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Global sensitivity analysis of biochemical, design and operational parameters of the Benchmark Simulation Model no. 2

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Abstract: Wastewater treatment plant control and monitoring can help to achieve good effluent quality, in a complex, highly non-linear process. The Benchmark Simulation Model no. 2 (BSM2) is a useful tool to competitively evaluate plant-wide control on a long-term basis. A key component to characterise the system for control is output-parameter sensitivity. This paper brings the results of a global sensitivity analysis performed on the BSM2 model in its open loop version, by means of Monte Carlo (MC) experiments and linear regression. This study presents methods that were applied to make computationally demanding MC experiments on such a complex model feasible, by reducing the computation time for a single simulation and by setting low but sufficient number of runs for the MC experiments; it was found that 50 times the number of uncertain parameters was necessary. The most sensitive parameters turned out to be the design and operation parameters, followed by the wastewater treatment model parameters, while the adopted BSM2 evaluation criteria are rather insensitive to variations in sludge treatment models parameters. The results are verified on a closed loop version of BSM2, and allow future uncertainty analysis studies on BSM2 to be conducted on a smaller set of parameters and to focus the attention on the most critical parameters.

***Keywords**:* activated sludge; anaerobic digestion; BSM2; mathematical modelling; numerical methods.

1. INTRODUCTION

The biological, physical and chemical phenomena taking place in activated sludge systems are complex, 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, monitoring and control of such plants can be very helpful but, given the 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.

Originated in the 90's, the Benchmark Simulation Model no. 1 (BSM1) was proposed as a tool to foster the dissemination of control and monitoring strategies [Copp, 2002]. 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 a well defined set of criteria.

Recently, the BSM2 [Jeppsson et al., 2007] was developed for plant-wide WWTP control strategy evaluation on a long-term basis, with a much more complex plant model. It consists of a pre-treatment process, an activated sludge process and sludge treatment processes.

This paper shows the results of a global sensitivity analysis (SA) performed on the BSM2 model in its open loop (without control) version, by means of Monte Carlo (MC) experiments and linear regression of the MC results [Saltelli et al., 2000]. The parameters for which the sensitivity is computed belong to the biochemical and physical models and to the design and operation of the plant. The study discusses the methods applied to reduce the computational efforts required by such a complex model, by testing possibilities to reduce the computation time of a single simulation, and by looking for a number of simulation runs for the MC experiments sufficient to accept the results of the sensitivity analysis.

2. METHODS

2. 1 The Model

The Benchmark Simulation Model no. 2 protocol [Jeppsson et al., 2007] consists of a plant wide (including wastewater and sludge treatment) model representing a general WWTP, a benchmarking procedure and a set of evaluation criteria. The three evaluation criteria used in this work are: (1) the Effluent Quality Index (EQI), a weighted sum of effluent pollutant loads with weight values set to 2 for BOD, 1 for COD, 2 for TSS, 30 for NH_4 and 10 for 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; (3) the fraction of time in which the effluent exceeds the limit of 4mgNH_4/l, expressed as percentage of the whole evaluation period (one year, the last 365 of the 609 simulated days).

2. 2 Solver Optimisation

The BSM2 contains 265 differential equations and requires a simulation time of 609 days in very dynamic conditions (the evaluation is based on the last 365 days). In order to perform a global sensitivity analysis of such a complex model, potentially involving a very large number of MC simulations, careful selection of numerical settings is needed to minimise the time required to run a single simulation.

The modelling and simulation software used in this work was WEST (MOSTforWATER, Kortrijk, Belgium) with its new numerical engine Tornado [Claeys et al., 2006a]. The starting point was the Runge-Kutta 4th order adaptive step-size (RK4ASC) solver [Forsythe et al., 1977] with accuracy, initial and minimum step size set to 10^{-6} – which are the solver settings normally used with this type of models to provide very accurate results at reasonable computation cost.

Advanced solvers such as CVODE [Hindmarsh et al., 2005] often show a better performance, and an approach based on scenario analysis was applied to find the best solver settings (see also Claeys et al. [2006b]), which provided as optimum: IterationMethod: Newton; LinearMultistepMethod: Adams; LinearSolver: SPGMR. Using those settings, results are shown in Table 1 with regard to computation time and difference from the reference (RK4ASC) for EQI, OCI and ammonium exceedance periods. The best compromise between solution difference and calculation time was found for a solver accuracy of 10^{-3}.

Another aspect evaluated to reduce computation time and storage requirement was the reduction of output frequency. The standard for BSM2 is 15 minutes, and output frequencies of 30, 45 and 60 minutes were tested (see Table 1). The frequency of 30 minutes was chosen since it still provided acceptable results – leaving EQI and OCI practically unchanged and with NH_4 exceedance 3% different – in shorter time and with half the output file size, which is an important factor for storage and post-processing of files. In other types of studies lower frequencies can be accepted [Ráduly et al., 2007]. The selected settings allow therefore, compared to the reference settings, a reduction to almost 1/5 of the computation time and to 1/2 of the output file size.

Table 1. Simulation performance for different solver settings and output frequencies; in dark grey the reference simulation settings, in light grey the best settings.

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

2. 3 Method for 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 Probability Density Functions (PDFs) – and linear regression to calculate the Standardised Regression Coefficients (SRCs) and the Partial Correlation Coefficients (PCCs) of the parameters 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 are the measure of linear dependence between an output variable and a parameter in the case where the influence of the other parameters is eliminated. A number N of simulations was run for each MC experiment, sampling from the PDFs of the parameters with Latin Hypercube Sampling (LHS) [Benedetti et al., 2008]. To evaluate the quality of the linear regression, the coefficient of determination R^2, i.e. the fraction of the input variance reproduced by the regression model, was calculated; the regression is considered of good quality when $R^2>0.7$. The calculation of the t-statistic on the SRCs and PCCs [Morrison, 1984] allowed classifying the parameters as significant at the 5% level with a t-statistic larger than 1.96.

The number N is equal to n times the number of uncertain parameters, and n was determined as follows. Running the MC experiments with uncertain design and operational parameters (19 parameters), n was set to 4/3, 3, 12 and 20, i.e. N was 26, 57, 228 and 380. Since the ranking of the parameter sensitivities made on the basis of the SRCs and PCCs was different in all MC experiments (including three different MC experiments with n=20), it was assumed that n=20 was not sufficient, in disagreement with Manache and Melching [2008], where n=3 was sufficient for a model with similar structure, but probably with lower complexity. Three more MC experiments were performed with n set to 50 (N=950), and in this case the differences were less pronounced, allowing to select n=50 for the rest of the MC experiments as a compromise between accuracy of results and feasibility of computation.

The parameters were divided into three groups (see Table 2 for details): (1) design and operational (DO) parameters, including volumes, recirculation rates, etc.; (2) wastewater treatment (WT) parameters, including some parameters of the ASM1 and of the primary and secondary settler models; (3) sludge treatment (ST) parameters, including some parameters of the ADM1 and interface parameters. Model parameters selected for testing were based on operational knowledge, previous studies, and our own sensitivity screening. Of course, a different choice for the PDFs might lead to different results [Benedetti et al., 2008].

The PDFs of the parameters regarding design and operation of the plant were defined as uniform with their mean set to the default value for BSM2 and boundaries set as +/-20% of the mean. The PDFs of the ASM1 parameters were taken from Rousseau et al. [2001], while for all the other parameters the PDFs were assumed to be triangular with median equal to the BSM2 default and boundaries at +/-20% of the median. The PDFs of the ADM1 parameters were mainly taken from Appendix A in Batstone et al. [2002], with additional information from Batstone et al. [2003; 2004] and Siegrist et al. [2002], while for the AD/AS model interfaces parameters they were assumed to be triangular with median equal to the BSM2 default and boundaries +/-20% of the median.

Table 2. PDFs of parameters; LB=lower bound, UB=upper bound, DO=design and operation, WT=wastewater treatment, ST=sludge treatment, 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	DO	U	-	240	360
AD.V_liq	Volume of liquid in AD tank, in m^3	DO	U	-	2720	4080
ASU3.Kla	kLa in AS reactor no.3, in d^{-1}	DO	U	-	96	144
ASU4.Kla	kLa in AS reactor no.4, in d^{-1}	DO	U	-	96	144
ASU5.Kla	kLa in AS reactor no.5, in d^{-1}	DO	U	-	48	72
C_source	C-source with COD=400000g/m^3, in m^3/d	DO	U	-	1.6	2.4
dewatering.rem_perc	TSS removal fraction in dewatering	DO	U	-	0.96	1
dewatering.X_under	TSS underflow concentration, as fraction	DO	U	-	0.224	0.336
internal_rec	Internal mixed liquor recirculation, in m^3/d	DO	U	-	49555.2	74332.8
PC.f_PS	Primary settler underflow as ratio on inflow	DO	U	-	0.0056	0.0084
PC.Vol	Primary settler volume, in m^3	DO	U	-	800	1200
SC.A	Surface area of secondary settler, in m^2	DO	U	-	1200	1800
SC.H	Height of secondary settler, in m	DO	U	-	3.2	4.8
SC.Q_Under	Underflow of secondary settler, in m^3/d	DO	U	-	16518.4	24777.6
sec_sludge_to_AD	Secondary sludge to AD, in m^3/d	DO	U	-	240	360
thickener.rem_perc	TSS removal fraction in thickener	DO	U	-	0.96	1
thickener.X_under	TSS underflow concentration, as fraction	DO	U	-	0.056	0.084
Vol_aer	Volume of each aerated tank, in m^3	DO	U	-	2400	3600
Vol_anox	Volume of each anoxic tank, in m^3	DO	U	-	1200	1800
f_P	Henze et al. [1987]	WT	T	0.08	0.076	0.084
F_TSS_COD	TSS/COD ratio	WT	T	0.75	0.7125	0.7875
i_X_B	Henze et al. [1987]	WT	T	0.08	0.076	0.084
i_X_P	Henze et al. [1987]	WT	T	0.06	0.057	0.063
k_a	Henze et al. [1987]	WT	T	0.05	0.025	0.075
k_h	Henze et al. [1987]	WT	T	3	1.5	4.5
K_NH	Henze et al. [1987]	WT	T	1	0.5	1.5
K_NO	Henze et al. [1987]	WT	T	0.5	0.25	0.75
K_OA	Henze et al. [1987]	WT	T	0.4	0.2	0.6
K_OH	Henze et al. [1987]	WT	T	0.2	0.1	0.3
K_S	Henze et al. [1987]	WT	T	10	5	15
K_X	Henze et al. [1987]	WT	T	0.1	0.05	0.15
mu_A	Henze et al. [1987]	WT	T	0.5	0.4	0.6
mu_A_b_A	mu_A/b_A ratio, for correlation	WT	U	-	9.5	10.5
mu_H	Henze et al. [1987]	WT	T	4	3.2	4.8
mu_H_b_H	mu_H/b_H ratio, for correlation	WT	U	-	12.66	13.99
n_g	Henze et al. [1987]	WT	T	0.8	0.64	0.96
n_h	Henze et al. [1987]	WT	T	0.8	0.64	0.96
PC.f_X	Otterpohl et al. [1994]	WT	T	0.86	0.765	0.935
SC.f_ns	Takács et al. [1991]	WT	T	0.0023	0.0018	0.0027
SC.r_H	Takács et al. [1991]	WT	T	0.0006	0.0005	0.0007
SC.r_P	Takács et al. [1991]	WT	T	0.00286	0.00228	0.00343
SC.v0	Takács et al. [1991]	WT	T	474	379.2	568.8
SC.v00	Takács et al. [1991]	WT	T	250	200	300
SC.X_Lim	Takács et al. [1991]	WT	T	900	720	1080
SC.X_T	Takács et al. [1991]	WT	T	3000	2400	3600
Y_A	Henze et al. [1987]	WT	T	0.67	0.6365	0.7035
Y_H	Henze et al. [1987]	WT	T	0.24	0.228	0.252
AD.kdis	Batstone et al. [2002]	ST	T	0.7	0.5	1
AD.khyd_ch	Batstone et al. [2002]	ST	T	0.8	0.5	1
AD.khyd_li	Batstone et al. [2002]	ST	T	1.1	0.7	1.5
AD.khyd_pr	Batstone et al. [2002]	ST	T	1.1	0.7	1.5
AD.KI_nh3_ac_km_ac	KI_nh3_ac/km_ac ratio, for correlation	ST	U	-	0.00013	0.00015
AD.kla	Batstone et al. [2002]	ST	T	150	50	200
AD.km_ac	Batstone et al. [2002]	ST	T	10	8	12
AD.km_c4	Batstone et al. [2002]	ST	T	15	10	20
AD.km_fa	Batstone et al. [2002]	ST	T	15	10	20
AD.km_pro	Batstone et al. [2002]	ST	T	10	8	12
AD.Ks_ac_km_ac	Ks_ac/km_ac ratio, for correlation	ST	U	-	0.025	0.083
AD.Ks_c4_km_pro	Ks_c4/km_pro ratio, for correlation	ST	U	-	0.025	0.1
AD.Ks_fa_km_pro	Ks_fa/km_pro ratio, for correlation	ST	U	-	0.025	0.1
AD.Ks_pro_km_pro	Ks_pro/km_pro ratio, for correlation	ST	U	-	0.025	0.083
ADM2ASM.frxs_AS	Nopens et al. [2008]	ST	T	0.7505	0.711	0.79
ASM2ADM.frlixb	Nopens et al. [2008]	ST	T	0.4	0.38	0.42
ASM2ADM.frlixs	Nopens et al. [2008]	ST	T	0.7	0.665	0.735
ASM2ADM.frxs	Nopens et al. [2008]	ST	T	0.646	0.612	0.68

3. RESULTS

Four different MC experiments were performed to conduct the SA on: (1) design and operational parameters, (2) wastewater treatment parameters, (3) sludge treatment parameters and (4) all parameters together.

Performing the SA on the design and operational parameters, no less than 17 out of 19 parameters are significant for all three criteria based on the SRCs and 12 based on the PCCs. PCCs are indeed known to produce a smaller number of significant parameters [Manache and 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. The surface of the secondary clarifier and the anoxic volume are very important for the EQI.

From the analysis on the wastewater treatment parameters, only 4 out of the 28 parameters were judged as not significant for the SRCs and 9 for the PCCs, in this case because of the very different importance of the parameters towards environmental and economic performance. The only ones that strongly influence both EQI (but not NH_4) and OCI are Y_H of ASM1 and r_P and v0 of the secondary clarifier model. Very important for EQI and NH_4 are both K_OA and K_OH.

For the sludge treatment parameters, only one parameter out of 18 can be considered as not significant for all three criteria based on the SRCs, and 7 based on the PCCs. Clearly the most significant are khyd_pr of ADM1 and frxs of the AS/AD interface.

From Table 3, which shows the results for the SA on all parameters together, the three BSM2 evaluation criteria are mostly sensitive to design and operational parameters, and largely not to sludge treatment parameters. Ten out of 65 parameters were identified as not sensitive based on their *t*-statistic for SRC. With the significance tested on the *t*-statistic for the PCCs, only 25 of the original 65 parameters are classified as significant, with most of the AD parameters being not significant. An R^2>0.7 indicates a good quality of the linear regression.

Figure 1 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 design and operational parameters, as suggested by the figures in Table 3.

The sludge treatment parameters only contribute to the OCI variability, because of the importance of methane production for cost recovery. The AD is largely dimensioned and is very stable in open loop. The complexity of ADM1 might be required in closed loop configurations which alter the AD influent and/or operation, pushing it towards instability.

Performing the uncertainty analysis on the BSM2 with the 25 most significant parameters only, the overall uncertainty in model output is practically unchanged, as can be seen in Figure 1. This means that sensitivity and uncertainty analyses on BSM2 can be performed by only assuming that reduced parameter set to be uncertain. Such reduced analysis will not lead to a loss of significant information and will be significantly faster to conduct.

To verify the transferability of these results to different configurations of the BSM2 (e.g. a control strategy), a SA was conducted for the open loop configuration on the 38 wastewater and sludge treatment parameters, which are the parameters to be considered for SA in case a specific design and operation configuration has to be evaluated. Based on the significance for the PCCs (see Table 3), a reduced set of 24 parameters can be accepted. Figure 2 shows the variability of the three evaluation criteria with the full and the reduced parameter sets for the open loop and a basic closed loop, consisting of a simple dissolved oxygen controller on the three aerated tanks, which strongly reduces the NH_4 exceedance period. It is evident that the changes in output variability from the full to the reduced parameter set are practically negligible in both BSM2 configurations.

Table 3. PCCs and ranking of all the parameters; 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; in bold face not significant for SRC and PCC from the SA on WT and ST parameters (fixed DO parameters).

		EQI R^2=0.71		NH_4 R^2=0.97		OCI R^2=0.99	
Parameter	Group	PCC	rank	PCC	rank	PCC	rank
AD.V_gas	DO	0.01731	27	0.00757	32	-0.00040	58
AD.V_liq	DO	0.00956	35	-0.00630	34	-0.07242	10
ASU3.Kla	DO	-0.08355	10	-0.18763	2	0.15281	5
ASU4.Kla	DO	-0.10341	7	-0.17658	3	0.15493	4
ASU5.Kla	DO	-0.05268	15	-0.11993	4	0.07767	9
C_source	DO	-0.02537	22	0.02833	13	0.24269	3
dewatering.rem_perc	DO	0.00081	61	0.01247	23	0.01504	23
dewatering.X_under	DO	0.00487	45	-0.00791	30	0.00023	62
internal_rec	DO	-0.04679	17	-0.01410	20	0.08078	8
PC.f_PS	DO	-0.01618	28	-0.01307	21	0.39139	1
PC.Vol	DO	-0.02056	23	-0.04589	7	-0.08159	7
SC.A	DO	-0.20355	2	-0.00406	46	0.05186	13
SC.H	DO	-0.01974	24	0.00036	61	0.00369	41
SC.Q_Under	DO	-0.01106	33	-0.00099	57	-0.01100	27
sec_sludge_to_AD	DO	-0.00290	53	0.00358	51	0.02354	20
thickener.rem_perc	DO	0.00886	37	0.00762	31	0.00679	32
thickener.X_under	DO	0.00879	38	0.00396	47	-0.08870	6
Vol_aer	DO	-0.41771	1	-0.50165	1	0.35651	2
Vol_anox	DO	-0.09818	9	0.00343	52	0.02873	18
f_P	WT	0.00571	43	-0.00442	44	0.01851	21
F_TSS_COD	WT	0.00002	65	0.00859	27	0.01617	22
i_X_B	WT	-0.00213	55	-0.01245	24	0.00064	54
i_X_P	WT	0.00279	54	-0.00097	58	0.00050	57
k_a	WT	-0.06743	12	0.01114	25	-0.00038	59
k_h	WT	-0.02652	21	0.03058	10	0.00836	29
K_NH	WT	0.07427	11	0.03390	9	0.00114	50
K_NO	WT	0.03002	19	0.00165	55	-0.00022	63
K_OA	WT	0.15490	3	0.08899	5	0.00052	56
K_OH	WT	-0.14524	4	-0.03852	8	-0.00098	52
K_S	WT	0.00911	36	0.00521	39	-0.00008	65
K_X	WT	0.01856	25	-0.01730	16	-0.00389	38
mu_A	WT	-0.05464	14	-0.03004	11	-0.00015	64
mu_A_b_A	WT	-0.00649	42	-0.00034	62	0.00097	53
mu_H	WT	0.00072	63	0.02927	12	-0.01045	28
mu_H_b_H	WT	-0.01421	31	-0.02033	14	0.00220	44
n_g	WT	-0.06272	13	-0.01773	15	0.00123	47
n_h	WT	-0.02662	20	0.01285	22	0.00117	49
PC.f_X	WT	-0.00212	57	-0.00491	42	-0.00423	35
SC.f_ns	WT	0.04716	16	0.00390	48	-0.01104	26
SC.r_H	WT	0.11410	6	0.00537	38	-0.03566	15
SC.r_P	WT	-0.10327	8	0.00817	28	0.03038	17
SC.v0	WT	-0.11726	5	0.00581	37	0.03212	16
SC.v00	WT	-0.00212	56	0.01428	19	0.00372	40
SC.X_Lim	WT	-0.00957	34	-0.00017	64	0.00024	61
SC.X_T	WT	-0.00106	59	-0.00050	60	0.00032	60
Y_A	WT	-0.01787	26	-0.01546	18	0.00118	48
Y_H	WT	0.04541	18	-0.08133	6	0.07165	11
AD.kdis	ST	0.00071	64	0.00165	54	-0.00384	39
AD.khyd_ch	ST	-0.00331	51	-0.00185	53	-0.01456	24
AD.khyd_li	ST	0.00150	58	0.01009	26	-0.02715	19
AD.khyd_pr	ST	0.01463	30	0.00588	36	-0.04839	14
AD.KI_nh3_ac_km_ac	ST	0.00667	41	0.00811	29	-0.00100	51
AD.kla	ST	-0.00352	50	0.00373	50	0.00132	46
AD.km_ac	ST	-0.00439	48	-0.00617	35	-0.00409	37
AD.km_c4	ST	0.00105	60	0.00030	63	-0.00245	42
AD.km_fa	ST	-0.00479	46	0.00141	56	-0.00226	43
AD.km_pro	ST	-0.00851	39	-0.00433	45	0.00421	36
AD.Ks_ac_km_ac	ST	-0.00331	52	0.00494	41	0.01417	25
AD.Ks_c4_km_pro	ST	-0.00466	47	0.00733	33	0.00811	30
AD.Ks_fa_km_pro	ST	-0.00383	49	-0.00002	65	0.00425	34
AD.Ks_pro_km_pro	ST	-0.01571	29	-0.01715	17	0.00729	31
ADM2ASM.frxs_AS	ST	0.00074	62	0.00088	59	-0.00056	55
ASM2ADM.frlixb	ST	-0.00560	44	-0.00519	40	0.00147	45
ASM2ADM.frlixs	ST	0.00774	40	0.00482	43	-0.00560	33
ASM2ADM.frxs	ST	0.01408	32	0.00386	49	-0.06466	12

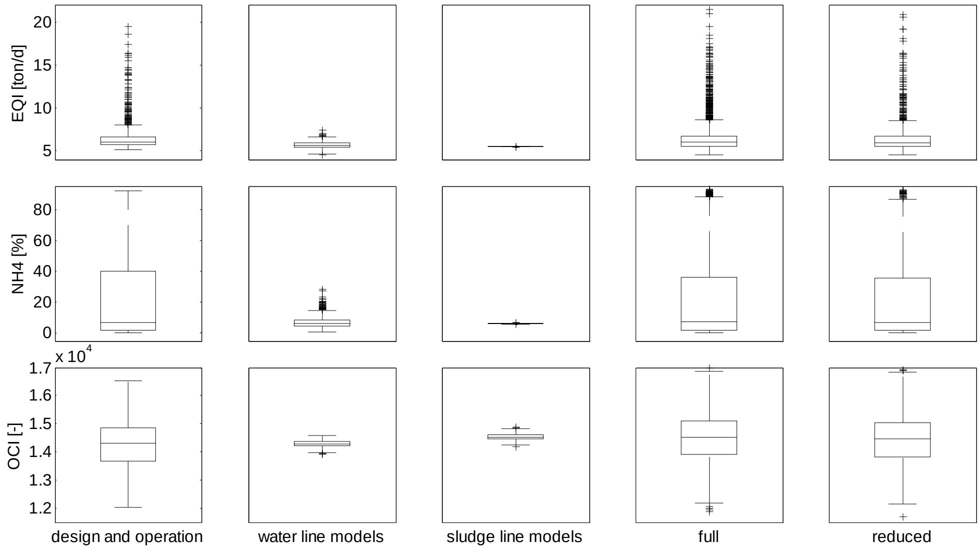

Figure 1. Variability box plots of the three BSM2 evaluation criteria for the three parameter categories separately, altogether ("full") and with the reduced set of uncertain parameters ("reduced").

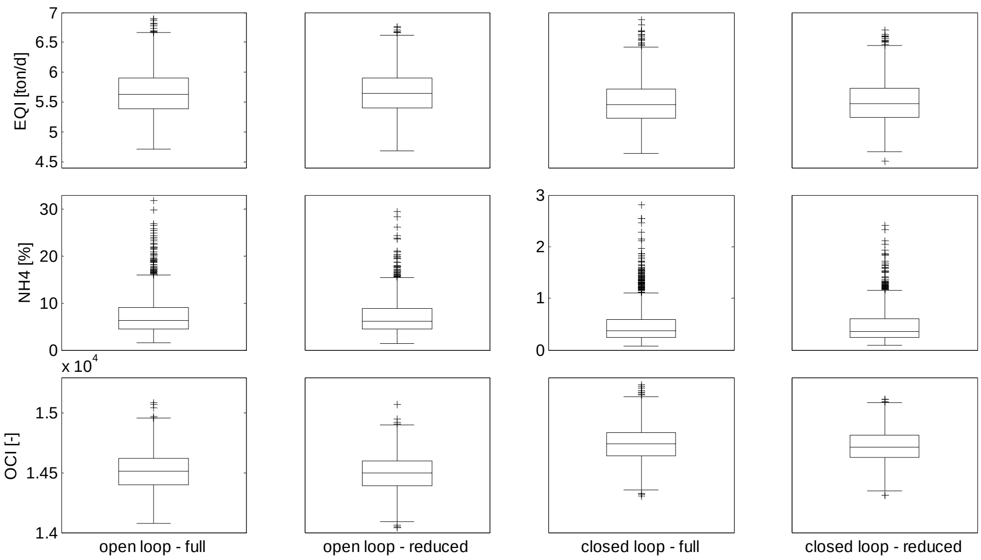

Figure 2. Variability box plots of the three BSM2 evaluation criteria for open loop and closed loop, with all wastewater and sludge treatment parameters ("full") and with the reduced set of uncertain parameters ("reduced").

4. CONCLUSIONS

Given the complexity of the BSM2 and the MC computational load, it is found useful to perform some preliminary numerical solver optimisation by means of solver setting exploration and downsampling of the output file. Proper solver selection could reduce the time required for computation by a factor of 5. This involved the use of the CVODE solver with specific settings for IterationMethod (Newton), LinearMultistepMethod (Adams), LinearSolver (SPGMR) and Accuracy (10^{-3}).

The required number of MC simulations was found to be 50 times the number of parameters to be tested.

The most sensitive BSM2 parameters belong to the design and operational group, especially for the OCI and NH_4 criteria, while for the EQI also some of the wastewater treatment parameters are of high importance. The sludge treatment parameters have hardly any significance for the three evaluation criteria. In particular, primary settling parameters are important with respect to the economic performance of the plant.

Based on our results, the output-parameter sensitivity Jacobian can be reduced from 65 to 25 key parameters in case all parameters are considered. When a specific design and operation parameter set has to be evaluated (e.g. to assess the output variability of a control strategy), the number of wastewater and sludge treatment uncertain parameters can be reduced from 38 to 24.

These results make the execution of future sensitivity and uncertainty analysis studies more feasible.

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REFERENCES

Batstone, D.J., J. Keller, I. Angelidaki, S.V. Kalyuzhnyi, S.G. Pavlostathis, A. Rozzi, W.T.M. Sanders, H. Siegrist and V.A. Vavilin, Anaerobic digestion model no.1., IWA STR no.13, IWA Publishing, London, UK, 2002.

Batstone, D.J., P.F. Pind and I. Angelidaki, Kinetics of thermophilic, anaerobic oxidation of straight and branched chain butyrate and valerate, *Biotechnology and Bioengineering*, 84(2), 195-204, 2003.

Batstone, D.J., M. Torrijos, C. Ruiz and J.E. Schmidt, Use of an anaerobic sequencing batch reactor for parameter estimation in modelling of anaerobic digestion, *Water Science and Technology*, 50(10), 295-303, 2004.

Benedetti, L., D. Bixio, F. Claeys and P.A Vanrolleghem, Tools to support a model-based methodology for emission/immission and benefit/cost/risk analysis of wastewater treatment systems which considers uncertainties. *Environmental Modelling & Software*, 23(8), 1082-1091, 2008.

Claeys, F., D. De Pauw, L. Benedetti, I. Nopens, and P.A. Vanrolleghem, Tornado: a versatile efficient modelling & virtual experimentation kernel for water quality systems, iEMSs 2006 Conference, Burlington, VT, 2006a.

Claeys, F., P.A. Vanrolleghem and P. Fritzson, Boosting the efficiency of compound virtual experiments through a priori exploration of the solver setting space, 2006 European Modelling and Simulation Symposium (EMSS), October 4-6, Barcelona, Spain, 2006b.

Copp J.B. (ed.) The COST simulation benchmark: description and simulator manual. Office for Official Publications of the European Community, Luxembourg. 154 pages, 2002.

Hindmarsh, A.C., P.N. Brown, K.E. Grant, S.L. Lee, R. Serban, D.E. Shumaker, and C.S. Woodward. SUNDIALS: suite of nonlinear and differential/algebraic equation solvers, *ACM Transactions on Mathematical Software*, 31(3), 363-396, 2005.

Jeppsson, U., M.-N. Pons, I. Nopens, J. Alex, J.B. Copp, K.V. Gernaey, C. Rosen, J.-P. Steyer and P.A. Vanrolleghem, Benchmark simulation model no 2: general protocol and exploratory case studies, *Water Science and Technology*, 56(8), 67-78, 2007.

Forsythe, G.E., M.A. Malcolm and C.B. Moler, Computer methods for mathematical computations, Englewood Cliffs, NJ Prentice-Hall, 1977.

Henze, H., C.P.L. Jr Grady, W. Gujer, G.v.R. Marais and T. Matsuo, Activated sludge model no.1. IWA STR no.1, IWA Publishing, London, UK, 1987.

Manache, G. and C.S. Melching, Identification of reliable regression- and correlation-based sensitivity measures for importance ranking of water-quality model parameters, *Environmental Modelling & Software*, 23(5), 549-562, 2008.

Morrison, D.F., Multivariate statistical methods, Mc-Graw Hill, Singapore, 1984.

Nopens, I., D. Batstone, J.B. Copp, U. Jeppsson, E. Volcke, J. Alex and P.A. Vanrolleghem, A new interface for ASM-ADM for use in the Benchmark simulation model no.2., *Water Research* (submitted), 2008.

Otterpohl, R., M. Raak and T. Rolfs, A mathematical model for the efficiency of the primary clarification, IAWQ 17th Biennial International Conference, 24–29 July, Budapest, Hungary, 1994.

Ráduly, B., K.V. Gernaey, A.G. Capodaglio, P.S. Mikkelsen and M. Henze, Artificial neural networks for rapid WWTP performance evaluation: methodology and case study. *Environmental Modelling & Software* 22(8), 1208-1216, 2007.

Rousseau, D., F. Verdonck, O. Moerman, R. Carrette, C. Thoeye, J. Meirlaen and P.A. Vanrolleghem, Development of a risk assessment based technique for design/retrofitting of WWTPs. *Water Science and Technology* 43(7), 287-294, 2001.

Saltelli A., K. Chan and E.M. Scott (eds.), Sensitivity analysis, Wileys series in probability and Statistics, 2000.

Siegrist H., D. Vogt, J. Garcia-Heras and W. Gujer, Mathematical model for meso and thermophilic anaerobic sewage sludge digestion, *Environmental Science and Technology* 36, 1113-1123, 2002.

Takács, I., G.G. Patry and D. Nolasco, A dynamic model of the clarification thickening process. *Water Research*, 25(10), 1263-1271, 1991.