Biotransformation kinetics and sorption of cocaine and its metabolites and the factors influencing their estimation in wastewater - DTU Orbit (15/01/2019)

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The quantitative analysis of human urinary metabolites as biomarkers in wastewater streams has been used to estimate the rates of illicit drug use in the wider community. The primary underlying assumption in such studies is that a sample of wastewater is equivalent to a cumulative sample of urine. Drug metabolism in humans is predominantly enzymatically mediated, but these processes are not exclusive to the human body, and are found to occur in the environment and the sewer network. Understanding what happens to drugs and their urinary metabolites in the sewer system between the point of excretion and sampling is particularly important since it is possible that in-sewer transformation may influence final biomarker concentration. The present study uses batch experiments to measure and assess the biotransformation processes of cocaine and its two major human metabolites, benzoylecgonine and ecgonine methyl ester. The activated sludge modelling framework for xenobiotic organic micro-pollutants (ASM-X) is used for model structure identification and calibration. Biotransformation was observed to follow pseudo first-order kinetics. The biodegradation kinetics of cocaine, benzoylecgonine and ecgonine methyl ester is not significantly affected by the availability of dissolved oxygen. Results obtained in this study show that omitting in-pipe biotransformation affects the accuracy of back-calculated cocaine use estimates. This varies markedly depending on the in-sewer hydraulic retention time, total biomass concentration and the relative concentration of each metabolite. However, back-calculated cocaine use estimates derived from wastewater concentrations of benzoylecgonine and ecgonine methyl ester do show very close agreement if ex-vivo biotransformation of these compounds is considered.

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