

# A simplified approach for activity monitoring in complex wastewater treatment processes

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**Abstract:** The stoichiometric relations between substrate and product are the first parameter obtained for novel processes. We propose here a method for process monitoring that uses the stoichiometry matrix and a linear least square optimisation as a simple approach for process monitoring. The new method is benchmarked versus a well-established method: the continuous-discrete extended Kalman filter (CD-EKF) and both are compared estimating biological rates of a novel technology. It is seen that, although inferior to the CD-EKF, the new method can be an alternative for process monitoring in wastewater treatment.

**Keywords:** Monitoring; wastewater treatment; observer; extended Kalman filter

## INTRODUCTION

Novel wastewater treatment technologies can take advantage of microbial activities that have only recently been discovered. In some cases, new technologies have already been implemented, such as autotrophic nitrogen removal based on anammox while others are still in development at different scales, such as the use of denitrifying anaerobic methane oxidizers (DAMO). As the number of biological processes that can take place in a reactor increases, it becomes more difficult to operators to monitor the reactor operation given macroscopic measurements.

Indeed the field of monitoring and estimation in bioreactors is mature with a large number of sophisticated algorithms, well adapted for wastewater treatment processes (see for instance Vargas *et al.* 2014). However, in a number of cases, approaches based on observers can be difficult to understand by plant managers. Expert and fuzzy based systems have been developed and implemented providing a more intuitive manner of monitoring reactors and providing insight over the biological processes (Boiocchi *et al.* 2015). Srinivasan *et al.* (2016) have used extent of reactions to identify chemical reaction rates, demonstrating the method with a considerable number of examples. A key aspect in the concept of extents is that the mass balance and reactions are used as constraints.

Inspired by the use of extent of reactions, we propose here a very simple approach based on using the stoichiometry matrix for estimating the biological processes by solving a linear least-square program. Stoichiometric yields are in general the most certain parameters when dealing with new technologies and microbial groups, in particular, the parameters that relate substrates and products. Stoichiometric yields that lead to the biomass production are, on the contrary, more uncertain. Hence, the monitoring method proposed here only uses the product/substrate stoichiometric yields. This novel approach is demonstrated by monitoring the biological processes in a complex and novel technology (SIAM) and benchmarked against a nonlinear observer, the continuous-discrete extended Kalman filter (Mauricio-Iglesias *et al.* 2015).

**METHODS**

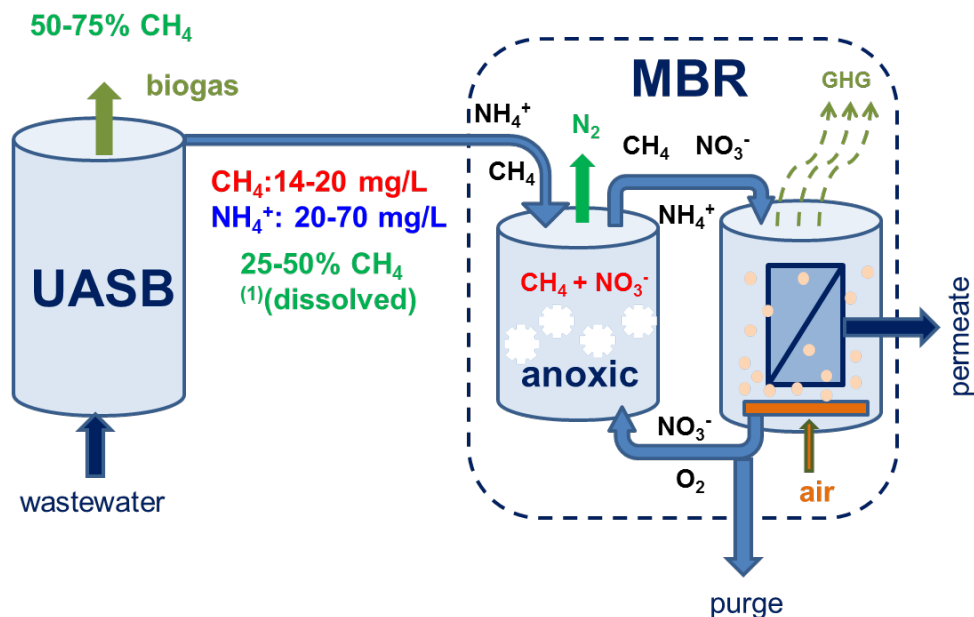
**Case-study description**

An innovative pilot plant located at the University of Santiago de Compostela (Spain) was chosen as a case study. The plant (fig. 1) is a novel two-stage MBR process referred to as SIAM, (Spanish acronym for *Integrated system of methanogenic anaerobic reactor and membrane bioreactor for COD and nitrogen removal in wastewater*). The plant and the operating conditions are described in detail elsewhere (Buntner *et al.* 2012) as well as the model developed, briefly summarised here for the sake of completeness (Mauricio-Iglesias *et al.* 2016). The model includes 21 states per chamber, namely the total hold-up and:

- 9 soluble compounds, namely dissolved oxygen, soluble COD, dissolved nitrogen, total ammonium nitrogen, total nitrite nitrogen, nitrate, soluble inerts, total inorganic carbon(TIC) and dissolved methane.

- 10 particulate compounds, namely particulate inerts, particulate COD, heterotrophs (Xh), storage product (Xsto), ammonium oxidizing bacteria (AOB), nitrite oxidizing bacteria (NOB), DAMO archaea (Xda), DAMO bacteria (Xdb), anaerobic ammonium oxidizing bacteria (Xan or anammox), aerobic methane oxidizers (Xamo) and total solids (TSS)

The microbial kinetics are modelled by 25 processes that are briefly summarised here. The heterotrophic metabolism was modelled using the activated sludge model no. 1 modified to include two step nitrification/denitrification as nitrite is the substrate of anammox and DAMO bacteria. The biological reactions of AOB, NOB and anammox were modelled as in Vangsgaard *et al.* (2012) using the unionized form of ammonium and nitrous acid as true substrates. The model of DAMO archaea and bacteria was taken from Chen *et al.* (2014) but modified in order to include the oxygen inhibition results obtained by Luesken *et al.* (2012).



**Figure 1.** Diagram of the SIAM technology used as a case-study. In particular, the microbial specific activity rates are monitored in the anoxic reactor

### Stoichiometry matrix method

The proposed monitoring method uses the stoichiometry matrix of the biological reactions to estimate the specific activity of the microbial groups present in the reactor. To make it realistic and in accordance with the uncertainty of yield coefficients, it is considered that only the substrate/product yields are known but not the substrate/biomass, as the latter are more uncertain. The method can be summarised in the following steps which illustrate the case-study:

*Step 1.* Determine the stoichiometry matrix ( $\mathbf{S}$ ), at least for substrate(s)/product(s) relationships. For the SIAM process, the stoichiometry matrix relates eight biological processes (activity rates of AOB, NOB, anammox, DAMO bacteria, DAMO archaea, aerobic methane oxidizers and heterotrophic denitrification) with five chemical species which are routinely monitored (methane, total ammonium, total nitrite, nitrate and oxygen)

*Step 2.* Estimate the vector of observable rates ( $\mathbf{r}$ ) based on macroscopic measurements by mass balances in appropriate control volumes in order to estimate the total consumption/production of each of the five species

*Step 3.* Solve the following constrained linear least-squares problem.

$$\min_{\rho} \frac{1}{2} \|\mathbf{S}\rho - \mathbf{r}\|^2 \quad s.t. \quad \rho_i \geq \mathbf{0} \quad \text{and} \quad \rho_{inf} \leq \rho_i \leq \rho_{sup} \quad (\text{eq. 1})$$

where  $\mathbf{S}$  is the stoichiometry matrix,  $\mathbf{r}$  are the observable rates and  $\rho$  is the vector of biological processes. In general,  $\mathbf{S}$  is not full rank which hinders solving the system of equations. However, as  $\rho$  is constrained to be non-negative, it is possible to find a solution to the problem in eq.1 although the unicity of the solution cannot be guaranteed *a priori*.

### Continuous Discrete Extended Kalman Filter

The system described in the case study section can be written in a general non-linear state-space form such as

$$\frac{dx}{dt} = f(x(t), u(t), d(t)) \quad (\text{eq. 2})$$

where the states ( $x$ ), inputs ( $u$ ) and disturbances ( $d$ ) represent:

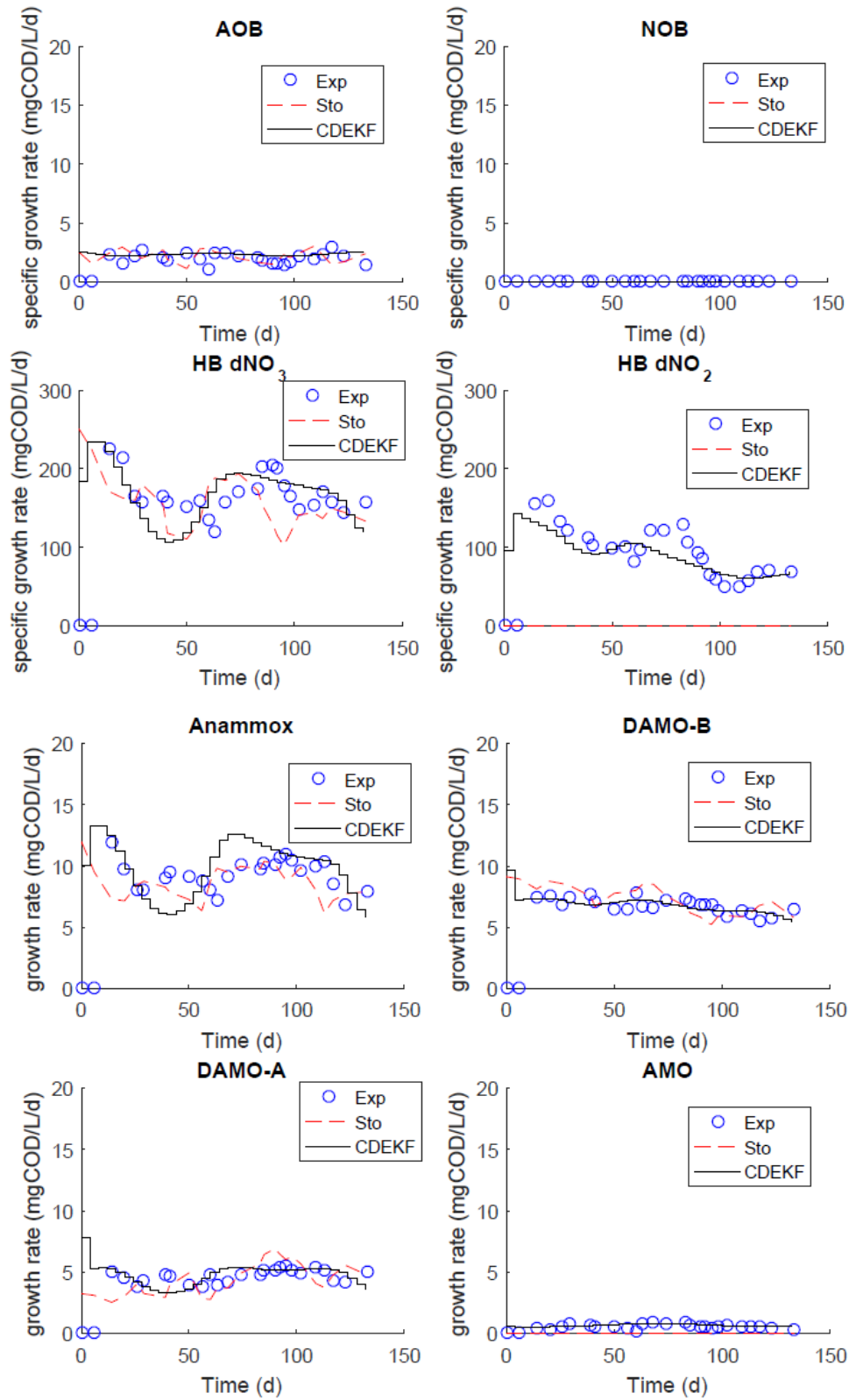
$$x = [M \ C_i]^T \quad u = [F_{in}] \quad d = [C_{i,in}] \quad (\text{eq. 3})$$

The estimation is indeed computed at discrete time step based on the sample rate in the control or monitoring system. The system (5) takes the following discrete step form:

$$x_{k+1} = F(x_k, u_k, d_k) = x_k + \int_{t_k}^{t_{k+1}} f(x(\tau), u(\tau), d(\tau)) d\tau \quad (\text{eq.4})$$

$$y_k = G(x_k) + v_k, \quad v_k \in N_{iid}(0, R_v)$$

The observer is formulated as a Continuous-Discrete Extended Kalman Filter as described in detail by Price *et al.* (2015). Ammonium, nitrate, nitrite, methane and oxygen were considered as measured variables for the CD-EKF.



**Figure 2.** Comparison of specific rates with the CD-EKF and the proposed simplified approach (Sto) for the eight biological processes taking place in the system. Heterotrophic denitrification is split in two independent steps (HB-dNO<sub>3</sub> and HB-dNO<sub>2</sub>)

## RESULTS

To test the validity of the newly proposed method and benchmark it against the CD-EKF, the model of SIAM was simulated for 140 days. To carry out a realistic simulation, the influent composition and flowrate changed as according real influent measurements obtained at pilot plant (Figure 2). For the CD-EKF estimation, input uncertainty in measurements and parameter uncertainty in the model was introduced. If no uncertainty was introduced, the CD-EKF was able to track all offset free the 18 model states and the reaction rates (results not shown). With uncertainty, the CD-EKF is still able to track the reaction rates but not all the states. The CD-EKF appears as a very reliable tool for monitoring biological processes but its development is certainly time-consuming as it requires a first principle model in order to properly determine the sensitivity equations.

For the stoichiometry-based method, the stoichiometry matrix coefficients provided (eq. 1) were also changed by simulating parameter uncertainty ( $\pm 10\%$  of nominal value). This method was able to detect most of the biological rates but, in particular, it failed in determining the heterotrophic denitrification processes. This is likely to happen because heterotrophic denitrification is not linked to any other measured co-substrate, contrarily to the rest of the processes. The advantage of this method is, indeed, its simplicity, as it is easily understood by those who have insight of the biological reactions.

## CONCLUSION

A simplified method was proposed for monitoring biological rates in wastewater treatment processes based on solving a linear least square program using the stoichiometry matrix and the observed reaction rates. The method was proved as successful in predicting most of the microbial rates of a complex novel technology and it is comparably more simple than other monitoring techniques. However, the validity of this method in other operating conditions and technologies remains to be tested and will be studied in the future.

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## REFERENCES

- Boiocchi, R., Mauricio-Iglesias, M., Vangsgaard, A.K., Gernaey, K.V., Sin, G. (2015) Aeration control by monitoring the microbiological activity using fuzzy logic diagnosis and control. Application to a complete autotrophic nitrogen removal reactor. *J Proc Cont*, 30, 22-23.
- Buntner, D., Sánchez-Sánchez, A., Garrido, J.M. (2011) Three stages MBR (methanogenic, aerobic biofilm and membrane filtration) for the treatment of low-strength wastewaters. *Water Sci.Tech*, 64(2), 397-402
- Chen, X. Guo, J. Shi, Y. Hu, S. Yuan, Z., Ni, B.J (2014) Modeling of simultaneous anaerobic methane and ammonium oxidation in a membrane biofilm reactor *Environ. Sci. Technol.*, 48, 9540–9547
- Luesken, F. Wu, M.L; Op den Camp, H.J.M. Keltjens, J.T Stunnenberg, H. Francoijs, K-J, Strous, M. Jetten, M.S.M (2014) Effect of oxygen on the anaerobic methanotroph 'Candidatus Methyloirabilis oxyfera': kinetic and transcriptional analysis. *Environmental Microbiology*. 14(4), 1024–1034
- Mauricio-Iglesias, M., Garrido, J.M., Lema, J.M. (2016) Operation of an innovative WWTP with environmental objectives. A model-based analysis. *IFAC-PapersOnLine*, 49 (7), 539-543
- Mauricio-Iglesias, M., Gernaey, K.V., Huusom, J.K. (2015) State Estimation in Fermentation of Lignocellulosic Ethanol. Focus on the Use of pH Measurements. *Comp Aid Chem Eng*, 37, 1769-1774

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- Price, J., Nordblad, M., Woodley, J.M., Huusom, J.K.(2015) Real-time model based process monitoring of enzymatic biodiesel production. *Biotechnol. Prog.*, 31 (2), 585-595.
- Srinivasan, S., Billeter, J., Bonvin, D. (2012) Extent-based incremental identification of reaction systems using concentration and calorimetric measurements, *Chemical Engineering Journal*, 207–208, 785-793
- Vangsgaard, A.K., Mauricio-Iglesias, M., Gernaey, K.V., Smets, B.F. and Sin, G. (2012). Sensitivity analysis of autotrophic N removal by a granule based bioreactor: Influence of mass transfer versus microbial kinetics. *BioresourceTechnology* 123, 230-241.
- Vargas, A., Moreno, J.A., Vande Wouwer, A. (2014) A weighted variable gain super-twisting observer for the estimation of kinetic rates in biological systems. *J. Proc. Cont.*, 24 (6), 957-965