

Uncertainty analysis of WWTP control strategies made feasible

Lorenzo Benedetti, Damien J. Batstone, Bernard De Baets, Ingmar Nopens and Peter A. Vanrolleghem

ABSTRACT

The control of wastewater treatment plants can help to achieve good effluent quality, in a complex, highly non-linear environment. A key but time-demanding component of such modelling studies is uncertainty analysis (UA). The general aims of this paper are (a) to evaluate methods for reduction of the time necessary to conduct an UA, and (b) to evaluate the sensitivity of parameters and model subsystems. Two UA studies on the Benchmark Simulation Model no. 2 (BSM2) are used to illustrate how the above mentioned aims can be achieved: (1) robustness of performance evaluations against changing operation and design conditions; and (2) uncertainty of performance evaluations for a given plant layout and operation. The main conclusions are: (1) solver settings have a large impact on simulation speed and require proper attention; (2) to reach convergence in Monte Carlo simulations with Latin Hypercube Sampling, the number of simulations should be at least 50 times the number of sampled parameters, which is more than what is reported in similar studies; and (3) the number of uncertain parameters that needs to be considered to make a proper uncertainty assessment of a model can be reduced significantly by omitting parameters that have little influence.

Key words | activated sludge, anaerobic digestion, BSM2, global sensitivity analysis, mathematical modelling, numerical methods

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INTRODUCTION

The biological, physical and chemical phenomena taking place in activated sludge (AS) systems are complex, closely interrelated and highly non-linear. Moreover, the operation of these systems should continuously meet effluent requirements, preferably at the lowest possible operational cost. In order to achieve this, control of such plants can be very helpful but, given its complexity, this is not an easy task. Operators are often reluctant to test new control strategies on the real plant because of their possibly unexpected behaviour.

Initiated in the 1990s, the Benchmark Simulation Model no. 1 (BSM1) was proposed as a tool to foster the dissemination of control and monitoring strategies (Spanjers *et al.* 1998). This benchmark is a simulation environment defining a plant layout, simulation models for all process units,

influent loads, test procedures and evaluation criteria. For each of these items, compromises were made to match model simplicity with realism and accepted standards. Once the user has verified the simulation code, any control strategy can be applied and the performance can be evaluated according to a well-defined set of criteria (Stare *et al.* 2007). Recently, the Benchmark Simulation Model no. 2 (BSM2) (Jeppsson *et al.* 2007; Nopens *et al.* 2010) was developed for plant-wide wastewater treatment plant (WWTP) control strategy evaluation on a long-term basis, with a much more complex plant model. It consists of a pre-treatment process, an AS process and sludge treatment processes.

One of the main and often neglected aspects of modelling – and therefore of the evaluations done and decisions made by using models – is the uncertainty associated with

the model predictions (Belia *et al.* 2009). In order to make informed decisions, such uncertainty should be made explicit by transparently using an uncertainty analysis (UA) method. The reasons to include UA in a WWTP (control) study may include the assessment of: (1) the robustness of the performance of a control strategy against deviating operation and design (OD) parameters (Vanrolleghem & Gillot 2002), i.e. the transferability of a control strategy to different plants or operating conditions; (2) the importance of uncertainty in a multi-criteria evaluation of control strategies (Flores-Alsina *et al.* 2008); (3) the probability of exceeding a legal effluent standard (Rousseau *et al.* 2001); and (4) process variability in WWTP design and upgrade options (Sin *et al.* 2009; Benedetti *et al.* 2010b). In many cases the uncertainty bounds for outcomes of interest are larger than the differences between the expected values of the outcomes for different alternatives (see Figure 1). Nevertheless, it is still possible to discriminate between such alternatives (Reichert & Borsuk 2005).

The main aims of this paper are: (1) to facilitate application of UA studies with the BSM2 – given the constraints introduced by the BSM2, i.e. a fixed model structure, a fixed influent time-series and some fixed parameters – by providing useful suggestions on how to reduce the time spent to finalise the analysis; and (2) to provide general methods to achieve such reduction that can be applied to other WWTP modelling studies.

Two UA applications are presented: (1) a global sensitivity analysis (GSA) to identify the most important parameters (including operational and design parameters), used to assess the transferability of strategies to other WWTPs (referred to as robustness study); and (2) a GSA

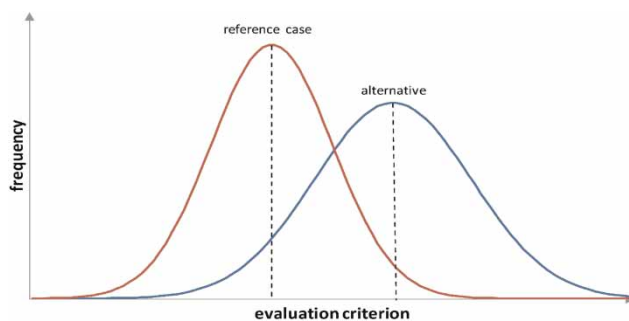


Figure 1 | Typical case of frequency distributions for the evaluation criterion of two scenarios.

to identify the model parameters that mostly influence the output uncertainty having fixed the design and operation of the plant (referred to as uncertainty study). To perform the GSAs, the most commonly used method was adopted, i.e. Monte Carlo (MC) experiments, which consist of performing multiple simulations sampling the parameter values from probability density functions (PDFs), and applying linear regression on the results to quantify parameter impact on objective function outputs (Saltelli *et al.* 2000).

Given the heavy computational load generated by MC experiments – function of the time required by a single simulation times the number of simulations required, which is in turn function of the number of uncertain parameters – the first focus of the work was to reduce the computation time of a single simulation. Next, the method for ranking and selecting parameters according to their sensitivity in the two UA applications (robustness study and uncertainty study) was studied, including the search for the number of simulation runs sufficient to accept the results of the GSA.

METHODS

The model

The BSM2 protocol (Jeppsson *et al.* 2007; Nopens *et al.* 2010) consists of a complete model representing a typical AS WWTP with on-site sludge treatment (Figure 2), a benchmarking procedure and a set of evaluation criteria.

The main components of the plant model (see Figure 2) are: (1) primary clarification, based on Otterpohl & Freund (1992) and Otterpohl *et al.* (1994), 50% solids removal efficiency, no biological activity; (2) five-reactor nitrogen removal AS system, based on ASM1 (Henze *et al.* 1987) – the first two anoxic and the last three aerobic as default – with temperature dependency for the biological parameters; (3) secondary clarification, based on Takács *et al.* (1991), no biological activity; (4) gravity thickening, ideal and continuous process, 98% solids removal efficiency, no biological activity; (5) anaerobic digestion (AD), based on ADM1 (Batstone *et al.* 2002); (6) dewatering, ideal and continuous process, 98% solids removal efficiency, no biological activity; (7) AS/AD/AS model interfaces, based on

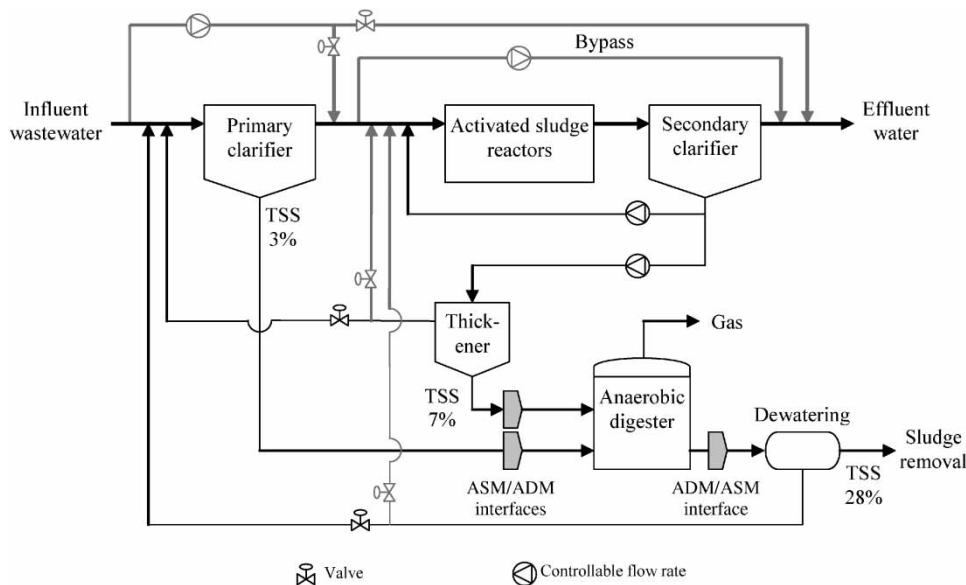


Figure 2 | Plant layout for BSM2 (from Nopens et al. 2010).

Nopens et al. (2009); (8) storage tank, continuous process, controllable output pumping capacity, no biological activity; and (9) influent wastewater characteristics, based on Ger-naey et al. (2006), 609-day dynamic influent data file (sampling frequency equal to a data point every 15 min) with daily dynamic temperature values.

The three model outputs, the uncertainty of which is being studied in this work, are the standard benchmark evaluation criteria: (1) the Effluent Quality Index (EQI), a weighted sum of effluent pollutant loads with weights set to 2 for biochemical oxygen demand (BOD), 1 for chemical oxygen demand (COD), 2 for total suspended solids (TSS), 30 for ammonium (NH_4) and 10 for nitrates (NO_3); (2) the Operating Cost Index (OCI) which takes into account energy consumption (aeration, pumping, mixing), external carbon addition, waste sludge production, heating of the digester and energy recovery from methane production (see Jeppsson et al. 2007; Nopens et al. 2010); and (3) the period of time in which the effluent exceeds the limit of $4 \text{ mg NH}_4\text{-N/l}$, expressed as a percentage of the whole evaluation period (52 weeks, the last 364 of the 609 simulated days).

If not otherwise specified, the BSM2 was used in this work in its open loop version, which means without any control strategy implemented.

Solver optimisation

The BSM2 has 265 derived state variables. In order to perform a GSA of such a complex model, potentially involving a very large number of MC simulations, optimisation of solver settings can dramatically reduce the overall simulation time.

The modelling and simulation software used in this work was WEST (Vanhooren et al. 2003; www.mikebydhi.com). The starting point for solving the model was the Runge–Kutta fourth order adaptive step-size (RK4ASC) solver (Forsythe et al. 1977). In general, advanced solvers such as the C initial value ordinary differential equation (CVODE) solver (Hindmarsh et al. 2005) often yield better performance than the more basic Runge–Kutta solver, but the performance of CVODE is highly dependent on solver settings, and inappropriate selection can result in poor performance (Claeys et al. 2010). However, CVODE has many combinations of solver settings, and it is very impractical to test each of these manually. Therefore, an approach based on solver setting scenario analysis was applied (see also Claeys et al. 2006). One solver setting (accuracy) was tested individually (see Results section). Another aspect evaluated was the reduction of output frequency. The standard for BSM2 is to produce data points every 15 min,

while output frequencies of data every 30, 45 and 60 min were also tested.

Sensitivity analysis

The sensitivity of the three BSM2 evaluation criteria towards model parameters was assessed by means of MC experiments, which consist of performing multiple simulations with parameter values sampled from their PDFs, and linear regression of the outputs to calculate the standardised regression coefficients (SRCs) and the partial correlation coefficients (PCCs) of the parameters that are considered uncertain (Saltelli *et al.* 2000). The SRCs

represent the change in an output variable that results from a change of one standard deviation in a parameter, while the PCCs measure the linear dependence between an output variable and a parameter in the case where the influence of the other parameters is eliminated. The SRCs and the PCCs result in the same ranking of parameters in case the parameters are not correlated, and in this case the set of parameters that is not significant for the PCCs is always a superset of the one for the SRCs.

The parameters were divided into three groups (see Table 1 for details): (1) OD parameters, including volumes, recirculation rates, etc.; (2) water line (WL) parameters, including some parameters of the ASM1 and of the primary

Table 1 | PDFs of parameters; LB = lower bound, UB = upper bound, OD = operation and design, WL = water line, SL = sludge line, *t* = triangular, *u* = uniform

Parameter	Description or reference	Group	PDF	Median	LB	UB
AD.V_gas	Volume of gas in AD tank, in m ³	OD	U	–	240	360
AD.V_liq	Volume of liquid in AD tank, in m ³	OD	U	–	2,720	4,080
ASU3.Kla	kLa in AS reactor no. 3, in d ⁻¹	OD	U	–	96	144
ASU4.Kla	kLa in AS reactor no. 4, in d ⁻¹	OD	U	–	96	144
ASU5.Kla	kLa in AS reactor no. 5, in d ⁻¹	OD	U	–	48	72
C_source	C-source, COD = 400,000 g/m ³ , in m ³ /d	OD	U	–	1.6	2.4
dewatering.rem_perc	TSS removal fraction in dewatering	OD	U	–	0.96	1
dewatering.X_under	TSS underflow concentration, as fraction	OD	U	–	0.224	0.336
internal_rec	Internal mixed liquor recircul., in m ³ /d	OD	U	–	49,555.2	74,332.8
PC.f_PS	Prim. settler underflow as ratio on inflow	OD	U	–	0.0056	0.0084
PC.Vol	Primary settler volume, in m ³	OD	U	–	800	1,200
SC.A	Surface area of secondary settler, in m ²	OD	U	–	1,200	1,800
SC.H	Height of secondary settler, in m	OD	U	–	3.2	4.8
SC.Q_Under	Underflow of secondary settler, in m ³ /d	OD	U	–	16,518.4	24,777.6
sec_sludge_to_AD	Secondary sludge to AD, in m ³ /d	OD	U	–	240	360
thickener.rem_perc	TSS removal fraction in thickener	OD	U	–	0.96	1
thickener.X_under	TSS underflow concentration, as fraction	OD	U	–	0.056	0.084
Vol_aer	Volume of each aerated tank, in m ³	OD	U	–	2,400	3,600
Vol_anox	Volume of each anoxic tank, in m ³	OD	U	–	1,200	1,800
f_P	Henze <i>et al.</i> (1987)	WL	T	0.08	0.076	0.084
F_TSS_COD	TSS/COD ratio	WL	T	0.75	0.7125	0.7875
i_X_B	Henze <i>et al.</i> (1987)	WL	T	0.08	0.076	0.084
i_X_P	Henze <i>et al.</i> (1987)	WL	T	0.06	0.057	0.063
k_a	Henze <i>et al.</i> (1987)	WL	T	0.05	0.025	0.075
k_h	Henze <i>et al.</i> (1987)	WL	T	3	1.5	4.5
K_NH	Henze <i>et al.</i> (1987)	WL	T	1	0.5	1.5

(continued)

Table 1 | continued

Parameter	Description or reference	Group	PDF	Median	LB	UB
K_NO	Henze <i>et al.</i> (1987)	WL	T	0.5	0.25	0.75
K_OA	Henze <i>et al.</i> (1987)	WL	T	0.4	0.2	0.6
K_OH	Henze <i>et al.</i> (1987)	WL	T	0.2	0.1	0.3
K_S	Henze <i>et al.</i> (1987)	WL	T	10	5	15
K_X	Henze <i>et al.</i> (1987)	WL	T	0.1	0.05	0.15
mu_A	Henze <i>et al.</i> (1987)	WL	T	0.5	0.4	0.6
mu_A_b_A	mu_A/b_A ratio, for correlation	WL	U	–	9.5	10.5
mu_H	Henze <i>et al.</i> (1987)	WL	T	4	3.2	4.8
mu_H_b_H	mu_H/b_H ratio, for correlation	WL	U	–	12.66	13.99
n_g	Henze <i>et al.</i> (1987)	WL	T	0.8	0.64	0.96
n_h	Henze <i>et al.</i> (1987)	WL	T	0.8	0.64	0.96
PC.f_X	Otterpohl <i>et al.</i> (1994)	WL	T	0.86	0.765	0.935
SC.f_ns	Takács <i>et al.</i> (1991)	WL	T	0.0023	0.0018	0.0027
SC.r_H	Takács <i>et al.</i> (1991)	WL	T	0.0006	0.0005	0.0007
SC.r_P	Takács <i>et al.</i> (1991)	WL	T	0.00286	0.00228	0.00343
SC.v0	Takács <i>et al.</i> (1991)	WL	T	474	379.2	568.8
SC.v00	Takács <i>et al.</i> (1991)	WL	T	250	200	300
SC.X_Lim	Takács <i>et al.</i> (1991)	WL	T	900	720	1,080
SC.X_T	Takács <i>et al.</i> (1991)	WL	T	3,000	2,400	3,600
Y_A	Henze <i>et al.</i> (1987)	WL	T	0.24	0.228	0.252
Y_H	Henze <i>et al.</i> (1987)	WL	T	0.67	0.6365	0.7035
AD.kdis	Batstone <i>et al.</i> (2002)	SL	T	0.7	0.5	1
AD.khyd_ch	Batstone <i>et al.</i> (2002)	SL	T	0.8	0.5	1
AD.khyd_li	Batstone <i>et al.</i> (2002)	SL	T	1.1	0.7	1.5
AD.khyd_pr	Batstone <i>et al.</i> (2002)	SL	T	1.1	0.7	1.5
AD.KI_nh3_ac_km_ac	KI_nh3_ac/km_ac ratio, for correlation	SL	U	–	0.00013	0.00015
AD.kla	Batstone <i>et al.</i> (2002)	SL	T	150	50	200
AD.km_ac	Batstone <i>et al.</i> (2002)	SL	T	10	8	12
AD.km_c4	Batstone <i>et al.</i> (2002)	SL	T	15	10	20
AD.km_fa	Batstone <i>et al.</i> (2002)	SL	T	15	10	20
AD.km_pro	Batstone <i>et al.</i> (2002)	SL	T	10	8	12
AD.Ks_ac_km_ac	Ks_ac/km_ac ratio, for correlation	SL	U	–	0.025	0.083
AD.Ks_c4_km_pro	Ks_c4/km_pro ratio, for correlation	SL	U	–	0.025	0.1
AD.Ks_fa_km_pro	Ks_fa/km_pro ratio, for correlation	SL	U	–	0.025	0.1
AD.Ks_pro_km_pro	Ks_pro/km_pro ratio, for correlation	SL	U	–	0.025	0.083
ADM2ASM.frxs_AS	Nopens <i>et al.</i> (2009)	SL	T	0.7505	0.711	0.79
ASM2ADM.frlixb	Nopens <i>et al.</i> (2009)	SL	T	0.4	0.38	0.42
ASM2ADM.frlixs	Nopens <i>et al.</i> (2009)	SL	T	0.7	0.665	0.735
ASM2ADM.frxs	Nopens <i>et al.</i> (2009)	SL	T	0.646	0.612	0.68

and secondary settler models; and (3) sludge line (SL) parameters, including some parameters of the ADM1 and interface parameters. Model parameters selected for testing were based on operational knowledge and previous studies. Of course, a different choice of PDFs might lead to different results (Benedetti *et al.* 2008).

The PDFs of the 19 parameters regarding OD of the plant (all OD parameters available in BSM2) were defined as uniform with mean value set to the default value for BSM2 and boundaries as $\pm 20\%$ of the mean, except for the dewatering and thickener removal rates, which were assumed to vary between 0.96 and 1. For the ASM1, the selection of the uncertain parameters and their PDFs were taken from Rousseau *et al.* (2001), while for the settling parameters (all settling parameters available in BSM2) the PDFs were assumed to be triangular with median value equal to the BSM2 default and boundaries $\pm 20\%$ of the median. The selection of the uncertain parameters and their PDFs of the ADM1 were taken from Batstone *et al.* (2002, 2003, 2004) and Siegrist *et al.* (2002), while the AS/AD/AS model interface parameter PDFs – the only four parameters (see Table 1, last four parameters) supposed to be variable in the interface (Nopens *et al.* 2009) – were assumed to originate from a triangular distribution with median equal to the BSM2 default and boundaries $\pm 5\%$ of the median.

For simplicity, no correlations were assumed between parameters, with the exception of maximum growth rates and decay rates of both autotrophs and heterotrophs. In this case, the ratios $\mu_{A_b_A}$ and $\mu_{H_b_H}$ were introduced as uncertain and used to calculate b_A and b_H from μ_A and μ_H .

A number of simulations, N , was run for each MC experiment, sampling from the PDFs of the parameters with Latin Hypercube Sampling (LHS) and making use of parallel computing to speed up the calculations (Claeys *et al.* 2006; Benedetti *et al.* 2008). To evaluate the quality of the linear regression, the coefficient of determination R^2 , i.e. the fraction of the output variance reproduced by the regression model, was calculated; the regression is considered of good quality when $R^2 > 0.7$ (Saltelli *et al.* 2000). The calculation of the t -statistic on the SRCs and PCCs (Morrison 1984) allows for classifying the parameters as significant at the 5% level with a t -statistic larger than 1.96. For the

parameter screening, only the parameters that resulted as being not significant for all evaluation criteria were considered as not significant and discarded from the parameter list for further UA studies.

The number of simulations N in a MC experiment was equal to n times the number of uncertain parameters, and n was determined by setting it to 4/3 (as originally suggested for LHS by McKay 1988) and then increasing it until stable parameters ranking is achieved. This ranking stability was assessed for each value of n tested by running three MC simulations (repeats) with three different seeds of the random number generator and qualitatively judging the stability of the ranking in the three simulations.

An automated procedure to assess the convergence on MC simulations is being developed (Benedetti *et al.* 2011).

Robustness study

For the evaluation of the transferability of strategies to different situations, a GSA was performed on all parameters together, after which insignificant parameters were removed and a new GSA was performed on the reduced list of parameters. The effect of adopting a smaller number of parameters on the output uncertainty was evaluated. Then, the GSA was performed on the three groups of parameters separately (OD, WL, SL, see above), to show the relative importance of the groups towards the total uncertainty in the output.

Uncertainty study

To illustrate how a practical comparison of alternatives would be carried out with the new methodology on a defined WWTP design and operation condition (the BSM2 in open loop, OD parameters fixed) by using UA, a GSA was performed on all WL and SL parameters together. After this, insignificant parameters were removed and a new GSA was performed on the reduced list of parameters. The same reduced GSA was conducted on a closed loop version of BSM2 (i.e. with control), consisting of a simple dissolved oxygen controller on the three aerated tanks, which strongly reduces the NH_4 exceedance period. The effect of adopting a smaller number of parameters on the output uncertainty was evaluated in both cases.

RESULTS

Solver optimisation

The results of the solver settings scenario analysis are shown in Table 2 with regard to computation time and difference (accuracy) from the reference for EQI, OCI and ammonium exceedance period. The best compromise between accuracy and computation time was found for a solver accuracy of 10^{-3} .

The output frequency of data every 30 min was chosen since it provided still acceptable results in a shorter time and with half the output file size, which is an important factor for storage and post-processing of simulation data. In other types of studies, lower frequencies can be accepted (Ráduly et al. 2007). Compared to the reference settings, the selected settings therefore allow an almost five times reduction of the computation time with only half the output file size.

Number of simulations

Running the MC experiments with all OD parameters (19 OD parameters) considered as uncertain, n was set to 4/3, 3, 12 and 20, i.e. N was set to 26, 57, 228 and 380 simulations. Since the ranking of the parameter sensitivities on the basis of the SRCs was different in all MC experiments (including three MC experiments with different seeds, each with $n = 20$, as shown in Table 3), it was assumed that $n = 20$ was not sufficient. This is in disagreement with Manache & Melching (2008) – where $n = 3$ was sufficient for a model with a similar structure, but probably with a lower

Table 3 | SRC analysis; NH_4 indicates the percentage of time that ammonium exceeded 4 mg NH_4-N/l ; numbers indicate the parameter ranking when it did not change (ideal situation); light grey boxes indicate cases where the ranking of the parameter was different in the three MC experiments with three different seeds (negative situation); dark grey boxes indicate when the parameter changed from significant to not significant or vice versa (very negative situation)

Parameter	$n = 20$			$n = 50$		
	EQI	NH_4	OCI	EQI	NH_4	OCI
AD.V_gas	█	█	█	█	█	█
AD.V_liq	█	█	9	█	█	9
ASU3.Kla	█	2	█	5	█	█
ASU4.Kla	█	3	█	4	█	█
ASU5.Kla	█	4	8	█	4	8
C_source	█	█	3	█	6	3
dewatering.rem_perc	█	█	14	█	█	14
dewatering.X_under	█	█	█	█	█	█
internal_rec	█	█	10	█	█	10
PC.f_PS	█	█	1	█	█	1
PC.Vol	█	5	7	█	5	7
SC.A	2	█	11	2	█	11
SC.H	█	█	█	█	█	█
SC.Q_Under	█	█	█	█	█	█
sec_sludge_to_AD	█	█	13	17	█	13
thickener.rem_perc	█	█	█	█	█	15
thickener.X_under	█	█	6	█	█	6
Vol_aer	1	1	2	1	1	2
Vol_anox	3	█	12	3	█	12

complexity – and with Rousseau et al. (2001) who found 300 simulations to be sufficient for 20 parameters ($n = 15$). Three more MC experiments were performed with n set to 50 ($N = 950$) with three different seeds, and in this case

Table 2 | Simulation performance for different solver settings and output frequencies; the reference simulation settings are in dark grey, the best settings are in light grey

Solver	Accuracy	Output freq. [min]	File size [MB]	Computation time [s]	ΔEQI [%]	ΔOCI [%]	ΔNH_4 [%]
RK4ASC	10^{-6}	15	13.4	571	0.0000	0.0000	0.0000
CVODE	10^{-5}	15	13.4	249	0.0000	0.0001	-0.1391
CVODE	10^{-4}	15	13.4	158	-0.0140	-0.0132	0.0585
CVODE	10^{-3}	15	13.4	131	-0.0170	-0.0127	-0.0804
CVODE	10^{-2}	15	13.4	133	0.1102	-0.0056	1.6840
CVODE	10^{-3}	30	6.7	121	-0.0223	-0.0003	-3.4363
CVODE	10^{-3}	45	5.0	119	-0.0589	-0.0091	-10.7498
CVODE	10^{-3}	60	3.3	118	-0.0528	0.0198	-20.2360

the differences were less pronounced (as can be concluded from visual inspection of Table 3), allowing to select $n = 50$ for the rest of the MC experiments as a compromise between accuracy of the results and feasibility of computation.

Robustness study

Four different MC experiments were performed to conduct the GSA on: (1) all parameters together; (2) OD parameters; (3) WL parameters; and (4) SL parameters.

From Table 4, which shows the results for the GSA on all parameters together, the three BSM2 evaluation criteria are mainly sensitive to OD parameters, and largely not to sludge treatment parameters. Ten out of 65 parameters were identified as not significant based on their t -value for SRC. With the significance tested on the t -statistic for the PCCs, 40 of the original 65 parameters are classified as not significant, with most of the AD parameters not being significant. It is to be noted that among the WL parameters, the most significant parameters are the ones concerning nitrification and secondary settling.

Performing the GSA on the OD parameters only (see Table 5), two out of 19 parameters are not significant for all three criteria based on the SRCs and seven based on the PCCs. PCCs are indeed known to produce a larger number of not significant parameters (Manache & Melching 2008). As expected, the aerated volume (Vol_aer) is in general the most important parameter, followed by the air supply (KLa) in the three aerated tanks and by the external carbon dosage (C_source). Also relevant is the highest importance of the primary clarifier underflow (PC.f_PS) for the OCI, given the fact that primary sludge is very well suited for methane production, which heavily influences OCI. The surface of the secondary clarifier and the anoxic volume are very important for the EQI, by affecting the effluent TSS and NO₃, respectively.

From the analysis on the wastewater treatment parameters only (see Table 6), only four out of the 28 parameters were judged as not significant (for all three performance criteria) for the SRCs and nine for the PCCs, in this case because most parameters are important for at least one performance criterion. The only ones that strongly influence both EQI (but not NH₄) and OCI are Y_H of

ASM1 and r_P and v0 of the secondary clarifier model. Very important for EQI and NH₄ are both K_OA and K_OH.

Only one parameter out of 18 sludge treatment parameters (see Table 7) can be considered as not significant for all three criteria based on the SRCs, and seven based on the PCCs.

Figure 3 shows the variability of the three evaluation criteria for the three parameter categories separately and altogether. It is clear that most of the output variability is due to the OD parameters, as suggested by the figures in Table 4.

The sludge treatment parameters only contribute to the OCI variability, because of the importance of methane production for cost recovery.

Performing the UA on the BSM2 with the 25 most significant parameters only (the ones with white cells in Table 4), the overall uncertainty in model output is practically unchanged, as can be seen in Figure 3 (right). This means that sensitivity and uncertainty analyses on BSM2 can be performed by only considering this reduced parameter set. Such reduced analysis does not lead to a loss of significant information but is significantly faster to conduct ($65/25 = 2.6$ times faster).

Uncertainty study

To verify the transferability of these parameter ranking results to different configurations of the BSM2 (e.g. modified by adding a control strategy), a GSA was first conducted for the open loop configuration on the 38 wastewater and sludge treatment parameters. Based on the significance for the PCCs (see Table 4), a reduced set of 24 parameters was adopted. Next, this output uncertainty was calculated for the basic closed loop version of BSM2 (DO control) adopting the reduced set.

Figure 4 shows the variability of the three evaluation criteria with the full and the reduced parameter sets for the open loop and the closed loop. It is evident that the changes in output variability from the full to the reduced parameter set are practically negligible in both BSM2 configurations, confirming that the reduced parameter set is sufficient for sensitivity and UA of BSM2 evaluation results.

Table 4 | PCCs and ranking of all parameters. Robustness study: in dark grey: the parameters not significant for all three criteria based on SRC and PCC; in light grey: significant for SRC but not for PCC, without shading significant for both SRC and PCC. Uncertainty study: in bold face not significant for SRC and PCC from GSA on WL and SL parameters (fixed OD parameters, see above under Uncertainty study)

Parameter	Group	EQI $R^2 = 0.71$		$NH_4 R^2 = 0.97$		OCI $R^2 = 0.99$	
		PCC	Rank	PCC	Rank	PCC	Rank
AD.V_gas	OD	0.01731	27	0.00757	32	-0.00040	58
AD.V_liq	OD	0.00956	35	-0.00630	34	-0.07242	10
ASU3.Kla	OD	-0.08355	10	-0.18763	2	0.15281	5
ASU4.Kla	OD	-0.10341	7	-0.17658	3	0.15493	4
ASU5.Kla	OD	-0.05268	15	-0.11993	4	0.07767	9
C_source	OD	-0.02537	22	0.02833	13	0.24269	3
dewatering.rem_perc	OD	0.00081	61	0.01247	23	0.01504	23
dewatering.X_under	OD	0.00487	45	-0.00791	30	0.00023	62
internal_rec	OD	-0.04679	17	-0.01410	20	0.08078	8
PC.f_PS	OD	-0.01618	28	-0.01307	21	0.39139	1
PC.Vol	OD	-0.02056	23	-0.04589	7	-0.08159	7
SC.A	OD	-0.20355	2	-0.00406	46	0.05186	13
SC.H	OD	-0.01974	24	0.00036	61	0.00369	41
SC.Q_Under	OD	-0.01106	33	-0.00099	57	-0.01100	27
sec_sludge_to_AD	OD	-0.00290	53	0.00358	51	0.02354	20
thickener.rem_perc	OD	0.00886	37	0.00762	31	0.00679	52
thickener.X_under	OD	0.00879	38	0.00396	47	-0.08870	6
Vol_aer	OD	-0.41771	1	-0.50165	1	0.35651	2
Vol_anox	OD	-0.09818	9	0.00343	52	0.02873	18
f_P	WL	0.00571	43	-0.00442	44	0.01851	21
F_TSS_COD	WL	0.00002	65	0.00859	27	0.01617	22
i_X_B	WL	-0.00213	55	-0.01245	24	0.00064	54
i_X_P	WL	0.00279	54	-0.00097	58	0.00050	57
k_a	WL	-0.06743	12	0.01114	25	-0.00038	59
k_h	WL	-0.02652	21	0.03058	10	0.00836	29
K_NH	WL	0.07427	11	0.03390	9	0.00114	50
K_NO	WL	0.03002	19	0.00165	55	-0.00022	63
K_OA	WL	0.15490	3	0.08899	5	0.00052	56
K_OH	WL	-0.14524	4	-0.03852	8	-0.00098	52
K_S	WL	0.00911	36	0.00521	39	-0.00008	65
K_X	WL	0.01856	25	-0.01730	16	-0.00389	38
mu_A	WL	-0.05464	14	-0.03004	11	-0.00015	64
mu_A_b_A	WL	-0.00649	42	-0.00034	62	0.00097	53
mu_H	WL	0.00072	63	0.02927	12	-0.01045	28
mu_H_b_H	WL	-0.01421	31	-0.02033	14	0.00220	44
n_g	WL	-0.06272	13	-0.01773	15	0.00123	47
n_h	WL	-0.02662	20	0.01285	22	0.00117	49
PC.f_X	WL	-0.00212	57	-0.00491	42	-0.00423	35
SC.f_ns	WL	0.04716	16	0.00390	48	-0.01104	26
SC.r_H	WL	0.11410	6	0.00537	38	-0.03566	15
SC.r_P	WL	-0.10327	8	0.00817	28	0.03038	17
SC.v0	WL	-0.11726	5	0.00581	37	0.03212	16
SC.v00	WL	-0.00212	56	0.01428	19	0.00372	40
SC.X_Lim	WL	-0.00957	34	-0.00017	64	0.00024	61

(continued)

Table 4 | continued

Parameter	Group	EQI $R^2 = 0.71$		$\text{NH}_4 R^2 = 0.97$		OCI $R^2 = 0.99$	
		PCC	Rank	PCC	Rank	PCC	Rank
SC.X_T	WL	-0.00106	59	-0.00050	60	0.00032	60
Y_A	WL	-0.01787	26	-0.01546	18	0.00118	48
Y_H	WL	0.04541	18	-0.08133	6	0.07165	11
AD.kdis	SL	0.00071	64	0.00165	54	-0.00384	39
AD.khyd_ch	SL	-0.00331	51	-0.00185	53	-0.01456	24
AD.khyd_li	SL	0.00150	58	0.01009	26	-0.02715	19
AD.khyd_pr	SL	0.01463	30	0.00588	36	-0.04839	14
AD.KI_nh3_ac_km_ac	SL	0.00667	41	0.00811	29	-0.00100	51
AD.kla	SL	-0.00352	50	0.00373	50	0.00132	46
AD.km_ac	SL	-0.00439	48	-0.00617	35	-0.00409	37
AD.km_c4	SL	0.00105	60	0.00030	63	-0.00245	42
AD.km_fa	SL	-0.00479	46	0.00141	56	-0.00226	43
AD.km_pro	SL	-0.00851	39	-0.00433	45	0.00421	36
AD.Ks_ac_km_ac	SL	-0.00331	52	0.00494	41	0.01417	25
AD.Ks_c4_km_pro	SL	-0.00466	47	0.00733	33	0.00811	30
AD.Ks_fa_km_pro	SL	-0.00383	49	-0.00002	65	0.00425	34
AD.Ks_pro_km_pro	SL	-0.01571	29	-0.01715	17	0.00729	31
ADM2ASM.frxs_AS	SL	0.00074	62	0.00088	59	-0.00056	55
ASM2ADM.frlxb	SL	-0.00560	44	-0.00519	40	0.00147	45
ASM2ADM.frlxs	SL	0.00774	40	0.00482	43	-0.00560	33
ASM2ADM.frxs	SL	0.01408	32	0.00386	49	-0.06466	12

Table 5 | Ranking of OD parameters; in dark grey the parameters that are not significant at 5% level for all three criteria, based on their t -statistic for SRC and in light grey the additional ones based on their t -statistic for PCC

Parameter	EQI $r^2 = 0.67$		$\text{NH}_4 r^2 = 0.80$		OCI $r^2 = 0.99$	
	SRC	Rank	SRC	Rank	SRC	Rank
AD.V_gas	0.01298	12	-0.00338	15	0.00041	18
AD.V_liq	-0.00582	14	-0.01732	8	-0.10400	9
ASU3.Kla	-0.08321	5	-0.26022	2	0.23033	4
ASU4.Kla	-0.14456	4	-0.25508	3	0.23043	5
ASU5.Kla	-0.04882	8	-0.13706	4	0.11560	8
C_source	-0.05282	6	0.05819	6	0.37044	3
dewatering.rem_perc	0.00140	19	0.01079	11	0.02588	14
dewatering.X_under	0.00186	18	-0.00540	14	-0.00034	19
internal_rec	-0.00936	13	-0.01437	10	0.09578	10
PC.f_PS	0.01682	11	0.00839	12	0.63136	1
PC.Vol	-0.02658	10	-0.07787	5	-0.12841	7
SC.A	-0.36227	2	0.00309	16	0.07186	11
SC.H	-0.05129	7	-0.02183	7	0.00279	17
SC.Q_Under	-0.03284	9	0.00584	13	-0.00541	16
sec_sludge_to_AD	0.00470	16	0.00233	18	0.0325	13

(continued)

Table 5 | continued

Parameter	EQI $r^2 = 0.67$		NH ₄ $r^2 = 0.80$		OCI $r^2 = 0.99$	
	SRC	Rank	SRC	Rank	SRC	Rank
thickener.rem_perc	-0.0035	17	-0.00238	17	0.01206	15
thickener.X_under	0.00518	15	0.00154	19	-0.13284	6
Vol_aer	-0.69071	1	-0.78075	1	0.57754	2
Vol_anox	-0.17295	3	0.01650	9	0.04960	12

Table 6 | Ranking of WL model parameters; in dark grey the parameters that are not significant at 5% level for all three criteria, based on their *t*-statistic for SRC and in light grey the additional ones based on their *t*-statistic for PCC

Parameter	EQI $r^2 = 0.94$		NH ₄ $r^2 = 0.88$		OCI $r^2 = 0.98$	
	SRC	Rank	SRC	Rank	SRC	Rank
f_P	-0.00391	22	-0.03844	14	0.22304	5
F_TSS_COD	-0.04051	18	-0.01042	21	0.17999	6
i_X_B	0.00601	20	-0.04869	13	0.00198	22
i_X_P	0.00519	21	-0.01655	19	-0.00103	26
k_a	-0.21688	6	0.06849	10	0.00613	20
k_h	-0.05382	15	0.22810	5	0.07976	8
K_NH	0.22293	5	0.26772	4	-0.00357	21
K_NO	0.09280	13	0.03093	15	-0.00127	24
K_OA	0.44432	2	0.64106	1	0.00729	18
K_OH	-0.45723	1	-0.31863	3	-0.01105	14
K_S	0.03395	19	0.00799	26	-0.00634	19
K_X	0.06123	14	-0.13404	7	-0.04371	10
mu_A	-0.16933	9	-0.20859	6	0.00122	25
mu_A_b_A	-0.04795	17	-0.06031	11	0.00920	15
mu_H	-0.04832	16	0.12611	8	-0.03459	11
mu_H_b_H	0.00314	23	-0.05116	12	0.01215	13
n_g	-0.19016	7	-0.11952	9	-0.00163	23
n_h	-0.10485	12	0.02805	16	0.00851	16
PC.f_X	0.00181	25	-0.02748	17	-0.07669	9
SC.f_ns	0.15253	11	0.00924	22	-0.14415	7
SC.r_H	0.18236	8	-0.00775	27	-0.23460	4
SC.r_P	-0.34679	3	0.00362	28	0.32184	3
SC.v0	-0.34587	4	-0.01474	20	0.32409	2
SC.v00	0.00097	27	0.00838	25	0.00767	17
SC.X_Lim	-0.00213	24	0.00903	23	-0.00004	28
SC.X_T	-0.00166	26	-0.00882	24	-0.00081	27
Y_A	0.00046	28	-0.02496	18	0.01523	12
Y_H	0.15734	10	-0.41395	2	0.77757	1

Table 7 | Ranking of SL models parameters; in dark grey the parameters that are not significant at 5% level for all three criteria, based on their *t*-statistic for SRC and in light grey the additional ones based on their *t*-statistic for PCC

Parameter	EQI $r^2 = 0.98$		NH ₄ $r^2 = 0.97$		OCI $r^2 = 0.99$	
	SRC	Rank	SRC	Rank	SRC	Rank
AD.kdis	0.02491	12	0.00898	15	-0.03422	12
AD.khyd_ch	0.00011	17	0.00393	17	-0.16450	4
AD.khyd_li	0.00209	16	-0.01128	14	-0.29627	3
AD.khyd_pr	0.69282	1	0.60394	1	-0.53288	2
AD.KI_nh3_ac_km_ac	0.01049	14	-0.03189	12	-0.00316	17
AD.kla	-0.00002	18	-0.00222	18	-0.00474	16
AD.km_ac	0.05671	9	-0.11429	8	-0.03583	11
AD.km_c4	0.07372	7	-0.12216	7	-0.04442	9
AD.km_fa	0.03336	11	-0.06877	10	-0.01645	14
AD.km_pro	-0.04602	10	0.09175	9	0.02586	13
AD.Ks_ac_km_ac	-0.23985	3	0.42886	3	0.14377	5
AD.Ks_c4_km_pro	-0.16717	5	0.28798	5	0.08672	7
AD.Ks_fa_km_pro	-0.07875	6	0.15004	6	0.04206	10
AD.Ks_pro_km_pro	-0.17258	4	0.30262	4	0.09555	6
ADM2ASM.frxs_AS	0.06754	8	0.06614	11	-0.00077	18
ASM2ADM.frlixb	-0.01031	15	-0.00594	16	0.00836	15
ASM2ADM.frlixs	0.02211	13	0.02755	13	-0.06134	8
ASM2ADM.frxs	0.56395	2	0.50161	2	-0.71721	1

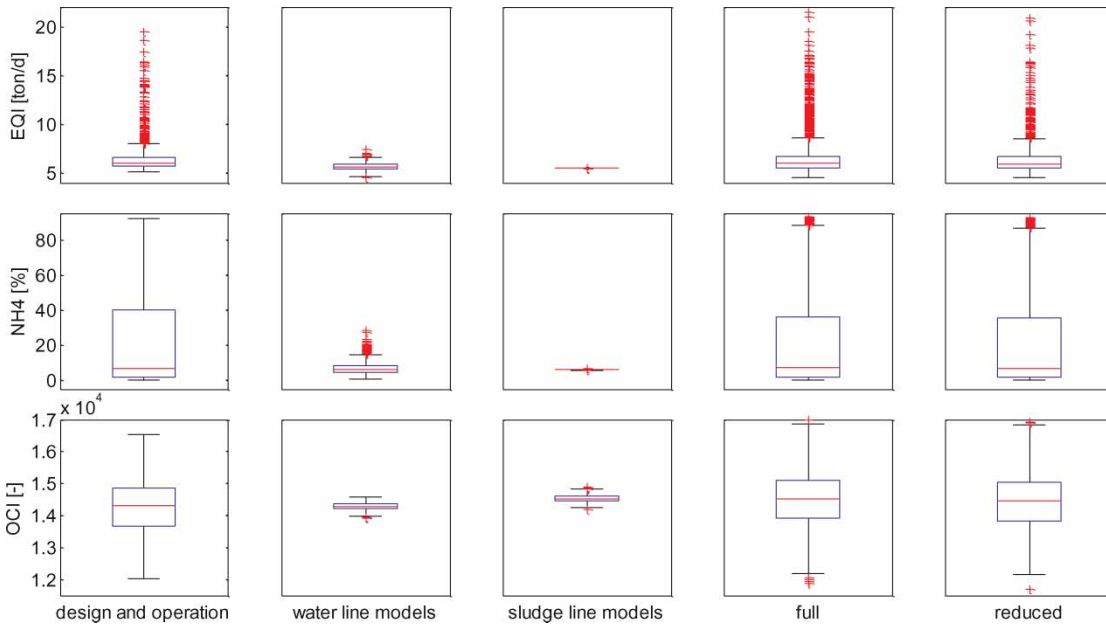


Figure 3 | Variability box plots of the three BSM2 evaluation criteria for the three parameter categories separately, altogether ('full') and with the reduced set of uncertain parameters ('reduced').

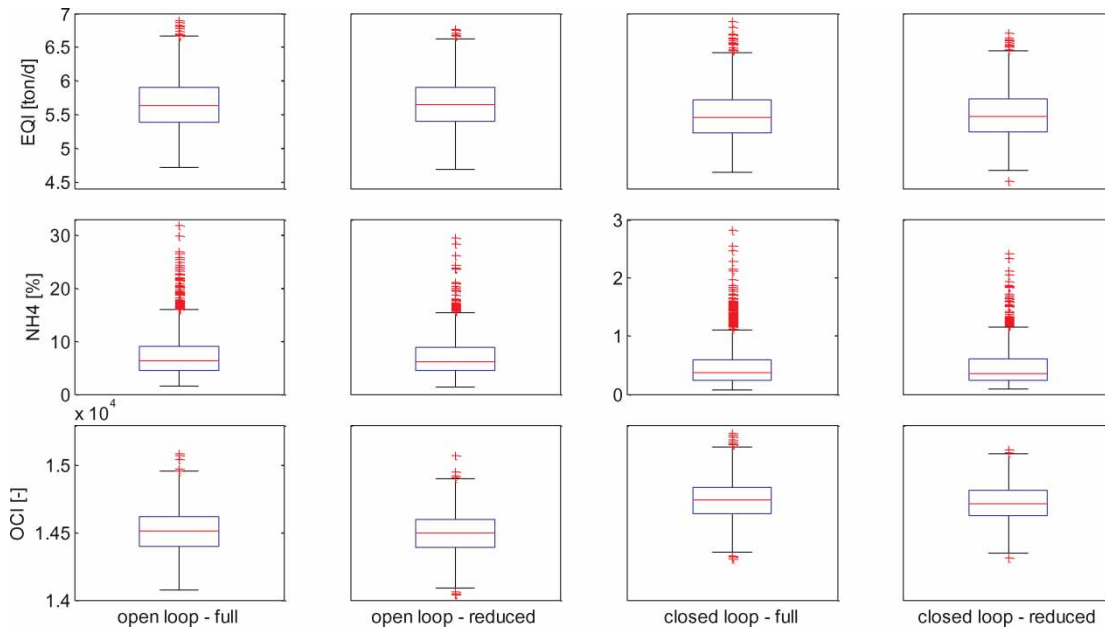


Figure 4 | Variability box plots of the three BSM2 evaluation criteria for open loop and closed loop, with all wastewater and sludge treatment parameters ('full') and with the reduced set of uncertain parameters ('reduced').

In general, these results allow conducting sensitivity and UA studies on control strategies with BSM2 (e.g. see [Benedetti et al. 2010a](#)) focusing attention on the most critical parameters. Nevertheless, it would always be possible that a control strategy changes the behaviour of the BSM2 to an extent where other parameters may become more important. For example, the SL becomes highly important during failure, when it will result in massive COD loads; the system is highly non-linear under these conditions, and therefore the sensitivity analysis is no longer valid.

DISCUSSION

Having acknowledged the need to include UA in modelling studies ([Belia et al. 2009](#)), this paper illustrates a general method to reduce the time needed to perform UA studies which require MC simulations, and provides specific results on simplification of UA for evaluation of control strategies with BSM2.

Given the complexity of the BSM2 and the MC computational load, it is necessary to perform some preliminary numerical solver optimisation by means of solver setting exploration and downsampling of the output file. Proper

solver settings selection could reduce the time required for computation by a factor of 5. For the BSM2, this involved the use of the advanced CVODE solver.

The second step was the definition of the minimum number of simulations to be run for each MC experiment. The required number of simulations was found to be at least 50 times the number of parameters to be tested, a value significantly higher than the ones found in literature about MC simulations conducted with similar models. Possible explanations could include different model complexity, different number of uncertain parameters and different objectives of the study.

A next development of the methodology would be to use incremental sampling to always have the sufficient number of simulations, specific for each different model, without the need to repeat MC simulations.

Being the two aims of this article: (1) to provide a method to reduce the number of uncertain parameters, in case it is foreseen to perform several UAs on the same (or similar) model; and (2) to provide the list of uncertain parameters to conduct UA on the BSM2, indeed the MC simulation had to be carried out twice, but this is justified by the production of a list of significant parameters that can be reused in other studies with the BSM2.

Concerning the results specific to BSM2, the most sensitive parameters belong to the OD group, especially for the OCI and NH_4 criteria. In particular, primary settling parameters are important with respect to the economic performance of the plant, affecting the biogas production (primary sludge yields double the methane production of secondary sludge, due to its higher degradability and energy content) and the treatment load (therefore aeration cost) to the AS units. For the EQI, some of the WL parameters are also of high importance, especially the ones that govern nitrification (acting on effluent NH_4 and NO_3 , which have high weights in the EQI) and secondary settling (acting on TSS and COD and on the capacity to retain the nitrifying sludge). The SL parameters have hardly any significance for the three evaluation criteria, probably because the simulated conditions did not provide sufficient stress to the SL to see the importance of its parameters.

Based on these results, the number of uncertain parameters to be studied can be reduced from 65 to 25 (38% of the original number) in cases where all parameters are considered (i.e. OD, WL and SL models parameters), without significant loss of information. This applies to UA for assessment of robustness (transferability) of control strategies evaluations to other design and operation conditions.

When a specific OD parameter set has to be evaluated (e.g. to assess the output variability of a control strategy for a specific layout), the number of uncertain parameters in the water and SL models can be reduced from 38 to 24 (63% of the original number), again leading to a reduction in computing time.

The more limited possibility to reduce the number of parameters in the latter case compared to the former can be explained by the fact that when considering the OD parameters, WL and SL parameters have a relatively small contribution to the total uncertainty. On the other hand, when only the WL and SL parameters are considered, there is not so much relative difference in their sensitivities.

CONCLUSIONS

This paper illustrates a general method to reduce the time needed to perform MC-based UA studies, and provides specific results on simplification of such studies for the evaluation of control strategies with BSM2.

The main results can be summarised as follows:

- Proper solver settings selection can reduce the time required for computation by a factor of 5 for the case studied. It involved the use of the CVODE solver.
- The required minimum number of simulations was found to be at least 50 times the number of parameters to be tested, a value significantly higher than the ones found in literature about MC simulations conducted with similar models.
- Specific for BSM2, the most sensitive parameters belong to the OD group, especially for the operational cost index and NH_4 criteria.
- Primary settling parameters are important with respect to the economic performance of the plant.
- For the EQI, some of the WL parameters are also of high importance, especially the ones that govern nitrification and secondary settling.
- For the conditions tested, the SL parameters have hardly any significance for the three evaluation criteria.
- The number of uncertain parameters to be considered can be reduced from 65 to 25 (allowing a 2.6 times shorter UA time) in cases where all parameters are considered to check the robustness of control strategies evaluations against other design and operation conditions.
- When a specific OD parameter set has to be evaluated (e.g. to assess the output variability of a control strategy on a fixed layout), the number of uncertain parameters in the water and SL models can be reduced from 38 to 24 (1.6 times shorter analysis time).

These results make the execution of future sensitivity and UA studies, especially with BSM2, more feasible.

ACKNOWLEDGEMENTS

Peter A. Vanrolleghem holds the Canada Research Chair in Water Quality Modelling. The authors gratefully acknowledge IWA for supporting the Task Group on Uncertainty Evaluation in WWTP Design and Operations.

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First received 24 November 2011; accepted in revised form 7 February 2012