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Generation of synthetic influent data to perform (micro)pollutant wastewater treatment modelling studies

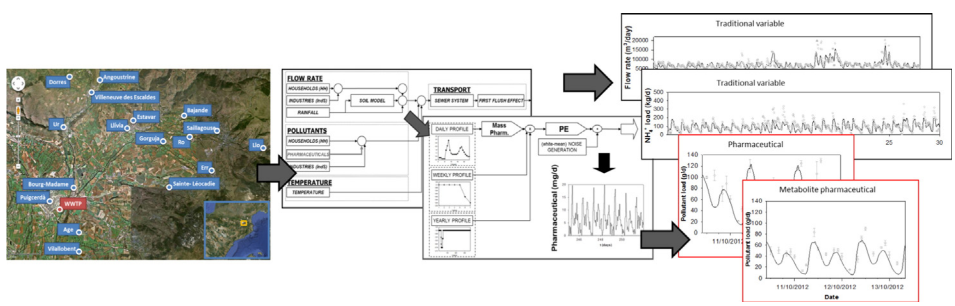
L.J.P. Snip [a], X. Flores-Alsina [a], I. Aymerich [b], S. Rodríguez-Mozaz [b], D. Barceló [b,c], B.G. Plósz [d], Ll. Corominas [b], I. Rodriguez-Roda [b,e], U. Jeppsson [f], K.V. Gernaey [a,*]

[a] CAPEC-PROCESS Research Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229, DK-2800 Kgs. Lyngby, Denmark
[b] ICRA, Catalan Institute for Water Research, Scientific and Technological Park of the University of Girona, Emili Grahit, 101, E-17003 Girona, Spain
[c] Water and Soil Quality Research Group, Department of Environmental Chemistry, IDAEA-CSIC, Jordi Girona 18-26, 08034 Barcelona, Spain
[d] Urban Water Engineering (UWE) Section, Department of Environmental Engineering, Technical University of Denmark, Building 115, DK-2800 Kgs. Lyngby, Denmark
[e] LEQUIA, Institute of the Environment, University of Girona, E17071 Girona, Spain
[f] Division of Industrial Electrical Engineering and Automation (IEA), Department of Biomedical Engineering (BME), Lund University, Box 118, SE-221 00 Lund, Sweden

HIGHLIGHTS

- The feasibility of a phenomenological influent generator model is demonstrated.
- The influent model can describe the dynamics of traditional variables as well as pharmaceuticals.
- The influent generator can effectively extrapolate time series.
- The importance of in-sewer biotransformation is shown when estimating consumption loads of drugs.

GRAPHICAL ABSTRACT



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ABSTRACT

The use of process models to simulate the fate of micropollutants in wastewater treatment plants is constantly growing. However, due to the high workload and cost of measuring campaigns, many simulation studies lack sufficiently long time series representing realistic wastewater influent dynamics. In this paper, the feasibility of the Benchmark Simulation Model No. 2 (BSM2) influent generator is tested to create realistic dynamic influent (micro)pollutant disturbance scenarios. The presented set of models is adjusted to describe the occurrence of three pharmaceutical compounds and one of each of its metabolites with samples taken every 2–4 h: the anti-inflammatory drug ibuprofen (*IBU*), the antibiotic sulfamethoxazole (*SMX*) and the psychoactive carbamazepine (*CMZ*). Information about type of excretion and total consumption rates forms the basis for creating the data-defined profiles used to generate the dynamic time series. In addition, the traditional influent characteristics such as flow rate, ammonium, particulate chemical oxygen demand and temperature are also modelled using the same framework with high frequency data. The calibration is performed semi-automatically with two different methods depending on data availability. The 'traditional' variables are calibrated with the Bootstrap method while the pharmaceutical loads are estimated with a least squares approach. The simulation results demonstrate that the BSM2 influent generator can describe the dynamics of both traditional variables and pharmaceuticals. Lastly, the study is complemented with: 1) the generation of longer time series for *IBU* following the same catchment principles; 2) the study of the impact of in-sewer *SMX* biotransformation when estimating the average daily

* Corresponding author at: CAPEC-PROCESS Research Center, DTU Chemical Engineering, Technical University of Denmark, Department of Chemical and Biochemical Engineering, Søltofts Plads, Building 227 (Postal address: Building 229), DK-2800 Kgs. Lyngby, Denmark.
E-mail address: kvg@kt.dtu.dk (K.V. Gernaey).

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load; and, 3) a critical discussion of the results, and the future opportunities of the presented approach balancing model structure/calibration procedure complexity versus predictive capabilities.

Nomenclature

A	Surface area of the variable volume tank, soil model block [m^2]
ASM	Activated Sludge Model
ASM1	Activated Sludge Model No. 1
ASM2	Activated Sludge Model No. 2
ASM2d	Activated Sludge Model No. 2d
ASM3	Activated Sludge Model No. 3
ASM-X	Activated Sludge Model for Xenobiotic trace chemical framework
BSM2	Benchmark Simulation Model No. 2
CMZ	Carbamazepine, antiepileptic drug
CMZ-2OH	Metabolite of carbamazepine, 2-hydroxy carbamazepine
$CMZ_{gperPEperd}$	Total average daily load of *CMZ* [g *CMZ*/(day·1000 PE)]
COD	Chemical Oxygen Demand [g COD/m^3]
CODpart	Particulate Chemical Oxygen Demand [g COD/m^3]
$CODpart_{gperPEperd}$	Total average daily load of *COD* particulates per day per PE [g *CODpart*/(day·PE)].
DS1	Long term dataset
DS2	Short term dataset
FFfraction	Fraction of suspended solids that can settle in the sewer, first flush effect model block [−]
G_{rain_Temp}	Proportional gain to adjust the temperature after a rain event, temperature model block [−]
HH	Households model block in influent generator
HRT	Hydraulic retention time [h]
IBU	Ibuprofen, non-steroidal anti-inflammatory compound
IBU-2OH	Metabolite of ibuprofen, 2-hydroxyibuprofen
$IBU_{gperPEperd}$	Total average daily load of IBU per day per 1000 PE [g IBU/(day·1000 PE)]
$IBU\text{-}2OH_{gperPEperd}$	Total average daily load of *IBU-2OH* per day per 1000 PE [g *IBU-2OH*/(day·1000 PE)].
IndS	Industry model block in influent generator
K_D	Solid-water distribution coefficient [L/g SS]
K_{down}	Gain for adjusting the flow rate to downstream aquifers, soil model block [m^2/d]
K_{inf}	Infiltration gain, soil model block [$m^{2.5}$/d]
M_{max}	Maximum mass of stored sediment in the sewer system, first flush effect model block [kg]
NH_4^+	Ammonium concentration [g N/m^3]
$NH4_{gperPEperd}$	Total average daily load of ammonium per day per PE [g NH_4–N/(day·PE)]
PE	Person equivalent
Q_{lim}	Flow rate limit triggering a first flush effect, first flush effect model block [m^3/d]
Qpermm	Flow rate per mm rain [m^3/mm]
QperPE	Wastewater flow rate per person equivalent [m^3/d]
SMX	Sulfamethoxazole, antibiotic drug
SMX-N4	Metabolite of sulfamethoxazole, N4-acetyl-sulfamethoxazole
$SMX_{gperPEperd}$	Total average daily load of *SMX* [g *SMX*/(day·1000 PE)]
Subarea	A parameter that forms a measure of the size of the catchment area. It will determine the number of variable volume tanks in series that will be used for describing the sewer system, sewer model block [−]
T	Temperature [°C]
T_{Bias}	Seasonal temperature variation, average, temperature model block [°C]
T_{dAmp}	Daily temperature variation, amplitude, temperature model block [°C]
WWTP	Wastewater treatment plant

1. Introduction

It has been >25 years since the publication of the Activated Sludge Model No. 1 (ASM1) (Henze et al. 1987). The ASM1 describes organic carbon and nitrogen removal processes in activated sludge systems and has been successfully applied to a large number of wastewater treatment plants (WWTPs). The successful results obtained in the early years have resulted in the further expansion of the number of phenomena included in activated sludge models (ASMs), e.g. by including the description of bacterial storage, 2-step nitrification, 4-step denitrification and phosphorus removal. In this way, ASM1 evolved to ASM2, ASM2d and finally ASM3 as well as many other versions of ASM inspired models. As a consequence, the use of ASMs (Henze et al. 2000) is constantly growing and practitioners in both industry and academia are increasingly applying these tools when performing WWTP engineering studies. Numerous publications demonstrate the usefulness of ASMs for benchmarking (Copp 2002; Jeppsson et al. 2007; Gernaey et al. 2014), diagnosis (Rodriguez-Roda et al. 2002; Olsson 2012), design (Flores et al. 2007; Rieger et al. 2012), teaching (Hug et al. 2009) and optimization (Rivas et al. 2008) of WWTPs.

The potential adverse effects of xenobiotics in aquatic environments (e.g. Ternes 1998) have promoted a substantial amount of research regarding the extension of ASMs to describe micropollutants (Clouzot et al. 2013; Plósz et al. 2013b). By micropollutants we mean compounds such as pharmaceuticals, personal care products, and biocides which are found in the environment in low concentrations (μg/L or ng/L). In many cases, these pollutants can pose a significant risk to the environment and human health. On aquatic life, such adverse effects can be characterized as spread and maintenance of antibacterial resistance (Baquero et al. 2008), sex reversal and/or intersexuality (Lange et al. 2009) or reduction of the reproductive behaviour (Coe et al. 2008).

Most models describing the fate of micropollutants in a WWTP include among others: volatilization (Lee et al. 1998), sorption/desorption (Joss et al. 2006; Lindblom et al. 2009), and biotransformation (Plósz et al. 2010; Suarez et al. 2010; Delgadillo-Mirquez et al. 2011). These models are used as decision support tools to help understand the underlying mechanisms of micropollutant fate in the WWTP, and thus they provide a prediction of the efficiency of different treatment technologies (Lindblom et al. 2006; Snip et al. 2014; Vezzaro et al. 2014).

In essence, the performance of WWTP modelling studies depends heavily on the availability of influent time series as these are the main disturbance of a typical WWTP (Rieger et al. 2012). These influent time series should represent the inherent natural variability of the traditional and/or micropollutant dynamics as accurately as possible (Ráduly et al. 2007). However, obtaining sufficiently long and qualitatively