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Publication date:
2015

Document Version
Peer reviewed version

Watermatex 2015
9th IWA Symposium on Systems Analysis and Integrated Assessment
11-14 June 2015, Gold Coast, Australia

Calibration and evaluation of predictive accuracy of a (micro)pollutant influent generator

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Keywords: Influent modelling; Quantitative evaluation; Xenobiotic trace chemicals

Summary of key findings

The Benchmark Simulation Model No. 2 influent generator upgraded with pharmaceutical occurrences is capable of reproducing both the long- and short-term dynamics of traditional variables as well as micropollutants. Several quantitative evaluation criteria are presented and used to assess the model's predictive capabilities and all show satisfactory results except for COD particulates. Ongoing research aims at improving this remaining issue.

Background and relevance

When performing wastewater treatment plant (WWTP) engineering studies, realistic data representing the influent dynamics are crucial (Rieger et al., 2012). This also applies when modelling micropollutants. However, due to the required time and costs of performing measuring campaigns, many simulation studies lack time series of adequate duration and quality. Therefore, influent generators are alternatives that have gained interest (Martin and Vanrolleghem, 2014).

In this study, the BSM2 influent generator (Gernaey et al., 2011) upgraded with pharmaceuticals (Snip et al., 2014) is used to produce dynamic influent characteristics of both 'traditional' variables and pharmaceuticals. The calibration is performed manually with high frequency data of a WWTP loaded for 16.000 population equivalent (PE) (**Figure A1**). Different quantitative evaluation methods are compared.

Results

Qualitative evaluation of calibration

A stepwise manual calibration procedure (Flores-Alsina et al., 2014) is used to adjust the most sensitive parameters (**Table A1**). By evaluating the calibration visually, it can be assumed that the model is capable of capturing dry weather dynamics (**Fig 1**). The morning peak, evening peak and late night and mid-day minima are well described for flow rate (**Fig 1a**), *COD* (Fig 1b) and NH_4^+ (**Fig 1c**). Also for temperature, daily variations are well described (**Fig 1d**). However, during wet weather there was rain data missing for additional peaks shown in the data of the flow rate (black line). In order to capture that rainfall, synthetic rainfall data was created (**Fig 1a**; grey line). Regarding the first flush effect, the model was able of capturing most. However, not all increases in particulates seem to have followed an increase in the flow rate and therefore were not captured by the model.

The calibration results of the pharmaceuticals can be seen in **Fig 2** and show that the generator can describe the daily variation. Even though ibuprofen (*IBU*) has an irregular administration pattern, a strong correlation with NH_4^+ was found, which indicates excretion via urine. The same correlation was found for sulfamethoxazole (*SMX*) and N-Acetyl Sulfamethazine-d4 (*SMX-N4*), however the length of the sewer had to be modified in order to describe the peaks. There are two possible explanations. Firstly, one must notice that *SMX* is considerably lower in load than *IBU* and therefore more sensitive to the error of sampling (Ort and Gujer, 2006). Secondly, we assume that the detected compound is consumed and excreted in an area close to the sampling point. Hence, the shorter residence time results in peak concentrations above the detection limits. Carbamazepine (*CMZ*) is correlated with

total suspended solids (*TSS*), due to the fact that *CMZ* is excreted only 1% in the urine and 28% in the faeces (Zhang et al., 2008). However, the metabolite 2-Hydroxy Carbamazepine (*CMZ-2OH*) is correlated with NH_4^+ and therefore two different profiles were used. The close link between *CMZ* and *TSS* dynamics could be associated with desorption in the sewer or filtering. Numerous studies report low sorption rates for *CMZ* in wastewater (e.g., Ternes et al., 2004).

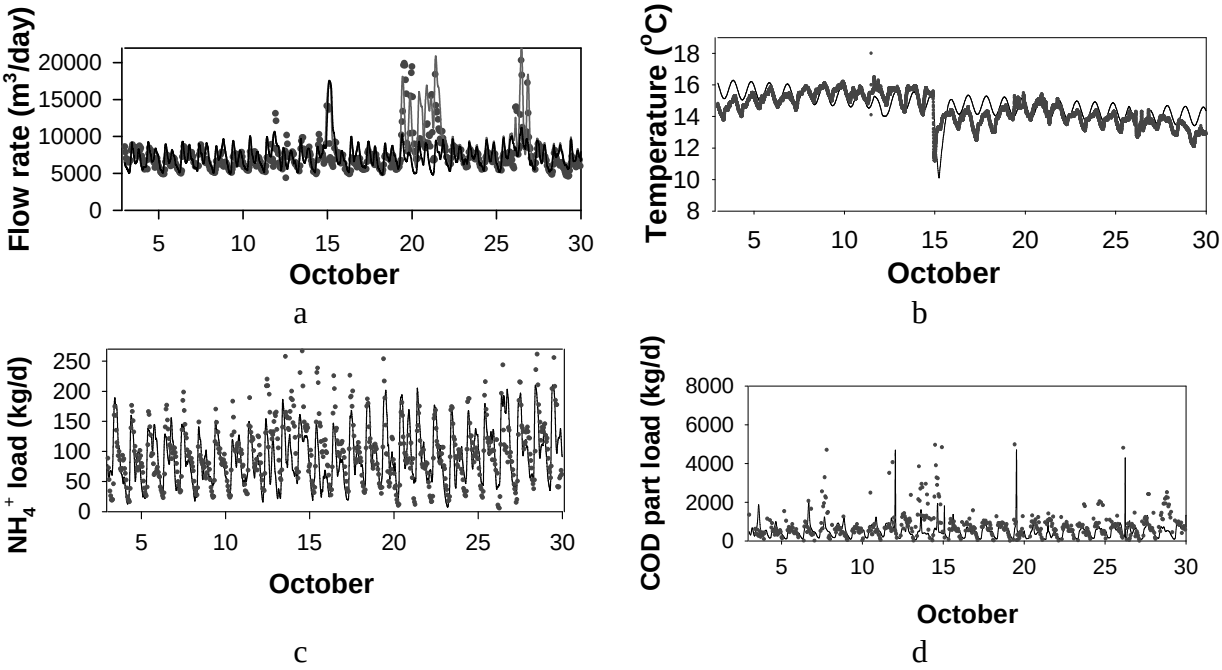

Figure 1. Comparison of the simulation results (black line) of flow rate (a), temperature (b), ammonia (c) and *COD* (d) with the measurements (grey dots). Synthetic rainfall data were created for the additional simulation of the flow rate (grey line).

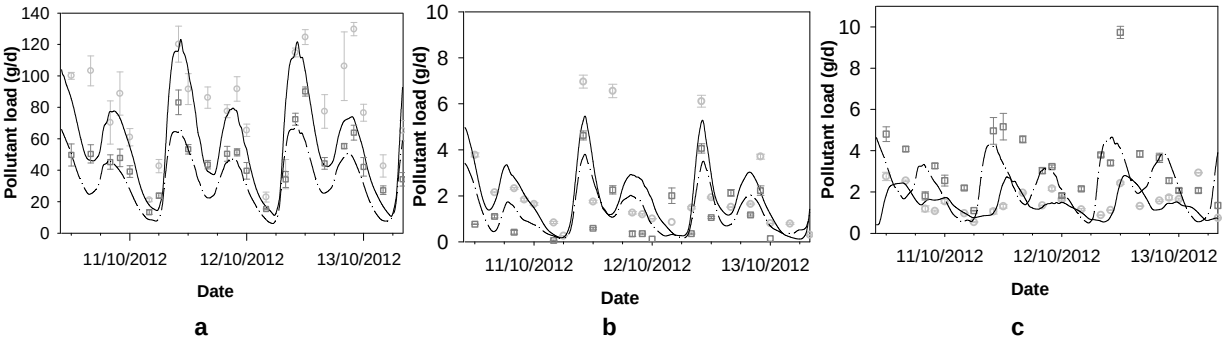

Figure 2. Simulations of influent *IBU* (black line) and metabolite *IBU-2OH* (line and dot) (a), *SMX* (black line) and metabolite *SMX-N4* (line and dot) (b), and *CMZ* (black line) and metabolite *CMZ-2OH* (line and dot) (c) and measurements with their standard deviation of the chemical analysis (dark grey dots.

Quantitative evaluation of calibration

The results of the quantitative evaluation can be found in **Table 1**, where the best and worst performances are presented in italics (calculations of criteria can be found in **Table A2**).

As *PDIFF* and *MSDE* are absolute criteria, the highest value for flow rate is expected. However, when comparing the relative criterion *PEP*, the magnitude of the simulated *SMX-N4* peaks differs the most compared with the observed peaks. As mentioned before, the sewer length was reduced for *SMX* and *SMX-N4* profiles and for *SMX-N4* the high peaks were still not captured. The best performance can be found for *CMZ*, which is also the compound with the most constant occurrence.

Regarding the absolute criteria, there seems to be little bias in the calibrations with respect to *ME*. However, it could be that negative and positive errors are cancelled out. Nevertheless, also *MSE* and *RMSE* show little bias.

About the relative criterion, the calibration of the temperature is the best, while the *COD* has the worst performance. One peculiarity (**Table 1, bold**) is the positive value for *ME* for NH_4^+, *COD* and *SMX-*

N4 while the *MPE* is negative. The positive *ME* is due to large positive errors at peak values, while overall negative errors are found (negative *MPE*).

Table 1. Quantitative evaluations of the BSM2 influent generator with high frequency data.

Quantitative method	Peak evaluation			Absolute criteria			Relative criterion		
Compound evaluated	*PDIFF*	*PEP*	*MSDE*	*ME*	*MAE*	*RMSE*	*MPE*	*IoAd*	*Corr*
NH_4^+	1.27	*0.60*	3.40	**1.83**	4.40	5.59	**-2.31**	0.60	0.71
CODpart	103.16	15.76	$9.15 \cdot 10^3$	**-21.64**	59.20	101.60	***107.86***	*-0.15*	0.33
Flow rate	*623.34*	3.42	$1.46 \cdot 10^6$	*181.5*	$1.07 \cdot 10^3$	$1.66 \cdot 10^3$	*0.12*	0.82	0.70
Temperature	0.16	0.94	0.37	-0.0084	0.4707	0.60	-0.15	0.78	*0.16*
IBU	$-7.76 \cdot 10^{-4}$	-9.02	$4.06 \cdot 10^{-5}$	$1.5 \cdot 10^{-3}$	$4.2 \cdot 10^{-3}$	$5.2 \cdot 10^{-3}$	7.41	0.71	0.50
IBU-2OH	$-6.34 \cdot 10^{-4}$	-11.85	$1.32 \cdot 10^{-5}$	$7.48 \cdot 10^{-4}$	$2.1 \cdot 10^{-3}$	$2.7 \cdot 10^{-3}$	9.47	0.77	0.62
SMX	$-2.27 \cdot 10^{-5}$	-6.43	$1.38 \cdot 10^{-7}$	$-5.27 \cdot 10^{-5}$	$1.57 \cdot 10^{-4}$	$2.24 \cdot 10^{-4}$	-71.58	0.84	*0.72*
SMX-N4	$2.23 \cdot 10^{-4}$	*-338.68*	$1.06 \cdot 10^{-7}$	$-1.03 \cdot 10^{-4}$	$1.89 \cdot 10^{-4}$	$2.91 \cdot 10^{-4}$	-78.16	*1.00*	*0.16*
CMZ	$-3.87 \cdot 10^{-4}$	-6.91	$1.31 \cdot 10^{-8}$	$\mathbf{-1.46 \cdot 10^{-5}}$	$6.39 \cdot 10^{-5}$	$9.06 \cdot 10^{-5}$	**0.63**	0.69	0.44
CMZ-2OH	$-3.50 \cdot 10^{-5}$	-8.38	$1.68 \cdot 10^{-7}$	$-7.04 \cdot 10^{-5}$	$2.17 \cdot 10^{-4}$	$2.84 \cdot 10^{-4}$	-3.17	0.51	0.26

The *IoAd* shows a fair fit only for flow rate, *SMX* and *SMX-N4*. Temperature performed the best for all relative criteria, however not for *IoAd*. The highest correlation between data and simulation is found in *SMX-N4*. It indicates that the trend of data was followed well, even though the magnitudes were not captured.

The *COD* particulates calibration scored low on many criteria and therefore other parameter values are chosen to compare the fit (**Table A3**). The relative criteria seem to worsen with the new parameters while the peak evaluation is improved. Therefore, there seems to be a trade-off between the relative error and the peak performance.

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Bio: Xavier Flores-Alsina joined the CAPEC PROCESS center at DTU as a Marie Curie Fellow in May 2013. He did his PhD between Spain, UK and Denmark. He worked as post doc in Canada, Sweden, Australia and South Africa. His field of expertise is modelling, control and benchmarking wastewater treatment systems.