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Generation of synthetic influent data for performing (micro) pollutant wastewater treatment modelling studies

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1. INTRODUCTION / OBJECTIVES

The use of Activated Sludge Models (ASM) (**Henze *et al.*, 2000**) is constantly growing and both industry and academia are increasingly applying these tools when performing wastewater treatment plant (WWTP) engineering studies. Besides describing the behaviour of traditional pollutants such as organic carbon (C), nitrogen(N) and phosphorus(P), ASM models have been successfully upgraded to predict the fate of different types of micro-pollutants (**Benedetti *et al*., 2013**). Indeed, the potential adverse effects of micro-pollutants in aquatic environments have been an object of intensive research during the last years (e.g. **Ferrari *et al.*, 2003**). However, due to the time and the high cost of measuring campaigns, many simulation studies of full-scale Wastewater Treatment Plants (WWTPs) suffer from a lack of sufficiently long and detailed time series representing realistic wastewater influent dynamics (**Gernaey *et al*., 2011**). This is an important point since realistic data representing the influent wastewater dynamics are crucial to accomplish any WWTP modelling project (**Rieger et al., 2012**). For this reason, model-based influent generators/synthetic data are an alternative that has recently gained considerable interest (**Flores-Alsina *et al*., 2014**, **Martin and Vanrolleghem 2014**).

The objective of this paper is to show the usefulness of model based influent generators to reproduce (micro) pollutant influent characteristics when performing WWTP modelling studies. Using a 30000 PE WWTP as a case base, three different types of pharmaceuticals (antibiotic, anti-inflammatory, model stabilizer) are the selected micro-pollutant to run the study. In addition, the paper is complemented describing the influent variation of flow-rate(Q), traditional pollutants (COD, N, P) and temperature (T). Two different data sets (short/long term) are used to calibrate the different model blocks comprising the influent generator. Preliminary simulation results show that the generated synthetic data follows the same pollutant/micro-pollutant dynamics. In addition, uncertainty in the assumed loads/natural stochasticity is assessed using the Monte Carlo simulation technique. The paper will be complemented with a scenario analysis demonstrating how additional influent characterises (following the same catchment) principles could be generated without the need to run (expensive) additional experimental campaigns.

2. METHODS

2.1. Compounds under study

In this paper the occurrence of a particular type of micro-pollutant (pharmaceuticals) is described using a model-based influent generator. These pharmaceuticals are one antibiotic; sulfamethoxazole (SMX), one non-steroidal anti-inflammatory compound; one non-steroidal anti-inflammatory compound; diclofenac (DCF) and one mood stabilising drug; carbamazepine (CMZ). Antibiotics are used to treat infections; DCF is used to reduce inflammation and as an analgesic reducing pain in certain conditions and CMZ is used primarily in the treatment of epilepsy and bipolar disorder, as well as trigeminal neuralgia. In addition, the study is complemented by describing the dynamics of flow-rate (Q), traditional pollutants (COD/N) and temperature (T)

2.2. WWTP under study and sampling campaign.

The wastewater treatment plant under study (*WWTP1*) is located in the North-East of Spain. The plant was constructed for a design capacity of 30000 Population Equivalent (PE). *WWTP1* has a high/low seasonal variation with an average flow (4100 / 8300 $m^3.hour^{-1}$) and an organic / nitrogen load of (595 / 1785 kg $BOD.day^{-1}$) and (123 / 349 kg $N.day^{-1}$) respectively. The catchment are under study is sparsely distributed (Area XXX) and covers urban (Spain / France) and agriculture areas. Nevertheless the major flow/loading contribution (30%) comes from medium village nearby (distance XXX)A data set comprising two (short/long) measuring campaigns is used for the case study. The short term data set comprises an intensive 3-day measuring campaign (8/10/2012 at 7am to 11/10/2012 at 7am). Samples were taken at the influent of WWTP1 to analyze (off-line) organic matter (COD), nutrients (nitrogen and phosphorus) and pharmaceutical products (12 parental compounds with their metabolites). Also, SCAN sensors were installed to get online data from organic matter (spectrolyzer) and nitrogen (ammolyzer) at 1 minute interval. 8/10/2012 at 7 AM to 11/10/2012 at 7 AM). The long term experimental campaign data only contains online measurements during the entire October 2012.

2.3. *Micro-pollutant model based influent generator*

The modelling approach proposed by **Gernaey et al. (2011),** which generates influent pollutant disturbance scenarios, is upgraded to describe pharmaceuticals according to the principles stated in **Snip et al., 2014.** (see **Fig1**)

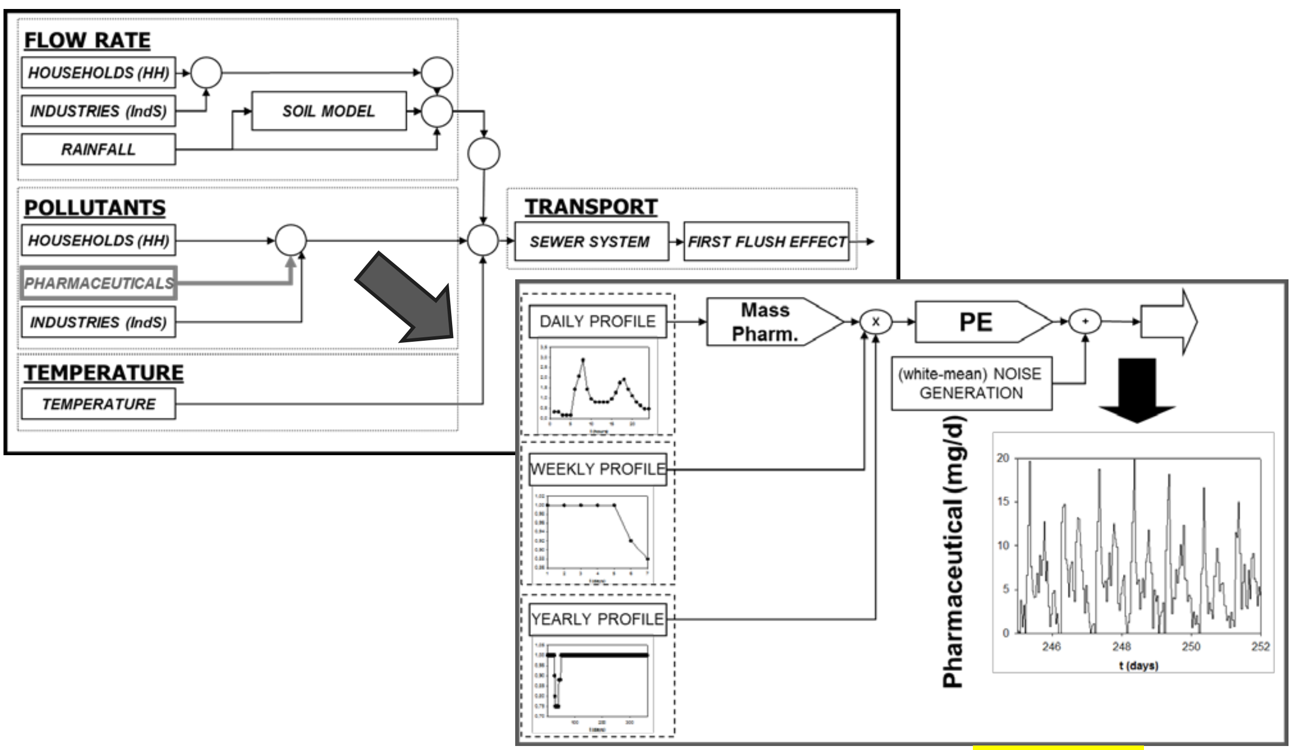


Figure 1. Model blocks to create the different pharmaceutical loading profiles [new schematics]

Daily, weekly and seasonal influent dynamics of micro-pollutants are generated based on user-defined pollutant flux profiles (and are strongly compound dependant). The basis of these user defined profiles are administration patterns, bioavailability, half-time and total annual consumption rates. The pollutant fluxes are transformed into $g.PE^{-1}$ (Person Equivalent), by multiplying the values in the input files – containing normalised information on the dynamics – with their loads (normally given in mg/(day.1000 PE)) and with *PE*, the number of person equivalents in the catchment area. Zero-mean white noise can be added to give more realism to the generated series using the noise variance as a tuning parameter (see **Fig1**)

3. PRELIMINARY RESULTS

Preliminary results show that the influent generator allows reproducing the daily variation of the influent nitrogen concentration data of *WWTP1* for the period comprising October 2012. As can be seen in **Fig2,** there is a daily flow rate profile that is repeated. Default user defined profiles for *HH* contribution are assumed. These profiles represent a general behaviour, namely one morning peak, one evening peak, and late night and mid-day minima. The morning and the evening peaks represent the residents going to or returning from work. The late night minimum flow rate corresponds to the sleeping hours with little water consumption. Finally, the daytime flow rate shows a small decline corresponding to the residents' working hours (**Gernaey et al., 2011**). The adjusted *SNH_gperPEperd* in the *HH* block is XXXX. *IndS* contribution was considered negligible and removed from the model. The sewer length time parameter (*subarea*) is adjusted to match and the system´s hydraulic retention time of XXX hours.

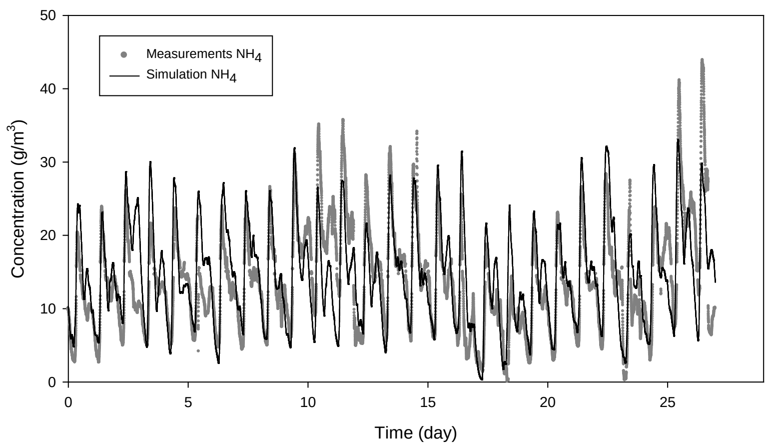
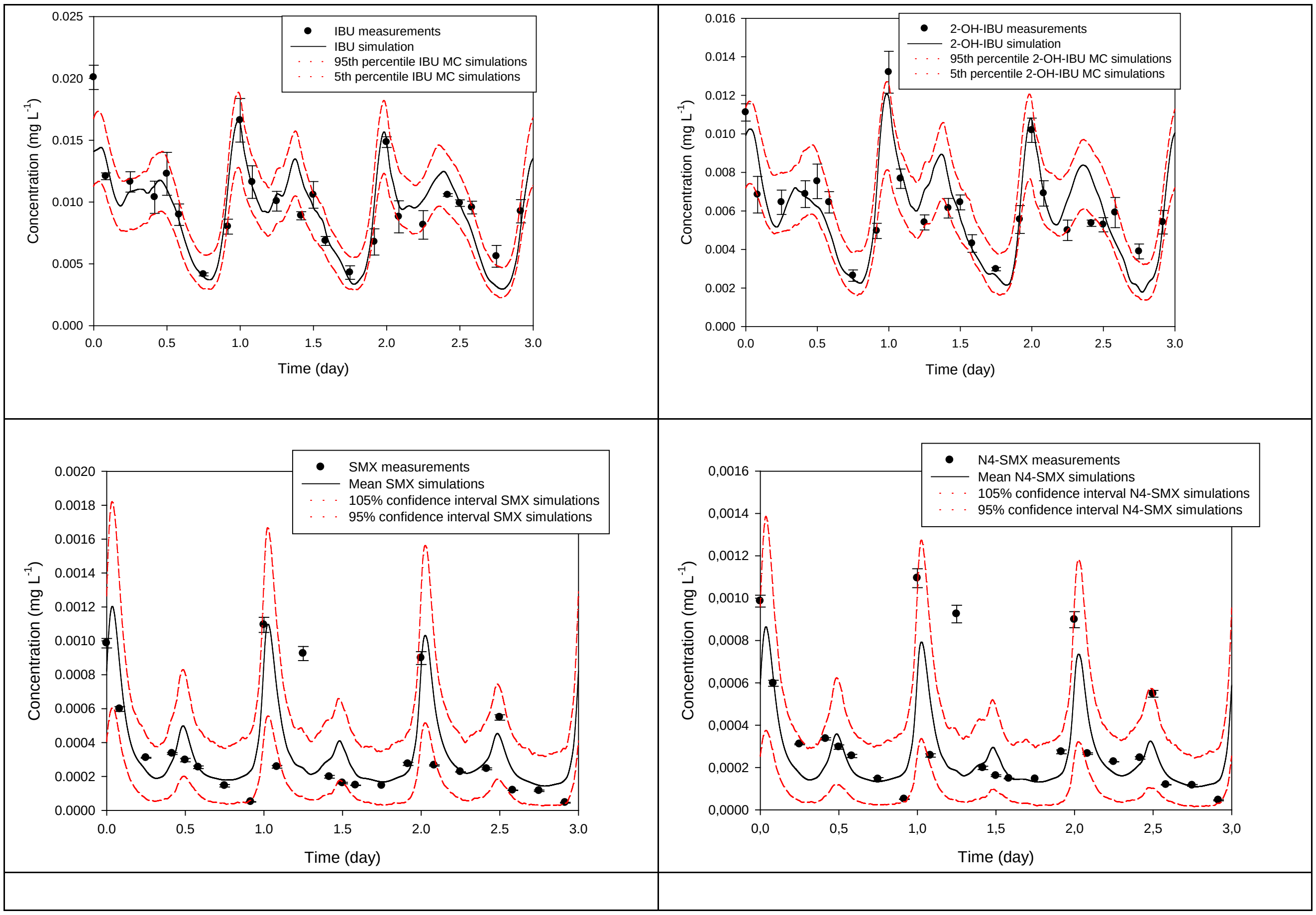


Figure1. Calibration of the influent ammonium at the inlet of WWTP1

Additional results show that proposed approach successfully describes the occurrence of the three selected compounds (and their metabolites). IBU and SMX present a high correlation with ammonium, which clearly indicates the impact of human urine (see **Fig3 a,b,c,d**). With a half-life of 10 h in the human body and a typically prescribed oral administration of twice a day, these findings correspond well with the theoretically expected distribution pattern (**Gobel et al., 2005**). The estimated total pollution loads are XXXX for IBU and XXX for SMX. It is important to highlight that to correctly describe the dynamics of SMX the parameter *subarea* had to be reduced. The authors find two possible explanations to this situation. First of all, one must notice that SMX is several orders of magnitude lower than IBU and consequently more sensitive to error in sampling method (toilet flushes were missing) (**Ort and Gujer, 2006**). Secondly, and due to the catchment distribution (see description above), the authors assume that most of the compound is consumed in the closest urban area (shorter hydraulic residence time). Indeed, the sources of NH4 and IBU are higher and more probably with a widest geographical distribution. The last studied compound (CMZ) present high correlation rate with TSS (results not shown). This is attributed to the fact that CMZ is only 1 % in the urine and 28 % in the faeces (**Miao et al., 2005**). Estimated pollution load for CMZ is XXX (see **Figure 3 e,f**). [residuals analysis]

Simulation results are complemented with uncertainty analyses based on the Monte Caro technique. Uncertainty ranges in the model parameters were assumed (calibrated loads, noise parameters), sampled and propagated through to the model outputs. This analysis will show a clearer view of the possible errors / natural stochasticity. These values can be combined with the inclusion of other uncertainties like sampling, analytical method calculating flow rate and the analytical method can have a paramount impact on the results (**Lai et al., 2011; Mathieu et al., 2011; Vezzaro et al., 2012**).



The study will be complemented with a scenario analysis where the calibrated model will be used to generate different influent characteristics. Increase of the length of the micro-pollutant data series, modification of the sewer configuration or simply predicts the seasonality variation will be presented alongside.

4. OUTLOOK

The preliminary presented results showed the usefulness of model based influent generators. The presented approach is capable to reproduce the behaviour of traditional/ non-traditional blocks with a set of generic blocks and minimal calibration effort. The scenario analysis and the creation of additional influent disturbances will show the model possibilities. Indeed, the presented set of models will be able to reduce cost/ workload of measuring campaigns when performing (micro)pollutant WWTP modelling studies