Supplementary information with:

Effective measuring campaigns for reliable and informative full-scale WWTP data

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Appendix A. Previous studies with data-reconciliation-related content

This appendix presents an overview of published studies which applied data reconciliation to wastewater treatment plants.

Table A1. Data reconciliation and related topic applied to WWTPs

#	Study	Data reconciliation-related content	System	software
Direct application to process data of WWTP				
1	(Strous et al., 1998)	Calculating stoichiometry of conversions of carbon and nitrogen compounds by Anammox	Lab-scale reactor	Macrobal
2	(Nowak et al., 1999)	Validating operational data for modelling purposes	Pilot WWTP	
3	(Meijer et al., 2002)	Validating and reconciliation data for modelling purposes	Full-scale municipal WWTP	Macrobal
4	(Puig et al., 2008)	Operational condition calculation (e.g. solid retention time, oxygen requirement) and benchmarking using reconciled data	Full-scale municipal WWTP	Macrobal
5	(Lim et al., 2012)	Estimate N_2O emission from the membrane reactor using reconciled flow data	Pilot municipal WWTP	
6	(Villez et al., 2013a)	Bilinear data reconciliation applied to flow and total suspended solid measurements to detect sensor fault	Simulated data from BSM1_LT	Matlab
7	(Lotti et al., 2014)	Calculating stoichiometry of conversions of carbon and nitrogen compounds by Anammox.	Lab-scale reactor	Macrobal
8	(Meijer et al., 2015)	Reconciled data for modelling calibrating and validating	Full-scale municipal WWTP	Macrobal
9	(Lee et al., 2015)	Demonstrate data reconciliation, raising the importance of reliable data	Simulated data from GPS-X	
10	(Behnami et al., 2016)	Evaluating the performance of a WWTP using reconciled data	Full-scale industrial WWTP	Matlab
Redundancy analysis and variable classification				
12	(Villez et al., 2013b)	Application of a graph-theoretical method for the classification of variables for a given sensor configuration	Simulated data from BSM1_LT	Matlab
13	(Spindler, 2014)	Deriving redundancy mass balances for a given WWTP configuration given measured and unmeasured variables (flows and concentrations)	WWTP	Sage Mathematics
14	(Villez et al., 2016)	Method to obtain Pareto optimal flow sensor layouts in terms of cost, observability, and	WWTP	Matlab

#	Study	Data reconciliation-related content	System	software
		redundancy that enable fault detection for a given WWTP configuration		
Substance flow analysis				
16	(Sokka et al., 2004)	Balanced data for examining the flows of nitrogen and phosphorus in the municipal waste	Municipality	STAN
17	(Benedetti et al., 2006)	Balancing data for water, BOD, COD, total nitrogen, total phosphorus, Zn of the wastewater collection and treatment system	Sewer catchment	
18	(Yoshida et al., 2015)	Examining the fate of organic carbon, heavy metals and organic pollutants in a WWTP	Full-scale municipal WWTP	STAN
19	(Kim et al., 2017)	Substance flow analysis of mercury from industrial and municipal wastewater treatment facilities	Full-scale industrial WWTP	STAN
Others				
20	(Rieger et al., 2010)	Mass balance-based to validate historical data from a WWTP for modelling purposes	WWTP	

Appendix B. Experimental design procedure for data reconciliation

B1. Overview

The experimental design procedure for practical application to wastewater treatment processes of Le et al. (2018) is summarized in Figure B1. The first three steps comprise the gathering of case-study-specific input information: the main goals and corresponding key variables are defined first (Step 1), followed by the set-up of an incidence matrix and mass balances based on the process flow diagram (Step 2), and by the inventory of available data (Step 3). The gathering of input information, which is most time-consuming, is followed by a fully automated procedure for finding optimal solutions. It is checked up-front that the combination of the given list of key variables and the given set of mass balances are relevant in the sense that key variables are identifiable (Step 4). Mass balances and their corresponding variables are clustered in groups of overlapping mass balances (Step 5), which greatly improves the efficiency of finding all solutions, i.e. sets of additionally measured variables that satisfy the defined main goal (Step 6). Steps 4-6 rely on a comprehensive redundancy analysis, following the method of van der Heijden et al. (1994). Among all solutions, a selection is made of optimal ones in terms of additional measurement costs and accuracy of identified key variables (Step 7). Step 4 to Step 7 were implemented in MATLAB 2014b (MathWorks®). More details on the individual steps are provided in Le et al. (2018).

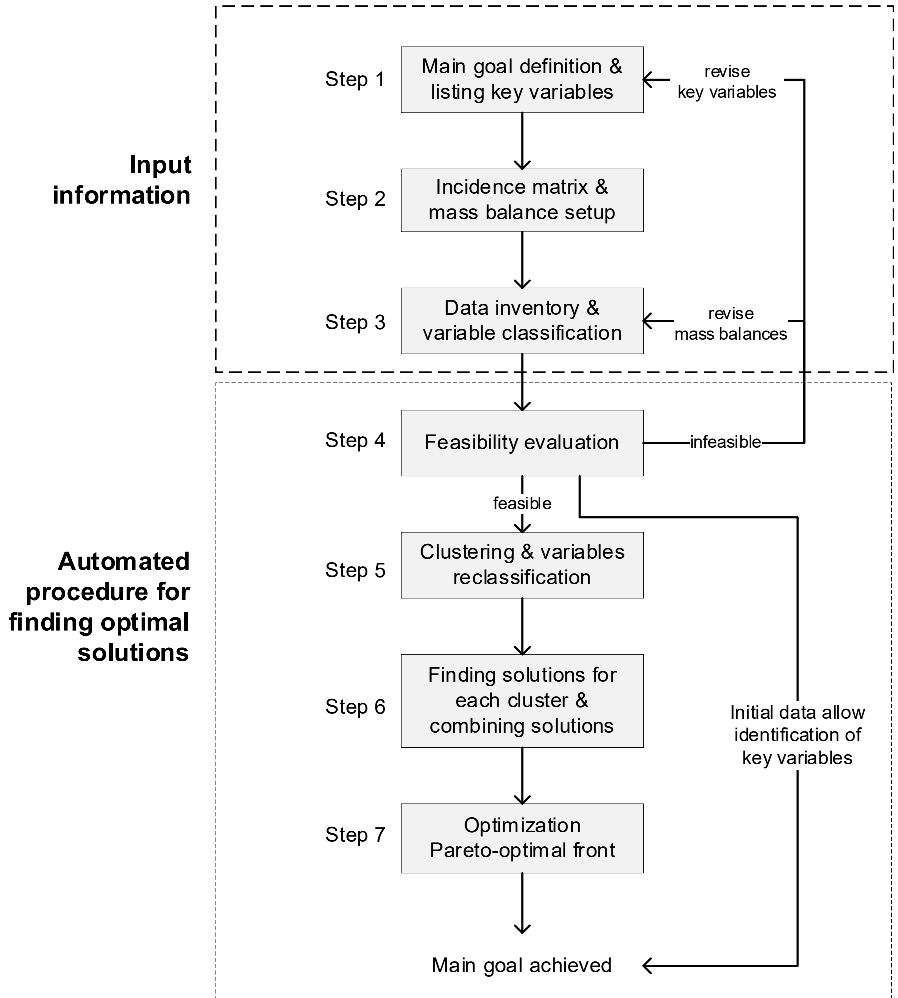

Figure B1. Experimental design procedure for the selection of sets of additionally measured variables that allow the identification of key variables (Le et al., 2018).

B2. Pareto-optimal solutions balancing cost and accuracy

The additional measurement costs and the accuracy of identified key variables were quantified through a cost function f_C and an accuracy function f_V, respectively, which are calculated according to Le et. al. (2018):

$$f_C = \sum_{j=1}^{n_P} w_{aj} \cdot a_j \qquad \text{(Eq. B1)}$$

$$f_V = \frac{1}{n_k} \sum_{i=1}^{n_k} v_i / v_i^r \qquad \text{(Eq. B2)}$$

in which

- n_P is the number of potential additional measurements
- a_j is a binary number indicating whether a potential additional measured variable with index j (=1,… n_P) is measured (1) or not measured (0) (see Tables C2b, C3b, C4b and C5b for application to the case studies).
- w_{aj} is the cost of additional measurement j (given in Table C1, C2a, C3a, C4a and C5a for the case studies).
- n_k is the number of key variables.
- v_i is the variance of new estimates (after data reconciliation) of key variables of a solution
- v_i^r is the variance of new estimates of key variable when the reference solution is implemented, i.e. when all additional measurements are performed.
- v_i and v_i^r were calculated from measurement uncertainty σ of the reported measured data (Table C1, C2a, C3a, C4a and C5a for the case studies) according to the procedures specified in the Supplementary Information of Le et al. (2018).

Appendix C. Measured data sets and Pareto-optimal solutions for the case studies considered

C1. Case study 1: Meijer et al. (2002), average data of one year

Table C1. Measured data set used for data reconciliation by (Meijer et al., 2002) - case study 1

	variable →	**Q** [$m^3 \cdot day^{-1}$]			**TP** [$g\ P \cdot m^{-3}$]			**COD** [$g\ COD \cdot m^{-3}$]			**TKN** [$g\ N \cdot m^{-3}$]			**NOx** [$g\ N \cdot m^{-3}$]		
	↓ stream	m	w_a	σ	m	w_a	σ	m	w_a	σ	m	w_a	σ	m	w_a	σ
in	influent	1*	10	2,000	1*	10	100	1*	10	2000	1*	10	1000	1*	10	2
ef	effluent		10	2,000	1*	10	10	1*	10	2000	1*	10	1000	1*	10	2
ce	inflow centrifuge	1*	10	100	1*	10	100	1*	10	100	1*	10	50	1*	10	2
cent	outflow centrifuge		10	100	1*	10	100	1*	10	100	1*	10	50		10	2
ex	excess sludge	1*	10	100	1*	10	100		10	100		10	50	1*	10	2

Note
Q = flow rate, TP = total phosphorus, COD = chemical oxygen demand, TKN = Kjeldahl nitrogen, NOx = nitrate.
m = measurement availability: 1 = measured, empty = unmeasured.
* variable included in initial data set provided by (Meijer et al., 2002)
w_a = cost of measurements (assumed to be the same for all measurements)
σ = magnitude of measurement uncertainty (derived from reported measured data)

C2. Case study 2: Meijer et al. (2002), data from measurement campaign of 8 days

Table C2a. Measured data set used for data reconciliation by Meijer et al. (2002) - case study 2

	Short Name	Q $[m^3 \cdot day^{-1}]$			TP $[g\ P \cdot m^{-3}]$			TKN $[g\ N \cdot m^{-3}]$		
		m	w_a	σ	m	w_a	σ	m	w_a	σ
in	influent	1*	10	1,000	1*	10	50	1*	10	500
r1	R1 to R2		10	1,000	1	10	50	1	10	500
rc	recycle R3 to R2	1	10	1,000	1	10	50	1	10	500
r2	R2 to R3		10	1,000	1	10	50		10	500
r3	R3 to clarifier		10	1,000		10	50		10	500
rt12	clarifier CL12 to R2 and TH	1	10	1,000	1	10	50	1	10	500
ef	effluent		10	1,000	1	10	50		10	500
rt34	clarifier CL34 to R1 and R2	1	10	1,000	1	10	10	1	10	10
th	inflow thickening	1	10	100	1	10	50		10	50
over	overflow thickening TH		10	100		10	50	1	10	50
ce	input centrifuge	1*	10	100	1*	10	50		10	50
cent	output centrifuge		10	100	1*	10	50	1*	10	50
ex	excess sludge	1*	10	100		10	50		10	50

Note:
Q = flow rate, TP = total phosphorus concentration, TKN = Kjeldahl nitrogen concentration
m = measurement availability, 1 = measured, empty = unmeasured
* variable included in initial data set provided by (Meijer et al., 2002)
w_a = cost of measurements (assumed to be the same for every measurement)
σ = magnitude of measurement uncertainty (derived from reported measured data)

Table C2b. Pareto-optimal solutions from experimental design procedure applied to the setup of Meijer et al. (2002). For all potential additional measurements, it is indicated whether (1) or not (empty) they should be included in the measurement campaign.

#	a	fc	fv	Q_{r1}	Q_{r2}	Q_{r3}	Q_{rc}	Q_{rt12}	Q_{rt34}	Q_{ef}	Q_{th}	Q_{ce}	Q_{over}	Q_{cent}	Q_{ex}
1	7	70	1.96		1		1	1	1		1	1		1	
2	8	80	1.55		1		1	1	1		1	1	1		1
3	9	90	1.39		1		1	1	1	1	1	1	1		1
4	10	100	1.24		1		1	1	1	1	1	1	1	1	1
5	11	110	1.13	1	1		1	1	1	1	1	1	1	1	1
6	12	120	1.05	1	1	1	1	1	1	1	1	1	1	1	1

= solution number, a = additional measurements, fc = cost of additional measurements (the lower the better), fv = accuracy of the solution (the smaller the more accurate)

C3. Case study 3: Puig et al. (2008)

Table C3a. Measured data set used for data reconciliation by Puig et al. (2008)

Short Name		Q [$m^3 \cdot day^{-1}$]			TP [$g\ P \cdot m^{-3}$]			COD [$g\ COD \cdot m^{-3}$]			NO [$g\ N \cdot m^{-3}$]			TKN [$g\ N \cdot m^{-3}$]		
		m	w_a	σ	m	w_a	σ	m	w_a	σ	m	w_a	σ	m	w_a	σ
in	influent	1*	10	1000	1*	10	100	1*	10	500	1*	10	2	1*	10	250
se	stripper effluent	1	10	100	1	10	10	1	10	50	1	10	2	1	10	25
2	outflow of anaerobic tank	1	10	1000	1	10	100		10	500		10	2		10	250
ras	return activated sludge	1	10	1000	1	10	200		10	500		10	2		10	250
a	sludge recycling from anoxic tank	1	10	100	1	10	100		10	50		10	2		10	25
6	outflow of anoxic tank	1	10	3000	1	10	300		10	1500		10	2		10	750
7	out flow of alternate aerated tank	1	10	3000		10	300		10	1500		10	2		10	750
c	sludge recycling from aerobic tank c	1	10	2000		10	200		10	1000		10	2		10	500
b	sludge recycling from aerobic tank b	1	10	2000	1	10	200		10	1000		10	2		10	500
8	settled sludge from clarifiers	1	10	1000	1	10	100		10	500		10	2		10	250
ef	effluent	1	10	1000	1*	10	100	1*	10	500	1*	10	2	1*	10	250
was	wasted activated sludge	1	10	10	1	10	10	1	10	5	1	10	2	1	10	2.5

Note
Q = flow rate, TP = total phosphorus, COD = chemical oxygen demand, TKN = Kjeldahl nitrogen, NO = nitrate.
m = measurement availability: 1 = measured, empty = unmeasured
* variable included in initial data set (assuming that only influent flow and concentration were measured)
w_a = cost of measurements (assumed to be the same for every measurement)
σ = magnitude of measurement uncertainty (derived from reported measured data)

Table C3b. Pareto-optimal solutions provided by the experimental design procedure to identify all key variables. Additional measurement should be included in measurement campaign (1) or not (empty).

				Q											TP								COD		NO		TKN	
#	a	fc	fv	se	2	ras	a	6	7	c	b	8	ef	was	se	2	ras	a	6	b	8	was	se	was	se	was	se	was
1	11	110	1.24	1									1	1	1							1	1	1	1	1	1	1
2	13	130	1.08	1	1		1						1	1	1							1	1	1	1	1	1	1
3	15	150	1.04	1	1	1	1					1	1	1	1							1	1	1	1	1	1	1
4	17	170	1.01	1	1	1	1					1	1	1	1	1		1				1	1	1	1	1	1	1
5	19	190	1	1	1	1	1					1	1	1	1	1	1	1			1	1	1	1	1	1	1	1
6	21	210	1	1	1	1	1	1			1	1	1	1	1	1	1	1			1	1	1	1	1	1	1	1
7	23	230	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1			1	1	1	1	1	1	1	1
8	25	250	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

= solution number, a = additional measurements, fc = cost of additional measurements (the lower the better), fv = accuracy of the solution (the smaller the more accurate)

C4. Case study 4: Meijer et al. (2015)

Table C4a. Measured data set used for data reconciliation by Meijer et al. (2015)

PFD	Short Name	Q $[m^3 \cdot day^{-1}]$			TP $[g\ P \cdot m^{-3}]$			COD $[g\ COD \cdot m^{-3}]$			TSS $[g \cdot m^{-3}]$		
		m	w_a	σ	m	w_a	σ	m	w_a	σ	m	w_a	σ
4	WWTP influent	1*	10	5,000	1*	10	50	1*	10	2000			
5	Reject water	1	10	500	1	10	50	1	10	1000			
7	Settled influent		10	5,000	1	10	50	1	10	2000			
15	Inflow secondary clarifiers		10	5,000	1	10	2000		10	1000			
17	WWTP effluent		10	5,000	1*	10	5	1*	10	100			
23	Return activated sludge	1	10	5,000	1	10	2000		10	50000			
26	Waste activated sludge (WAS)	1	10	100	1	10	50	1	10	1000	1	10	1000
27	Thickened WAS	1	10	10		10	10	1	10	1000	1	10	1000
28	Primary sludge	1	10	500	1	10	50	1	10	1000			
31	Thickened primary sludge	1	10	50		10	20	1	10	1000			
34	Digested sludge	1	10	50		10	50	1	10	1000			
35	WWTP waste sludge	1	10	10	1	10	50	1	10	1500			
37	Centrate WAS thickening		10	100		10	50		10	500	1	10	1000
38	Centrate dewatering		10	50		10	50		10	500			
39	Overflow primary thickener		10	1,000		10	100		10	500			
40	Process water	1*	10	5	x	10	2	x	10	2			
43	Biogas	1*	10	500	x	10	10	1*	10	1000			

Note:
Q = flow rate, TP = total phosphorus, COD = chemical oxygen demand, TSS = total suspended solids
m = measurement availability: 1 = measured, empty = unmeasured
* variable included in initial data set (assuming that influent, effluent, process water and biogas flow and concentration were measured)
w_a = cost of measurements (assumed to be the same for every measurement)
σ = magnitude of measurement uncertainty (derived from reported measured data)

Table C4b. Pareto-optimal solutions provided by the experimental design procedure to identify all key variables. Additional measurement should be included in measurement campaign (1) or not (empty).

#	a	fc	fv	Q														TP							COD								TSS		
				5	7	15	17	23	26	27	28	31	34	35	37	38	39	5	7	15	23	26	28	35	5	7	26	27	28	31	34	35	26	27	37
1	18	180	2.21		1	1		1	1	1		1	1	1			1		1			1		1		1	1	1		1	1	1			
2	19	190	1.47	1	1	1		1	1	1	1	1	1	1					1			1		1		1	1	1		1	1	1			
3	20	200	1.25	1	1	1	1	1	1	1	1	1	1	1					1			1		1		1	1	1		1	1	1			
4	21	210	1.16	1	1	1	1	1	1	1	1	1	1	1	1				1			1		1		1	1	1		1	1	1			
5	22	220	1.09	1	1	1	1	1	1	1	1	1	1	1	1	1			1			1		1		1	1	1		1	1	1			
6	23	230	1.07	1	1	1	1	1	1	1	1	1	1	1	1	1	1		1			1		1		1	1	1		1	1	1			
7	24	240	1.05	1	1	1	1	1	1	1	1	1	1	1	1	1			1			1		1	1	1	1	1	1	1	1	1			
8	25	250	1.04	1	1	1	1	1	1	1	1	1	1	1	1	1	1		1			1		1	1	1	1	1	1	1	1	1			
9	26	260	1.03	1	1	1	1	1	1	1	1	1	1	1	1	1		1	1			1	1	1	1	1	1	1	1	1	1	1			
10	27	270	1.01	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1			1	1	1	1	1	1	1	1	1	1	1			
11	28	280	1.01	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1		1	1	1	1	1	1	1	1	1	1	1	1			
12	29	290	1.01	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1			
X	29	29	1.38	1	1*	1*	1	1	1	1	1	1	1	1				1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

= solution number, a = additional measurements, fc = cost of additional measurements (the lower the better), fv = accuracy of the solution (the smaller the more accurate). **x** = a solution when two more crucial additional variables (*) were added to the set of measurements used by Meijer et al. (2015)

C5. Case study 5: Behnami et al. (2016)

Table C5a. Measured data set used for data reconciliation by Behnami et al. (2016).

PFD	Short Name	**Q** [$m^3 \cdot day^{-1}$]		
		m	w_a	σ
in1	Influent process wastewater	**1***	10	500
in2	Sanitary wastewater	**1***	10	100
1	Screened influent	1	10	500
2	API	1	10	500
3	Equalization	1	10	500
4	DAF	1	10	500
5	Aeration	1	10	1,000
6	Clarifier 1	1	10	500
7	Clarifier 2	1	10	500
8	Treated effluent	1	10	500
9	Oily sludge from API	1	10	2
10	Sand & grit from API	1	10	2
11	Return effluent from DAF	1	10	2
12	Oily sludge from DAF	1	10	2
13	Returned activated sludge	1	10	500
14	Waste sludge clarifier 1	1	10	2
15	Waste sludge clarifier 2	1	10	2
16	Backwash water	1	10	2
17	Backwash eff	1	10	2

Q = flow rate
m = measurement availability: 1 = measured, empty = unmeasured
* variable included in initial data set (assuming that influents were measured)
wa = cost of measurements (assumed to be the same for every measurement)
σ = magnitude of measurement uncertainty (derived from reported measured data)

Table C5b. Pareto-optimal solutions provided by the experimental design procedure to balance all key variables.

#	a	fc	fv	Q_1	Q_2	Q_3	Q_4	Q_5	Q_6	Q_7	Q_8	Q_9	Q_{10}	Q_{11}	Q_{12}	Q_{13}	Q_{14}	Q_{15}	Q_{16}	Q_{17}
1	7	70	1.72								1	1	1		1		1	1	1	
2	8	80	1.41				1				1	1	1		1		1	1	1	
3	9	90	1.41				1		1		1	1	1		1		1	1	1	
4	10	100	1.25	1			1				1	1	1	1	1		1	1	1	
5	11	110	1.15	1		1	1				1	1	1	1	1		1	1	1	
6	12	120	1.09	1	1	1	1				1	1	1	1	1		1	1	1	
7	13	130	1.09	1	1		1			1	1	1	1	1	1		1	1	1	1
8	14	140	1.04	1	1		1		1	1	1	1	1	1	1		1	1	1	1
9	15	150	1.01	1	1	1	1		1	1	1	1	1	1	1		1	1	1	1
10	17	170	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

= solution number, a = additional measurements, fc = cost of additional measurements (the lower the better), fv = accuracy of the solution (the smaller the more accurate)

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