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Application of data reconciliation to a dynamically operated wastewater treatment process with off-gas measurements

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SUPPLEMENTARY INFORMATION

Supplementary Information A: Materials and methods

A1. Data reconciliation and gross error detection procedure

Data reconciliation

The general procedure for mass balance-based data reconciliation applied in this study was proposed by Le (2019), based on the work of Verheijen (2010), and is schematically represented in Figure A1. Data reconciliation requires three types of input information:
(1) A list of key process variables to be identified. These variables can be either measured or unmeasured ones.
(2) A pre-processed raw data set which contains mean values and standard error of the means of the measured variables.
(3) A set of mass balances based on the plant configuration, which the variables need to adhere to. The input form of mass balances determines the formulation of the objective function and the pre-processing of the input data

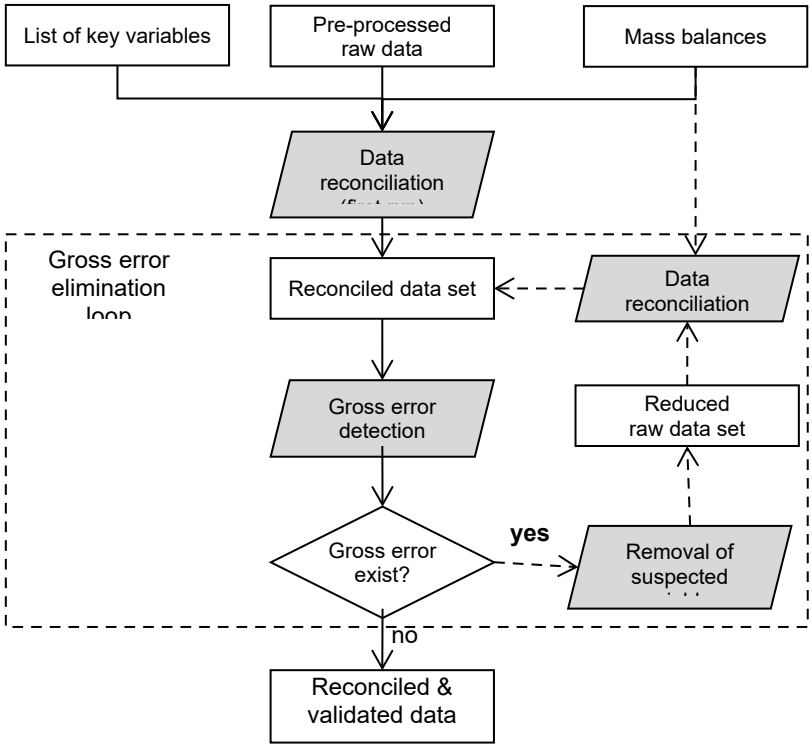

Figure A1. General mass-balance-based data reconciliation procedure (Le, 2019) applied in this study

The **identification of key process variables** means that their value is calculated from other, measured variables and from the prevailing constraints, such that improved estimates of their values are obtained. These new estimates, i.e., reconciled values, meet all the constraints (i.e., fit all mass balances) and are therefore considered more reliable and accurate (have a smaller standard deviation or error) than the original values. Key variables may be measured or not. In case a key variable is measured, the new estimate is considered improved compared to the original measurements. In case the key variable is not measured, the new estimate is considered improved compared to the value directly calculated from original measurements (using the available set of mass balances).

The objective function of the data reconciliation problem in this work was defined as the weighted least squares of the distance between the measurements vector and the vector of reconciled values weighted by the measurement error (Eq. 1).

$$\left.\begin{array}{l} min \sum \frac{(y-\bar{x})^2}{\sigma_y^2} \\ subject\ to\ \ f(\bar{x},u)=0 \end{array}\right\} \qquad \text{Eq.1}$$

in which y denotes measured variables, $\bar{x}$ reconciled variables and u unmeasured variables. $f(\bar{x},u)=0$ is a set of equality constraint equations or mass balances. σ_y^2 is a weighing factor, which usually the standard error of the mean of y. If it is assumed that the measurement errors are normally distributed with zero mean, the solution for this constrained optimization problem gives maximum likelihood estimates of process variables, so they are minimum variance and unbiased estimators (Verheijen, 2010).

The equality constrained nonlinear data reconciliation problem defined by Eq. 1 was solved using the classical method of Lagrange multiplier (Fletcher 2000).

The implementation of the data reconciliation procedure using the raw data set and a set of constraints will result in a reconciled data set. This reconciled data set typically contains four types of variables: reconciled measured variables, unreconciled measured variables, reconciled unmeasured variables and unreconciled unmeasured variables.

Gross error detection

The gross error is based on testing the data set against the alternative hypothesis: (1) the null hypothesis H_o that is no gross error is present and the alternative hypothesis H1: that gross errors are present.

Three common test reported in literature were used in this study namely the global, measurement, and nodal tests (Table 1). The global test compares each of the new estimates with the original measurements, $y - \bar{x}$. The nodal test substitutes each of the measurements into the active constraints, f(y). In these two cases the variances of the respective residuals can be derived easily. The measurement test makes use of the sum-of-squares of the residuals, which has a known distribution. All three tests calculated p-values, for the dataset (global and nodal test) or for individual variables (for the measurement test). When $p<0.05$ there is something wrong which could be a gross error, when $p \geqslant 0.05$ no gross error is detected.

Table 1. Basic tests in gross error detection (Verheijen, 2010)

Test	Description	Measure
Global test	Weighted sum of residuals squared gives an overall view	$y - \bar{x}$
Nodal test	Each individual constraint misfit is considered	f(y)
Measurement test	Each individual measurement is considered	$\sum (y-\bar{x})^2$

For more details on the data reconciliation and gross error detection procedures, the reader is referred to Le, 2019.

A2. Mass balances - stoichiometric and conversion factors

The information summarized in Table 2 results in the following mass balances (all in mol·h^{-1}), which have been applied in this study:

Mass balances including off-gas measurements

m1 (total nitrogen): $Q_{in}\cdot NH_{in}\cdot 1.053 - Q_{in}\cdot(1.053\cdot NH_{eff} + NO_{2eff} + NO3_{eff}) - Q_{off}\cdot K_{off}\cdot NO_{off} - Q_{off}\cdot K_{off}\cdot N_2O_{off} = 0$

m2 (oxygen): $(Q_{aer} + Q_{inf})\cdot O_{2aer}\cdot K_{aer} - Q_{in}\cdot(1.434\cdot NO_{2eff} + 1.934\cdot NO_{3eff}) - Q_{off}\cdot(N_2O_{off} + 1.25\cdot NO_{off})\cdot K_{off} - Q_{off}\cdot O_{2off}\cdot K_{off} - 0.428\cdot bCOD_{in}\cdot Q_{in} = 0$

m3 (carbon): $(TIC:NH)_{in}\ Q_{in}\cdot 1.053\cdot NH_{in} + (Q_{aer} + Q_{inf})\cdot CO_{2aer}\cdot K_{aer} + 0.303\cdot COD_{in}\cdot Q_{in} - Q_{off}\cdot CO_{2off}\cdot K_{off} - 0.067\cdot Q_{in}\cdot(NO_{2eff} + NO3_{eff}) = 0$

m4 (nitrogen gas): $(Q_{aer} + Q_{inf})\cdot(10^6 - O_{2aer} - CO_{2aer})\cdot K_{aer} - Q_{off}\cdot(10^6 - O_{2off} - CO_{2off})\cdot K_{off} = 0$

Mass balances without off-gas measurements

m5 (total nitrogen): $Q_{in}\cdot NH_{in}\cdot 1.053 - Q_{in}\cdot(1.053\cdot NH_{eff} + NO_{2eff} + NO3_{eff}) = 0$

m6 (oxygen): $OC - Q_{in}\cdot(1.434\cdot NO_{2eff} + 1.934\cdot NO3_{eff}) - 0.428\cdot COD_{in}\cdot Q_{in} = 0$

Table A1. Stoichiometric matrix of the biological conversions. Negative values denote consumption, positive values denote production.

components → [mole m^{-3}] **conversions ↓**	CH_xO_y (bCOD = organic carbon)	NH_4^+	CO_2	O_2	$C_5H_7NO_2$ (biomass)	NO_2^-	NO_3^-	N_2O	NO
NH_4^+ to NO_2^-		-1	$-5Y_N$	$-\frac{3-13Y_N}{2}$	Y_N	$1-Y_N$			
NH_4^+ to NO_3^-		-1	$-5Y_N$	$-2+7Y_N$	Y_N	$1-Y_N$			
NH_4^+ to N_2O		-2		-2				1	
NH_4^+ to NO		-4		-5					4
bCOD conversion	-1	$-Y$	$1-5Y$	$1+\frac{x}{4}-\frac{y}{2}-5Y$	Y				

yield of ammonium oxidizers Y_N= =0.0131 *mol*·mol-1 or 0.15 gCOD.gN^{-1} (de Kreuk et al., 2007)
yield of heterotrophs Y = 0.1395 *mol*·mol-1 or 0.67 gCOD.gCOD^{-1} (Henze et al., 2000)
a composition $CH_xO_y = CH_{1.5}O_{0.5}$ was assumed, corresponding with a COD content of 36 gCOD/mole

Table A2. Other conversion factors

#	factor	value	unit	description	assumption
1	K_{aer}	$\frac{10^{-6}}{R.(273.15+T_{aer})}$	mol· ppm^{-1}	conversion factor from ppm to mol	R = 8.2005.10^{-5} m^3·atm.K^{-1}·mol^{-1} T_{aer} = temperature of aeration air
2	K_{off}	$\frac{10^{-6}}{R.(273.15+T_{off})}$	mol· ppm^{-1}	conversion factor from ppm to mol	T_{off} = temperature of off- gas
3		1.053	mol .mol^{-1}	conversion factor from ammonium-nitrogen (NH_{in}) to total Kjeldahl nitrogen	Mampaey et al. (2016)

Supplementary Information B: Raw and reconciled data set with off-gas data

List of abbreviations

Notation	Description
var	variable name
measured	measured value
calculated	calculated values from raw data
reconciled	reconciled value
std	standard error of the mean
%sd	relative standard deviation
Δ(%)	ratio of reconciled value to measured value
i(%)	Improvement of a variables
M	measured variable
U	unmeasured variable
I	identified variable (i.e., reconciled & checked by gross error detection)

Result for the whole data set

Table B0a. Data reconciliation (iteration = 3, convergence tolerance = 3.4×10^{-10}, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	591	10	1.70	591	10	1.70	100.00	0.00	M	I
2	CO_{2off}	22,052	88	0.40	22,052	88	0.40	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	345	3	0.88	345	3	0.88	100.00	0.00	M	I
5	NH_{eff}	43.8	2.2	5.00	44.0	2.0	4.59	100.61	7.69	M	I
6	NH_{in}	93.7	4.7	5.00	92.5	2.7	2.87	98.69	43.26	M	I
7	NO_{2eff}	48.1	2.4	5.00	48.5	2.2	4.51	100.66	9.12	M	I
8	NO_{3eff}	0.6	0.0	5.00	0.6	0.0	5.00	100.01	0.00	M	I
9	NO_{off}	26	0	0.54	26	0	0.54	100.00	0.00	M	I
10	O_{2aer}	209,653	94	0.04	209,653	94	0.04	100.00	0.00	M	I
11	O_{2off}	193,865	66	0.03	193,865	66	0.03	100.00	0.00	M	I
12	Q_{aer}	1,653	9	1	1,653	9	0.54	100.00	0.00	M	I
13	Q_{in}	25.04	0.08	0.30	25.04	0.08	0.30	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**		
14	Q_{inf}	1,434	153	11	1,454	140	9.63	101.39	8.63	U	I
15	Q_{off}	3,243	161	5	3,263	147	4.50	100.64	8.65	U	I
16	$(TIC:NH)_{in}$	1.14	0.08	7	1.17	0.04	3.48	101.99	49.91	U	I

Table B0b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 1.12, $\chi^{2}_{1-0.05,1}$ = 3.84 p-value = 0.39	no gross error detected
Measurement test Degree of freedom = 1 t-statistic$_{max}$ = 1.96 p-value$_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 t-statistic$_{max}$ = 1.96 p-value$_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.00	0.32	0.37
2	CO_{2off}	0.02	0.05	0.32	0.37
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.00	0.01	0.32	0.37
5	NH_{eff}	0.27	0.84	0.32	0.37
6	NH_{in}	1.23	3.86	0.32	0.37
7	NO_{2eff}	0.32	1.00	0.32	0.37
8	NO_{off}	0.00	0.00	0.32	0.37
9	O_{2aer}	0.00	0.00	0.32	0.37
10	O_{2off}	0.08	0.26	0.32	0.37
11	Q_{aer}	0.04	0.13	0.32	0.37
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	1,791	5,617	0.32	0.37

Results for S1

Table B1a. Data reconciliation (iteration = 3, convergence tolerance = 3.8×10^{-09}, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	611	52	8.54	611	52	8.54	100.00	0.00	M	I
2	CO_{2off}	30,052	157	0.52	30,052	157	0.52	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	264	6	2.23	264	6	2.23	100.00	0.00	M	I
5	NH_{eff}	39.7	2.0	5.00	40.1	1.8	4.60	100.95	7.06	M	I
6	NH_{in}	88.9	4.4	5.00	87.0	2.5	2.88	97.87	43.58	M	I
7	NO_{2eff}	47.3	2.4	5.00	47.8	2.1	4.47	101.10	9.56	M	I
8	NO_{3eff}	0.4	0.0	5.00	0.4	0.0	5.00	100.01	0.00	M	I
9	NO_{off}	36	0	0.70	36	0	0.70	100.00	0.00	M	I
10	O_{2aer}	209,886	38	0.02	209,886	38	0.02	100.00	0.00	M	I
11	O_{2off}	188,072	101	0.05	188,072	101	0.05	100.00	0.00	M	I
12	Q_{aer}	2,119	23	1	2,119	23	1.10	100.00	0.00	M	I
13	Q_{in}	34.61	0.15	0.42	34.61	0.15	0.42	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**		
14	Q_{inf}	852	148	17	884	135	15.26	103.73	9.01	U	I
15	Q_{off}	3,130	154	5	3,163	140	4.43	101.07	9.24	U	I
16	$(TIC:NH)_{in}$	1.15	0.08	7	1.19	0.04	3.33	103.28	51.34	U	I

Table B2b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 2.92, $\chi^2_{1-0.05,1}$ = 3.84 p-value = 0.09	no gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.01	0.52	0.30
2	CO_{2off}	0.03	0.06	0.52	0.30
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.01	0.02	0.52	0.30
5	NH_{eff}	0.38	0.73	0.52	0.30
6	NH_{in}	1.89	3.67	0.52	0.30
7	NO_{2eff}	0.52	1.01	0.52	0.30
8	NO_{off}	0.00	0.00	0.52	0.30
9	O_{2aer}	0.00	0.00	0.52	0.30
10	O_{2off}	0.01	0.02	0.52	0.30
11	Q_{aer}	0.07	0.13	0.52	0.30
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	6,563	12,733	0.52	0.30

Results for S2

Table B2a. Data reconciliation (iteration = 3, convergence tolerance = 2.3×10^{-07}, CPU time = 0.8s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	550	12	2.27	550	12	2.27	100.00	0.00	M	I
2	CO_{2off}	30,496	159	0.52	30,496	159	0.52	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	296	9	3.09	296	9	3.09	99.96	0.00	M	I
5	NH_{eff}	44.8	2.2	5.00	43.1	2.1	4.85	96.16	6.72	M	I
6	NH_{in}	96.6	4.8	5.00	104.6	3.0	2.91	108.28	37.02	M	I
7	NO_{2eff}	66.0	3.3	5.00	62.4	2.8	4.53	94.50	14.37	M	I
8	NO_{3eff}	0.8	0.0	5.00	0.8	0.0	5.00	99.93	0.00	M	I
9	NO_{off}	44	0	0.54	44	0	0.54	100.00	0.00	M	I
10	O_{2aer}	210,280	13	0.01	210,280	13	0.01	100.00	0.00	M	I
11	O_{2off}	187,767	93	0.05	187,766	93	0.05	100.00	0.00	M	I
12	Q_{aer}	2,292	35	2	2,292	35	1.51	100.00	0.00	M	I
13	Q_{in}	36.48	0.05	0.13	36.48	0.05	0.13	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**		
14	Q_{inf}	1,924	209	11	1,671	179	10.73	86.86	14.38	U	I
15	Q_{off}	4,438	218	5	4,201	187	4.44	94.65	14.22	U	I
16	$(TIC:NH)_{in}$	1.46	0.10	7	1.27	0.04	3.12	87.38	61.35	U	I

Table B2b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 49.96, $\chi^2_{1-0.05,1}$ = 3.84 p-value = 0.00	gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$= 1.96 $p\text{-value}_{min}$ = 0.03	gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.00	2.13	0.02
2	CO_{2off}	0.17	0.08	2.13	0.02
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.13	0.06	2.13	0.02
5	NH_{eff}	1.72	0.81	2.13	0.02
6	NH_{in}	7.99	3.75	2.13	0.02
7	NO_{2eff}	3.63	1.70	2.13	0.02
8	NO_{off}	0.00	0.00	2.13	0.02
9	O_{2aer}	0.00	0.00	2.13	0.02
10	O_{2off}	0.01	0.00	2.13	0.02
11	Q_{aer}	0.28	0.13	2.13	0.02
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	-30,228	14,203	2.13	0.02

Results for S3

Table B3a. Data reconciliation (iteration = 4, convergence tolerance = 3.2×10^{-08}, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	833	147	17.60	833	147	17.60	100.01	0.00	M	I
2	CO_{2off}	26,135	353	1.35	26,135	353	1.35	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	386	13	3.30	386	13	3.30	99.98	0.00	M	I
5	NH_{eff}	36.7	1.8	5.00	36.3	1.7	4.67	98.96	7.52	M	I
6	NH_{in}	78.0	3.9	5.00	79.7	2.3	2.88	102.21	41.10	M	I
7	NO_{2eff}	44.1	2.2	5.00	43.6	2.0	4.52	98.77	10.68	M	I
8	NO_{3eff}	0.5	0.0	5.00	0.5	0.0	5.00	99.99	0.00	M	I
9	NO_{off}	36	1	1.57	36	1	1.57	100.00	0.00	M	I
10	O_{2aer}	210,375	108	0.05	210,375	108	0.05	100.00	0.00	M	I
11	O_{2off}	191,161	244	0.13	191,160	244	0.13	100.00	0.00	M	I
12	Q_{aer}	2,001	44	2	2,001	44	2.19	100.00	0.00	M	I
13	Q_{in}	30.75	0.05	0.16	30.75	0.05	0.16	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**		
14	Q_{inf}	812	154	19	760	140	18.40	93.52	9.11	U	I
15	Q_{off}	2,957	155	5	2,921	141	4.83	98.80	9.28	U	I
16	$(TIC:NH)_{in}$	1.20	0.09	8	1.16	0.05	4.24	96.66	45.62	U	I

Table B3b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 3.28, $\chi^2_{1-0.05,1}$ = 3.84, p-value = 0.07	no gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.06	0.10	0.55	0.29
2	CO_{2off}	0.33	0.61	0.55	0.29
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.07	0.12	0.55	0.29
5	NH_{eff}	0.38	0.70	0.55	0.29
6	NH_{in}	1.72	3.15	0.55	0.29
7	NO_{2eff}	0.54	0.99	0.55	0.29
8	NO_{off}	0.00	0.00	0.55	0.29
9	O_{2aer}	0.00	0.00	0.55	0.29
10	O_{2off}	0.15	0.27	0.55	0.29
11	Q_{aer}	0.75	1.38	0.55	0.29
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	-3,477	6,362	0.55	0.29

Results for S4

Table B4a. Data reconciliation (iteration = 3, convergence tolerance = 2.1×10^{-09}, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	511	5	0.91	511	5	0.91	100.00	0.00	M	I
2	CO_{2off}	28,438	247	0.87	28,438	247	0.87	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	265	6	2.11	265	6	2.11	100.00	0.00	M	I
5	NH_{eff}	37.3	1.9	5.00	37.6	1.7	4.63	100.97	6.45	M	I
6	NH_{in}	87.1	4.4	5.00	85.2	2.5	2.89	97.74	43.57	M	I
7	NO_{2eff}	47.8	2.4	5.00	48.4	2.1	4.44	101.21	10.20	M	I
8	NO_{3eff}	0.5	0.0	5.00	0.5	0.0	5.00	100.01	0.00	M	I
9	NO_{off}	42	0	0.98	42	0	0.98	100.00	0.00	M	I
10	O_{2aer}	210,534	15	0.01	210,534	15	0.01	100.00	0.00	M	I
11	O_{2off}	189,705	161	0.08	189,705	161	0.08	100.00	0.00	M	I
12	Q_{aer}	2,160	36	2	2,160	36	1.68	100.00	0.00	M	I
13	Q_{in}	33.45	0.08	0.23	33.45	0.08	0.23	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**		
14	Q_{inf}	881	156	18	896	141	15.73	101.66	9.62	U	I
15	Q_{off}	3,201	160	5	3,239	144	4.46	101.17	9.56	U	I
16	$(TIC:NH)_{in}$	1.18	0.08	7	1.22	0.04	3.43	103.53	50.50	U	I

Table B4b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 3.31, $\chi^2_{1-0.05,1}$ = 3.84 p-value = 0.07	no gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.00	0.55	0.29
2	CO_{2off}	0.10	0.19	0.55	0.29
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.01	0.02	0.55	0.29
5	NH_{eff}	0.36	0.66	0.55	0.29
6	NH_{in}	1.97	3.60	0.55	0.29
7	NO_{2eff}	0.58	1.05	0.55	0.29
8	NO_{off}	0.00	0.00	0.55	0.29
9	O_{2aer}	0.00	0.00	0.55	0.29
10	O_{2off}	0.00	0.00	0.55	0.29
11	Q_{aer}	0.21	0.37	0.55	0.29
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	6,188	11,280	0.55	0.29

Results for S5

Table B5a. Data reconciliation (iteration = 4, convergence tolerance = $1.6x10^{-07}$, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	494	3	0.65	494	3	0.65	100.00	0.00	M	I
2	CO_{2off}	22,551	253	1.12	22,551	253	1.12	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	309	7	2.12	309	7	2.12	100.01	0.00	M	I
5	NH_{eff}	35.5	1.8	5.00	35.8	1.7	4.64	100.86	6.50	M	I
6	NH_{in}	82.6	4.1	5.00	80.9	2.3	2.89	97.99	43.44	M	I
7	NO_{2eff}	45.0	2.3	5.00	45.5	2.0	4.44	101.07	10.23	M	I
8	NO_{3eff}	0.5	0.0	5.00	0.5	0.0	5.00	100.01	0.00	M	I
9	NO_{off}	31	0	1.43	31	0	1.43	100.00	0.00	M	I
10	O_{2aer}	210,702	11	0.01	210,702	11	0.01	100.00	0.00	M	I
11	O_{2off}	193,806	181	0.09	193,806	181	0.09	100.00	0.00	M	I
12	Q_{aer}	1,682	30	2	1,682	30	1.80	100.00	0.00	M	I
13	Q_{in}	25.63	0.03	0.11	25.63	0.03	0.11	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**		
14	Q_{inf}	1,023	141	14	1,033	128	12.36	100.93	9.32	U	I
15	Q_{off}	2,839	145	5	2,869	131	4.58	101.04	9.14	U	I
16	$(TIC:NH)_{in}$	1.14	0.08	7	1.18	0.04	3.71	103.13	47.71	U	I

Table B5b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 2.62, $\chi^2_{1-0.05,1}$ = 3.84 p-value = 0.11	no gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.00	0.49	0.31
2	CO_{2off}	0.16	0.32	0.49	0.31
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.02	0.04	0.49	0.31
5	NH_{eff}	0.31	0.63	0.49	0.31
6	NH_{in}	1.66	3.40	0.49	0.31
7	NO_{2eff}	0.48	0.99	0.49	0.31
8	NO_{off}	0.00	0.00	0.49	0.31
9	O_{2aer}	0.00	0.00	0.49	0.31
10	O_{2off}	0.00	0.00	0.49	0.31
11	Q_{aer}	0.38	0.78	0.49	0.31
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	2,938	6,026	0.49	0.31

Results for S6

Table B6a. Data reconciliation (iteration = 4, convergence tolerance = $1.5x10^{-07}$, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	539	16	2.96	539	16	2.96	100.00	0.00	M	I
2	CO_{2off}	7,490	299	3.99	7,495	299	3.98	100.07	0.01	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	263	12	4.71	263	12	4.70	100.24	0.06	M	I
5	NH_{eff}	42.0	2.1	5.00	43.0	2.0	4.58	102.54	6.02	M	I
6	NH_{in}	103.1	5.2	5.00	96.7	2.8	2.90	93.76	45.66	M	I
7	NO_{2eff}	49.9	2.5	5.00	51.4	2.3	4.40	103.11	9.18	M	I
8	NO_{3eff}	0.5	0.0	5.00	0.5	0.0	5.00	100.03	0.00	M	I
9	NO_{off}	8	0	5.40	8	0	5.40	100.01	0.00	M	I
10	O_{2aer}	210,758	19	0.01	210,758	19	0.01	100.00	0.00	M	I
11	O_{2off}	205,474	233	0.11	205,490	233	0.11	100.01	0.10	M	I
12	Q_{aer}	593	29	5	593	29	4.94	100.00	0.00	M	I
13	Q_{in}	7.33	0.26	3.61	7.33	0.26	3.61	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**	**M**	**I**
14	Q_{inf}	2,263	259	11	2,354	257	10.93	104.00	0.83	U	I
15	Q_{off}	2,985	270	9	3,090	269	8.70	103.52	0.47	U	I
16	$(TIC:NH)_{in}$	1.06	0.12	11	1.17	0.10	8.96	110.51	11.29	U	I

Table B6b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 24.31, $\chi^2_{1-0.05,1}$ = 3.84 p-value = 0.00	Gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.02	0.01	1.49	0.07
2	CO_{2off}	5.47	3.68	1.49	0.07
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.62	0.42	1.49	0.07
5	NH_{eff}	1.07	0.72	1.49	0.07
6	NH_{in}	6.43	4.33	1.49	0.07
7	NO_{2eff}	1.55	1.04	1.49	0.07
8	NO_{off}	0.00	0.00	1.49	0.07
9	O_{2aer}	0.00	0.00	1.49	0.07
10	O_{2off}	0.10	0.07	1.49	0.07
11	Q_{aer}	15.87	10.68	1.49	0.07
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	1,187	811	1.46	0.07

Results for S7

Table B7a. Data reconciliation (iteration = 3, convergence tolerance = 2.8×10^{-09}, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	545	8	1.48	545	8	1.48	100.00	0.00	M	I
2	CO_{2off}	24,375	180	0.74	24,375	180	0.74	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	252	5	2.18	252	5	2.18	100.01	0.00	M	I
5	NH_{eff}	41.0	2.1	5.00	41.6	1.9	4.58	101.37	7.18	M	I
6	NH_{in}	91.4	4.6	5.00	88.6	2.6	2.88	96.95	44.17	M	I
7	NO_{2eff}	47.1	2.4	5.00	47.9	2.1	4.48	101.53	9.07	M	I
8	NO_{3eff}	0.5	0.0	5.00	0.5	0.0	5.00	100.02	0.00	M	I
9	NO_{off}	28	0	1.07	28	0	1.07	100.00	0.00	M	I
10	O_{2aer}	210,407	13	0.01	210,407	13	0.01	100.00	0.00	M	I
11	O_{2off}	192,234	121	0.06	192,234	121	0.06	100.00	0.00	M	I
12	Q_{aer}	2,112	34	2	2,112	34	1.60	100.00	0.00	M	I
13	Q_{in}	28.99	0.03	0.11	28.99	0.03	0.11	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**	**M**	**I**
14	Q_{inf}	851	150	18	884	137	15.55	103.96	8.50	U	I
15	Q_{off}	3,112	154	5	3,158	141	4.45	101.48	8.65	U	I
16	$(TIC:NH)_{in}$	1.08	0.08	7	1.13	0.04	3.49	104.69	48.74	U	I

Table B7b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 5.95, $\chi^2_{1-0.05,11}$ = 3.84 p-value = 0.01	Gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.00	0.74	0.23
2	CO_{2off}	0.08	0.11	0.74	0.23
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.02	0.02	0.74	0.23
5	NH_{eff}	0.56	0.76	0.74	0.23
6	NH_{in}	2.79	3.79	0.74	0.23
7	NO_{2eff}	0.72	0.98	0.74	0.23
8	NO_{off}	0.00	0.00	0.74	0.23
9	O_{2aer}	0.00	0.00	0.74	0.23
10	O_{2off}	0.00	0.00	0.74	0.23
11	Q_{aer}	0.17	0.24	0.74	0.23
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	7,234	9,841	0.74	0.23

Results for S8

Table B8a. Data reconciliation (iteration = 3, convergence tolerance = 2.8×10^{-09}, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	630	14	2.26	630	14	2.26	100.00	0.00	M	I
2	CO_{2off}	28,059	98	0.35	28,059	98	0.35	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	176	8	4.50	176	8	4.50	100.04	0.00	M	I
5	NH_{eff}	42.4	2.1	5.00	43.6	2.0	4.53	102.74	6.92	M	I
6	NH_{in}	98.0	4.9	5.00	91.8	2.6	2.86	93.68	46.43	M	I
7	NO_{2eff}	47.0	2.4	5.00	48.4	2.2	4.47	102.93	7.97	M	I
8	NO_{3eff}	1.5	0.1	5.00	1.5	0.1	4.99	100.09	0.01	M	I
9	NO_{off}	47	0	0.56	47	0	0.56	100.00	0.00	M	I
10	O_{2aer}	210,447	16	0.01	210,447	16	0.01	100.00	0.00	M	I
11	O_{2off}	190,022	73	0.04	190,022	73	0.04	100.00	0.00	M	I
12	Q_{aer}	2,056	16	1	2,056	16	0.77	100.00	0.00	M	I
13	Q_{in}	28.73	0.13	0.46	28.73	0.13	0.46	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**	**M**	**I**
14	Q_{inf}	629	129	21	599	115	19.16	95.29	11.03	U	I
15	Q_{off}	2,825	135	5	2,903	124	4.28	102.77	7.73	U	I
16	$(TIC:NH)_{in}$	1.06	0.07	7	1.16	0.04	3.24	109.73	48.80	U	I

Table B8b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 24.66, $\chi^2_{1-0.05,1}$ = 3.84 p-value = 0.00	Gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.00	1.50	0.07
2	CO_{2off}	0.03	0.02	1.50	0.07
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.06	0.04	1.50	0.07
5	NH_{eff}	1.16	0.78	1.50	0.07
6	NH_{in}	6.20	4.14	1.50	0.07
7	NO_{2eff}	1.38	0.92	1.50	0.07
8	NO_{off}	0.00	0.00	1.50	0.07
9	O_{2aer}	0.00	0.00	1.50	0.07
10	O_{2off}	0.00	0.00	1.50	0.07
11	Q_{aer}	0.08	0.05	1.50	0.07
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	21,653	14,487	1.49	0.07

Results of S9

Table B9a. Data reconciliation (iteration = 3, convergence tolerance = 2.4×10^{-07}, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	583	11	1.86	583	11	1.86	100.00	0.00	M	I
2	CO_{2off}	26,390	305	1.15	26,391	305	1.15	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	601	15	2.53	601	15	2.53	100.04	0.01	M	I
5	NH_{eff}	39.8	2.0	5.00	40.8	1.9	4.58	102.47	6.18	M	I
6	NH_{in}	96.6	4.8	5.00	90.8	2.6	2.89	93.99	45.71	M	I
7	NO_{2eff}	48.3	2.4	5.00	49.7	2.2	4.41	102.99	9.16	M	I
8	NO_{3eff}	0.4	0.0	5.00	0.4	0.0	5.00	100.03	0.00	M	I
9	NO_{off}	30	0	1.56	30	0	1.56	100.00	0.00	M	I
10	O_{2aer}	210,674	12	0.01	210,674	12	0.01	100.00	0.00	M	I
11	O_{2off}	190,091	216	0.11	190,093	216	0.11	100.00	0.00	M	I
12	Q_{aer}	1,938	39	2	1,938	39	1.99	100.00	0.00	M	I
13	Q_{in}	28.10	0.10	0.34	28.10	0.10	0.34	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**	**M**	**I**
14	Q_{inf}	653	138	21	677	125	18.49	103.63	9.05	U	I
15	Q_{off}	2,721	139	5	2,801	128	4.57	102.92	8.02	U	I
16	$(TIC:NH)_{in}$	1.00	0.07	7	1.09	0.04	3.70	109.53	44.65	U	I

Table B9b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 22.50, $\chi^2_{1-0.05,1}$ = 3.84 p-value = 0.00	Gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.00	1.43	0.08
2	CO_{2off}	0.79	0.55	1.43	0.08
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.22	0.16	1.43	0.08
5	NH_{eff}	0.98	0.69	1.43	0.08
6	NH_{in}	5.80	4.06	1.43	0.08
7	NO_{2eff}	1.44	1.01	1.43	0.08
8	NO_{off}	0.00	0.00	1.43	0.08
9	O_{2aer}	0.00	0.00	1.43	0.08
10	O_{2off}	0.01	0.00	1.43	0.08
11	Q_{aer}	1.88	1.31	1.43	0.08
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	7,163	5,015	1.43	0.08

Results of S10

Table B10a. Data reconciliation (iteration = 3, convergence tolerance = $1.4x10^{-07}$, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	484	1	0.12	484	1	0.12	100.00	0.00	M	I
2	CO_{2off}	23,938	247	1.03	23,939	247	1.03	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	594	15	2.45	595	15	2.45	100.04	0.01	M	I
5	NH_{eff}	42.1	2.1	5.00	43.4	2.0	4.52	102.91	7.03	M	I
6	NH_{in}	96.5	4.8	5.00	90.1	2.6	2.88	93.35	46.27	M	I
7	NO_{2eff}	44.7	2.2	5.00	46.1	2.1	4.46	103.08	7.96	M	I
8	NO_{3eff}	0.5	0.0	5.00	0.5	0.0	5.00	100.04	0.00	M	I
9	NO_{off}	28	0	1.45	28	0	1.45	100.00	0.00	M	I
10	O_{2aer}	210,184	11	0.01	210,184	11	0.01	100.00	0.00	M	I
11	O_{2off}	191,631	176	0.09	191,632	176	0.09	100.00	0.00	M	I
12	Q_{aer}	1,735	31	2	1,735	31	1.76	100.00	0.00	M	I
13	Q_{in}	25.73	0.03	0.11	25.73	0.03	0.11	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**	**M**	**I**
14	Q_{inf}	732	128	17	797	119	14.89	108.91	7.03	U	I
15	Q_{off}	2,589	130	5	2,667	121	4.54	103.00	7.12	U	I
16	$(TIC:NH)_{in}$	0.94	0.07	7	1.04	0.04	3.76	110.37	42.73	U	I

Table B10b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 27.38, $\chi^2_{1-0.05,1}$ = 3.84 p-value = 0.00	Gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.00	1.58	0.06
2	CO_{2off}	0.65	0.41	1.58	0.06
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.24	0.15	1.58	0.06
5	NH_{eff}	1.22	0.78	1.58	0.06
6	NH_{in}	6.42	4.07	1.58	0.06
7	NO_{2eff}	1.38	0.87	1.58	0.06
8	NO_{off}	0.00	0.00	1.58	0.06
9	O_{2aer}	0.00	0.00	1.58	0.06
10	O_{2off}	0.01	0.00	1.58	0.06
11	Q_{aer}	1.59	1.01	1.58	0.06
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	6,534	4,148	1.58	0.06

Results for S11

Table B11a. Data reconciliation (iteration = 3, convergence tolerance = 6.7×10^{-09}, CPU time = 0.7s)

#	Var	measured	std	sD%	reconciled	std	sD%	Δ(%)	i(%)		
1	CO_{2aer}	529	10	1.85	529	10	1.85	100.00	0.00	M	I
2	CO_{2off}	24,260	318	1.31	24,260	318	1.31	100.00	0.00	M	I
3	COD_{in}	2.78	0.01	0.36	2.78	0.01	0.36	100.00	0.00	M	I
4	N_2O_{off}	541	20	3.76	541	20	3.76	100.02	0.01	M	I
5	NH_{eff}	44.8	2.2	5.00	45.1	2.1	4.60	100.74	7.33	M	I
6	NH_{in}	98.1	4.9	5.00	96.5	2.8	2.88	98.37	43.31	M	I
7	NO_{2eff}	50.6	2.5	5.00	51.1	2.3	4.49	100.84	9.43	M	I
8	NO_{3eff}	0.4	0.0	5.00	0.4	0.0	5.00	100.01	0.00	M	I
9	NO_{off}	33	1	1.73	33	1	1.73	100.00	0.00	M	I
10	O_{2aer}	210,170	12	0.01	210,170	12	0.01	100.00	0.00	M	I
11	O_{2off}	191,611	224	0.12	191,612	224	0.12	100.00	0.00	M	I
12	Q_{aer}	2,114	44	2	2,114	44	2.06	100.00	0.00	M	I
13	Q_{in}	27.28	0.15	0.55	27.28	0.15	0.55	100.00	0.00	M	I
#	**Var**	**calculated**	**std**	**sD%**	**reconciled**	**std**	**sD%**	**Δ(%)**	**i(%)**	**M**	**I**
14	Q_{inf}	832	159	19	877	148	16.89	105.36	7.00	U	I
15	Q_{off}	3,093	161	5	3,118	148	4.75	100.82	8.17	U	I
16	$(TIC:NH)_{in}$	1.06	0.08	7	1.09	0.04	4.03	102.50	44.30	U	I

Table B11b. Gross error detection

Test	Evaluation
Global test System degree of redundancy = 1 t-statistic = 1.72, $\chi^2_{1-0.05,1}$ = 3.84 p-value = 0.19	no gross error detected
Measurement test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected
Nodal test Degree of freedom = 1 $t\text{-statistic}_{max}$ = 1.96 $p\text{-value}_{min}$ = 0.03	no gross error detected

#	Var	residual	error	t-statistic	p-value
1	CO_{2aer}	0.00	0.00	0.40	0.35
2	CO_{2off}	0.27	0.67	0.40	0.35
3	COD_{in}	-	0.00	-	0.50
4	N_2O_{off}	0.12	0.31	0.40	0.35
5	NH_{eff}	0.33	0.84	0.40	0.35
6	NH_{in}	1.60	4.04	0.40	0.35
7	NO_{2eff}	0.42	1.07	0.40	0.35
8	NO_{off}	0.00	0.00	0.40	0.35
9	O_{2aer}	0.00	0.00	0.40	0.35
10	O_{2off}	0.00	0.00	0.40	0.35
11	Q_{aer}	0.63	1.58	0.40	0.35
12	Q_{in}	-	0.00	-	0.50

#	misbalance	error	t-statistic	p-value
1	1,954	4,948	0.39	0.35

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