Non-Linear Data Reconciliation for a Partial Nitritation (SHARON) Reactor

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Abstract

This work demonstrates the usefulness of non-linear data reconciliation to evaluate available measurements and estimate unmeasured variables for a full-scale partial nitritation (SHARON) reactor for the treatment of wastewater with high ammonium concentrations. Despite a lack of measured data, the bilinear approach of formulating system constraints allowed to satisfy the requirements for data reconciliation and gross error detection, leading to a balanced data set and the estimation of unmeasured variables.

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1 INTRODUCTION

Data reconciliation is a procedure of optimally adjusting measured data such that the estimates satisfy the conservation laws and other constraints (Crowe, 1996). The estimates are expected to be more accurate than the measurements and, more importantly, to satisfy known relationships between process variables defined by constraints. In wastewater treatment, however, the concept of data reconciliation has received relatively little attention so far. Its application is typically aimed at data validation and/or the identification of structural observability/redundancy.

1.1 Data validation for WWT processes

Data reconciliation demonstrated its usefulness to derive balanced data (where measurements fit the mass balances) sets for modelling and process assessment. Since the work of Nowak et al. (1999), the use of mass balances was put forward as a tool for the evaluation of wastewater treatment plant (WWTP) operation parameters in order to estimate fluxes of COD, phosphorus and nitrogen. Meijer et al. (2002) performed data reconciliation for a WWTP using yearly average measurements, aiming to obtain a balanced data set for a simulation study. Their study showed that data reconciliation improves the accuracy of estimations and that the use of a balanced data set simplifies the model calibration procedure. Puig et al. (2008) continued this line by proposing a practical stepwise methodology to check the historical data of a full-scale WWTP. Results indicated that poor quality of historical WWTP data leads to large errors when calculating key operational conditions. Performing a proper data evaluation by data reconciliation should make the modelling task easier and constitutes a reliable and an effective tool for operational troubleshooting, plant design and performance improvement (Meijer et al. 2015). The abovementioned works all applied the method developed by Vanderheijden et al. (1994) for linear steady-state data reconciliation which was implemented in the software Macrobal (Hellinga and Romein, 1992).

1.2 Redundancy analysis and variable classification for WWT processes

With regard to the classical approach of data reconciliation concerning the redundancy problem of data reconciliation (meaning that at least 02 measurements can be balanced), Villez et al. (2013a) presented a method based on mass balances, providing an initial step towards the optimization of sensor networks. Villez et al. (2013b) applied a graph-theoretical approach to structural observability and redundancy classification, allowing the automated classification of sensors and process variables for any plant and sensor configuration. Recently, Spindler (2014) proposed a procedure to determine all theoretically possible redundancy equations for a given plant layout and classification of variables. The proposed procedure could also be applied to assess the necessity of existing or additional measurements to the improvement of the data’s redundancy.

1.3 Research aim

This contribution focuses on the application of data reconciliation by setting constraints in the form of non-linear mass balances to evaluate the consistency of measurements (i.e. data validation) and to estimate unmeasured parameters for a wastewater treatment process. More specifically a partial nitritation (SHARON) process was studied.

2 MATERIAL AND METHODS

2.1 Measurement description

The SHARON reactor at the WWTP Dokhaven (Rotterdam) serves for biological nitrogen removal from wastewater. In this reactor, ammonium, the dominant form, is oxidized to nitrite, while further oxidation to nitrate is prevented, by keeping the aerobic retention time optimally for the process (Hellinga et al., 1998). Only about half of the ammonium in the influent is converted to nitrite; the reactor effluent thus contains ammonium and nitrite in about equimolar amounts, which is
ideally suited to feed the subsequent anammox process (van Dongen et al., 2001). The SHARON reactor is a covered reactor with a constant liquid volume of 1500 m³ and a headspace volume of approximately 300 m³ above the liquid (Mulder et al., 2001). It is operated in a cyclic way, with alternating aerobic-anoxic periods, in order to maintain a mean aerobic retention time of about 1.35 days. The duration of each aeration period is controlled by the influent flow rate during the previous cycle. During aeration, the DO (dissolved oxygen) level in the reactor is controlled at a fixed set point of 2 g O₂.m⁻³ by adjusting the aeration flow rate. Figure 2.1 illustrates the schematic diagram of this SHARON reactor and all measurements. The data used in this study were collected during a monitoring campaign during the of period 15-06-2010 to 08-07-2010 (Mampaey et al., 2016). An overview of the measured data is presented in Table 2.1.

Figure 2.1 Schematic view of the SHARON reactor and measurement variables (detailed in Table 2.1).

Table 2.1 Parameter/variable measurement and description.

| #  | Parameter (variable) | Mean(1) | Error(2) | Unit | Describing |
|----|----------------------|---------|----------|------|------------|
| 1  | Taer                 | 16.2    | 1.1      | °C   | Aeration air temperature |
| 2  | Toff                 | 30      | 1        | °C   | Off-gas temperature |
| 3  | Qaer                 | 2005    | 272      | m³.h⁻¹ | Aeration air flow rate |
| 4  | Qin                  | NA      | NA       | m³.h⁻¹ | Infiltration air flow rate |
| 5  | Qoff                 | NA      | NA       | m³.h⁻¹ | Off-gas flow rate |
| 6  | O₂aer (=O₂inf)       | 282.86  | 0.14     | g O₂.m⁻³ | Oxygen concentration in the aeration (infiltration) air |
| 7  | CO₂aer (=CO₂inf)     | 1.21    | 0.25     | g C.m⁻³ | Carbon dioxide concentration in the aeration (infiltration) air |
| 8  | NOaer (=NOinf)       | NA      | NA       | g N.m⁻³ | Nitric oxide concentration in the aeration (infiltration) air |
| 9  | N₂Oaer (=N₂Oinf)     | NA      | NA       | g N.m⁻³ | Nitrous oxide concentration in the aeration (infiltration) air |
| 10 | O₂off                | 240.47  | 0.35     | g O₂.m⁻³ | Oxygen concentration in the off-gas |
| 11 | CO₂off               | 56.70   | 0.86     | g C.m⁻³ | Carbon dioxide concentration in the off-gas |
| 12 | NOoff                | 0.0208  | 0.0008   | g N.m⁻³ | Nitric oxide concentration in the off-gas |
| 13 | N₂Ooff               | 0.37    | 0.06     | g N.m⁻³ | Nitrous oxide concentration in the off-gas |
| 14 | Qin                  | 34      | 2        | m³.h⁻¹ | Influent flow rate |
| 15 | Qeff                 | NA      | NA       | m³.h⁻¹ | Effluent flow rate |
| 16 | NHin                 | 1244    | 20       | g N.m⁻³ | Ammonium concentration in the influent |
| 17 | TIC                  | NA      | NA       | g C.m⁻³ | Total inorganic carbon (CO₂, HCO⁻₃, CO₃²⁻) |
| 18 | NHeff                | 556     | 37       | g N.m⁻³ | Ammonium concentration in the effluent |
| 19 | NO₃eff               | 6.0     | 0.6      | g N.m⁻³ | Nitrate concentration in the effluent |
| 20 | NO₂eff               | 663     | 9        | g N.m⁻³ | Nitrite concentration in the effluent |

(1) Mean/average of measured parameters/variables
(2) Standard error of the mean that takes into account sampling size
(3) NA = not analysed/unmeasured variables
(4) Variables in brackets were not measured but considered equal to corresponding measured one
2.2 Data pre-processing

Steady state operation is one of the prerequisites for data reconciliation. In this study, the process dynamics of the SHARON reactor have a low frequency, which allows to identify pseudo-steady state periods. As the feed temperature (35°C) and pH (6.8) were rather constant over time but the grab sampling frequency was too low compare to the one of the other measurements, it was not possible to evaluate the loading rate of the reactor over time nor to perform steady state assessment based on influent and effluent nitrogen. Only the variations in the feed flow rate of the reject water and the duration of the aeration cycle were taken into account to select the periods corresponding to pseudo steady-state operation (subset data). In this study, one data subset including 1000 sampling points for each parameter was selected. Their mean and error are presented in Table 2.1.

2.3 Constraint formulation

The steady-state constraints used to perform the data reconciliation were primarily composed of conservation balances, specifically nitrogen, oxygen and carbon around the SHARON reactor. In contrast with previous work in which mass balances were expressed in linear terms, namely fluxes of flows and components (Meijer et al., 2002, Puig et al., 2008, Meijer et al., 2015), in this study bilinear terms of flows and concentration of components were applied to utilize all the measurements. The linear approach would result in having 11 unknowns in 04 mass balances. Fluxes or any term related to Qeff, Qin and α (ratio of total inorganic carbon (TIC) to total ammonium nitrogen (NHin or TAN) in the influent; the TIC:TAN ratio) would be unknowns terms (Table 2.2) which then lead to the fact that no gross error test could be performed and possibly that no variable could be balanced and/or calculated. In contrast, the bilinear approach (linear terms in Table 2.3 are expressed as bilinear relation between flows and concentrations) has only 03 unknowns which then resulted in one redundancy which allow all procedures of reconciliation and gross error detection to be carried out. To set up these mass balances, the following assumptions were made:

- Evaporation was negligible compared to influent flow rate resulting in equality of influent and effluent (Qin = Qeff).
- N2O and NO in the aeration air, infiltration air and in liquid were negligible.
- All CO2 produced from bicarbonate or COD oxidation was stripped due to aeration.
- N2 gas produced by the SHARON process is negligible.
- Nitrogen and oxygen incorporated into biomass were negligible because the concentration of sludge in reactor was about 140 mg VSS.L-1.
- Influent COD was 150 ± 50 g.m-3

| Table 2.2 Linear mass balances as constraint equations for data reconciliation |
|---|---|
| # | Balance | Expression |
| 1 | Nitrogen (g N.h⁻¹) | MNHin − MNHoff − MO2eff − MN3eff − MN2Oeff − MN0off = 0 |
| 2 | Oxygen (g O₂.h⁻¹) | M02aer + MO2inf − MO2eff × 3.429 − MN3eff × 4.571 − MN2Oeff − 2.286 − MN0off × 1.429 − M02off − MCODin = 0 |
| 3 | Carbon (g C.h⁻¹) | MHO3in + MCODin × 12/32 + MO2aer × 12/44 + MO2inf × 12/44 − MO2off × 12/44 = 0 |
| 4 | Gas flow rate (m³.h⁻¹) | (Qaer + Qin)/(273.15 + Taer) − Qoff/(273.15 + Toff) = 0 |

Note: Prefix “M” means mass of the corresponding component, which is product of flow and concentration. For example: MNHin = Qin × NHin. Note: The variables in bold represent unmeasured variables for which no additional assumptions could be made.

| Table 2.3 Bilinear mass balances as constraint equations for data reconciliation |
|---|---|
| # | Balance | Expression |
| 1 | Nitrogen (g N.h⁻¹) | Qin × NHin − Qin × NHoff − Qin × NO2eff − Qin × NO3eff − Qin × N2Ooff − Qin × N0off = 0 |
| 2 | Oxygen (g O₂.h⁻¹) | Qaer × 02aer + Qin × 02aer − Qin × NO2eff × 3.43 − Qin × NO3eff × 4.57 − Qin × N2Ooff × 2.29 − Qin × N0off × 1.43 − Qin × Noff × 02off − Qin × CODin × 0.27 − Qin × CO2off × 0.27 = 0 |
| 3 | Carbon (g C.h⁻¹) | α × Qin × NHin × 0.86 + CODin × Qin × 0.38 + Qaer × CO2aer × 0.27 + Qin × CO2aer × 0.27 = 0 |
| 4 | Gas flow rate (m³.h⁻¹) | (Qaer + Qin)/(273.15 + Taer) − Qoff/(273.15 + Toff) = 0 |

Note: Variables in bold were not measured.

2.4 Data reconciliation and gross error detection

Data reconciliation and gross error detection were based on the method of Verheijen (2010). A detailed procedure is the subject of an upcoming article. The procedure was implemented using MATLAB 2013b (The MathWorks, Inc., Natick, Massachusetts, United States).
3 RESULT AND DISCUSSION

3.1 Gross error detection

Besides steady state condition mentioned in 2.2, measurement redundancy is a requirement for data reconciliation. The system redundancy need to be at least one for gross error tests to be performed and measurements to be balanced (Verheijen, 2010). Based on defined constraints and the available measurements of this case, the required redundancy was one indicating that there was enough redundancy to guaranty that some measured variables could be balanced and other unmeasured could be calculated. No gross errors were detected, confirming the consistency of the measurements.

3.2 Reconciliation and estimation of variables

Table 3.1 summarizes the data reconciliation results for the selected data set. The estimations did not differ much from the measured data, confirming their consistency. The reconciliation results were also consistent for all subsets of data in which the measurement of oxygen and nitrogen could be balanced. Three unmeasured variables were calculated. The uncontrolled infiltration air (Qinf) was found to be about 25% of all air that went into the reactor. The α ratio was about 1.1 for all data subset, which is a typical value for a SHARON reactor (Table 3.2). This ratio, however, was slightly underestimated because it was based on the assumption that all CO2 was stripped. In reality, a relatively very small amount of CO2 (not measured) remained in the effluent.

Table 3.1 Reconciliation result

| #  | Variable  | Measured(1) | Error(2) | Reconciled(3) | Error | Classification(5) |
|----|-----------|-------------|----------|---------------|-------|-------------------|
| 1  | CO2aer    | 1.21        | 0.25     | 1.21          | 0.25  | Measured Unbalanced |
| 2  | CO2off    | 56.7        | 0.86     | 56.70         | 0.86  | Measured Unbalanced |
| 3  | CODin     | 150         | 50       | 149.74        | 49.99 | Measured Balanced  |
| 4  | N2Ooff    | 0.37        | 0.06     | 0.37          | 0.06  | Measured Balanced  |
| 5  | NHeff     | 556         | 37       | 545.53        | 19.41 | Measured Balanced  |
| 6  | NHin      | 1244        | 20       | 1,247.06      | 17.76 | Measured Balanced  |
| 7  | NO2eff    | 663         | 9        | 662.35        | 8.79  | Measured Balanced  |
| 8  | NO3eff    | 6           | 0.6      | 6.00          | 0.60  | Measured Balanced  |
| 9  | NOoff     | 0.0208      | 0.0008   | 0.02          | 0.0008| Measured Balanced  |
| 10 | O2aer     | 282.86      | 0.14     | 282.86        | 0.14  | Measured Balanced  |
| 11 | O2off     | 240.47      | 0.35     | 240.47        | 0.35  | Measured Balanced  |
| 12 | Qaer      | 2005        | 272      | 2,005.00      | 272.00| Measured Unbalanced|
| 13 | Qin       | 34          | 2        | 34            | 2.00  | Measured Unbalanced|
| 14 | Taer      | 16.2        | 1.1      | 16.21         | 1.10  | Measured Balanced  |
| 15 | Toff      | 30          | 1        | 29.99         | 1.00  | Measured Balanced  |

Table 3.2 Estimation of unknown variables for others subset of data (S2, S3, S4) and all data (full)

|           | S2  | S3  | S4  | Full |
|-----------|-----|-----|-----|------|
| Qinf (m³.h⁻¹) | 578 | 629 | 448 | 394  |
| Qoff (m³.h⁻¹) | 2096| 2782| 233 | 253  |
| α         | 1.17| 1.12| 0.08| 1.10 |

(1) Mean measurement of variables
(2) Standard error of the mean, which take into account number of samples.
(3) Estimated mean of variables as result of data reconciliation.
(4) Calculated value of unmeasured variables that directly derived from solving set of mass balance equations
(5) Classification: Measured = measured variable; Unmeasured = variable that was not measured; Balanced = measured variables that was calculated from other measured variables using set of constraints. Unbalanced = measured variable that could not be calculated from other measured variables using set of constraint. Calculated = unmeasured variable that was calculated from other measured variables using set of constraint.
4 CONCLUSION

This study demonstrated the application of combined bilinear steady-state data reconciliation and gross error detection for the effective assessment of measured data from a wastewater treatment process. Data from a full-scale partial nitration SHARON reactor were applied to test the algorithm. The bilinear setup of mass balances allowed to reduce the number of unknown variables and to increase number of variables that can be estimated and balanced. This approach can be further applied to full-scale wastewater treatment processes where process dynamics stay in a narrow bound, exhibiting low frequency dynamics and/or even with high dynamic process for deriving balanced data sets in view of modelling and simulation.
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