SPATIALLY EXPLICIT RIVER CATCHMENT MODELLING OF DECAMETHYLCYCLOPENTASILOXANE

Oliver R. Price†, Richard J. Williams‡, Zhong Zhang‡, Roger van Egmond†
†SEAC, Unilever Colworth Laboratory, Sharnbrook, Bedfordshire, MK44 1LQ, UK
‡Centre of Ecology and Hydrology, Crowmarsh Gifford, Wallingford, Oxfordshire, OX10 8BB, UK

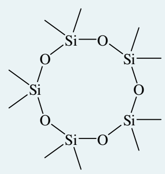
INTRODUCTION

• 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℃)	64 d (pH 8) 449 d (pH 7)
Log K_{OC}	4.4 to 6.6
Water Solubility (μg L^{-1} at 23℃)	17
Vapour Pressure (Pa at 25℃)	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.

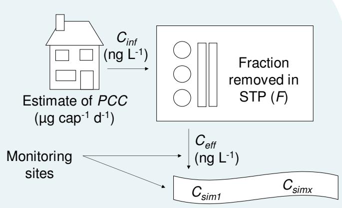


Figure 1: Schematic of chemical entry

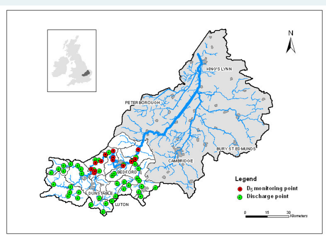


Figure 2: Great Ouse simulated region

• 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

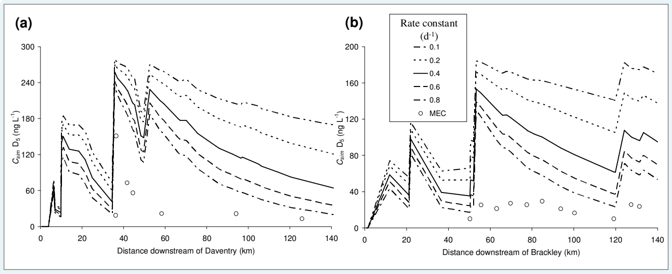


Figure 3: Concentrations of D_5 in (a) the river Nene and (b) the river Great Ouse assuming 98% removal in STP

• 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.

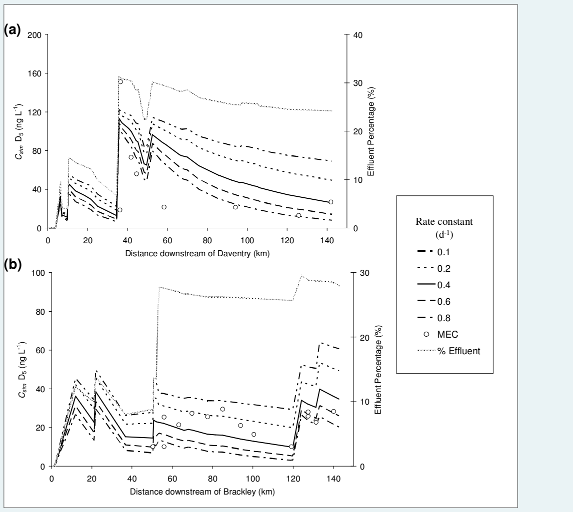


Figure 4: Concentrations of D_5 in (a) the river Nene and (b) the river Great Ouse using measured effluent concentrations

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.