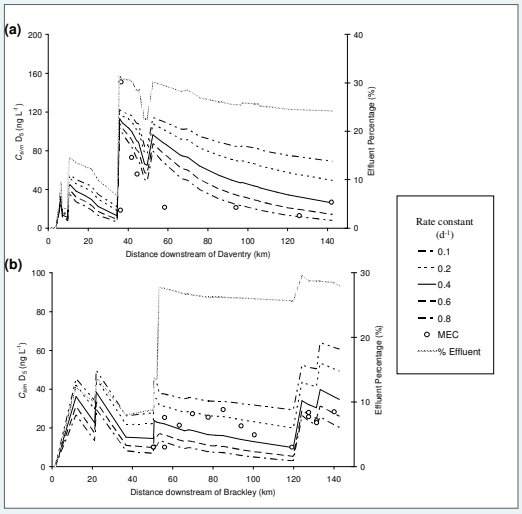


Figure 4: Concentrations of D_5 in (a) the river Nene and (b) the river Great Ouse using measured effluent concentrations

CONCLUSIONS

• Estimates of *PCC* and removal rates in STP for D_5 used in exposure assessments made by EUSES and LF2000-WQX (PEC_{local} and $PEC_{initial}$) resulted in predicted in-river concentrations that exceeded measured concentrations;

• $PEC_{regional}$ predicted by EUSES significantly overestimate D_5 exposure in surface waters;

• LF2000-WQX was able to give good estimates of the spatial and temporal distribution of D5 concentrations in two UK catchments using measured effluent concentrations from two STPs;

• The dissipation rate of D_5 in the water column of rivers is variable and a function of a rivers morphology, which may influence observed volatilisation and sedimentation rates.