Downloaded from orbit.dtu.dk on: Dec 16, 2017

Technical University of Denmark

Stochastic Greybox Modeling for Control of an Alternating Activated Sludge Process

Halvgaard, Rasmus Fogtmann; Vezzaro, Luca; Grum, M.; Munk-Nielsen, Thomas; Tychsen, Peter; Madsen, Henrik

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):
Halvgaard, R. F., Vezzaro, L., Grum, M., Munk-Nielsen, T., Tychsen, P., & Madsen, H. (2017). Stochastic Greybox Modeling for Control of an Alternating Activated Sludge Process. DTU Compute. (DTU Compute-Technical Report-2017, Vol. 08).

DTU Library
Technical Information Center of Denmark

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Stochastic Greybox Modeling for Control of an Alternating Activated Sludge Process

R. Halvgaard[a,b,*], L. Vezzaro[a,b], M. Grum[b], T. Munk-Nielsen[b], P. Tychsen[b], H. Madsen[a]

[a] *Technical University of Denmark, Matematiktorvet, DK-2800 Kgs. Lyngby, Denmark*
[b] *Krüger A/S, Gladsaxevej 363, DK-2860 Sborg, Denmark*

Abstract

We present a stochastic greybox model of a BioDenitro WWTP that can be used for short time horizon Model Predictive Control. The model is based on a simplified ASM1 model and takes model uncertainty into account. It estimates unmeasured state variables in the system, e.g. the inlet concentration or the sensor measurements in case of temporary sensor faults. This improves control performance without adding additional or redundant sensors. We fitted the parameters of the model to actual plant data and demonstrate the state estimation capabilities with this data set. The model now runs online at a WWTP in Denmark.

Keywords: WWTP, ASM1, Stochastic, Greybox, Alternating, BioDenitro
DTU Compute-Technical Report-2017, Vol. 8

1. Introduction

Automation and advanced control methods are some of the key tools to improve the performance of existing Waste Water Treatment Plants (WWTPs) [1]. New online control methods improve nutrient recovery, carbon neutrality, or energy neutral plants [2, 3, 4].

The control strategies can be evaluated by using the available simulation models based on the family of Activated Sludge Models (ASM) [5, 6], i.e. the Benchmark Simulation Model (BSM) [7]. The ASM models are great tools for simulation and provide a detailed description of the biological processes. However, this level of detail is not well suited for Model Predictive Control (MPC). As mentioned in [1], current MPCs in WWTP utilize "significantly simple“ models. When focusing on alternating plants, that are widely applied in Danish WWTPs, simple linear models of WWTPs were developed by [8, 9] including several heuristic model based control strategies [10, 11, 12, 13, 14, 15]. [16] also developed several models and control strategies for a pilot scale implementation of an alternating process, where [17] specifically focused on the BioDenitro process. [18] investigated a nonlinear observer for an alternating process. [19, 20, 21, 16] provide great summaries of other literature that deals with control and modeling of alternating plants.

Important obstacles on the road to widespread usage of MPC are data quality and measurements encumbered with uncertainty [1]. Although several approaches for data validation are available in literature [22, 23, 24, 25], their full-scale utilization in combination with MPC is still limited [26]. Focus for allowing the practical implementation of complex MPC approaches in WWTPs are therefore

1. handling of uncertainty
2. fault-tolerant control of sensor failures
3. parameter estimation
4. forecasting of inlet flows and concentrations
5. numerical computational times

These points can be addressed by stochastic greybox models that combine simple and fast model structures with data assimilation routines, e.g. in the form of an extended Kalman filter. [27, 28] showed the first applications of greybox models in the 1990s, who applied parameter estimation of reduced ASM1 models on alternating plants with the aim of process prediction and control. [27] concludes that greybox models of the wastewater processes performs significantly better than traditional blackbox models like ARMAX models.

The aim of this paper is to present a stochastic greybox model for Model Predictive Control of a WWTP that also accounts for uncertainty. The model is based on a simplification of the ASM1 model for a control horizon of 24 hours since this short time horizon is the most important for control. The model continuously adapts to the slower time-varying effects of the process described in the ASM1. The proposed model is formulated as a continous-discrete time state space model and is capable of estimating unmeasured variables in the system. This improves control performance without adding additional sensors.

This paper is organized as follows. Section 2.1 reduces the original ASM1 model to a practical greybox model. Section 3 describes the framework for estimating stochastic greybox model parameters using maximum likelihood estimation and the Extended Kalman Filter for state estimation. Section 4 describes our case study and the treatment process. The case

*Corresponding author
Email addresses: rhal@dtu.dk (R. Halvgaard), luve@env.dtu.dk (L. Vezzaro), mg@kruger.dk (M. Grum), thm@kruger.dk (T. Munk-Nielsen), ptt@kruger.dk (P. Tychsen), hmad@dtu.dk (H. Madsen)
URL: www.compute.dtu.dk/~rhal (R. Halvgaard)

study applies the greybox model and state estimation to real plant data. Finally, Section 5 provides conclusions.

2. Model of the activated sludge process

Since one of the most promising fields for MPC in WWTP is energy optimization, we focus our model on nitrogen removal. This removal processs requires aeration of wastewater, which is the most energy demanding process in treatment plants. Among the available models for modelling processes in WWTPs [5], we selected the ASM1 model [29], since the additional processes included in the later ASM models (e.g. P removal) are not relevant for our purpose. The ASM1 and its expansions [6] serve as great tools for detailed simulation studies of activated sludge processes, and are widely used for benchmarking control strategies [7].
However, the full model (see section 6) is not well-suited for practical online process control purposes in WWTPs. Partly due to the large amount of parameters entering its nonlinear model equations that change over different time scales, and partly because online sensors for measuring all variables in the model are simply not technologically available, too costly, or too difficult to maintain in practice. So all parameters can not be identified by statistical methods and the currently available measurements [28]. Fortunately, the most important parameters in the processes can be identified in reduced versions of the ASM. Ammonium NH_4, nitrate NO_3 and phosphate PO_4 (which is not included in ASM1) can be measured online and combined with stochastic greybox models to provide a sufficient model for control and short term prediction.

2.1. Reduced greybox model of BioDenitro process

Based on the assumptions made in Section 6.2, the equations for simulating removal of nitrogen in WWTP can be reduced to the following :

$$\dot{S}_{NH} = -k^{O}_{NH}\rho_O - k^{NO}_{NH}\rho_{NO} - k^{NH}_{NH}\rho_{NH} \tag{1a}$$

$$\dot{S}_{NO} = -k^{NO}_{NO}\rho_{NO} + k^{NH}_{NO}\rho_{NH} \tag{1b}$$

$$\dot{S}_{O} = -k^{O}_{O}\rho_O - k^{NO}_{O}\rho_{NO} \tag{1c}$$

$$\tag{1d}$$

Where the reactions rates are

$$\rho_O = \frac{S_{O_2}}{K_{O_2,OHO} + S_{O_2}} \tag{2a}$$

$$\rho_{NO} = \frac{S_{O_2}}{K_{O_2,OHO} + S_{O_2}} \frac{S_{NO_x}}{K_{NO_x,OHO} + S_{NO_x}} \tag{2b}$$

$$\rho_{NH} = \frac{S_{O_2}}{K_{O_2,ANO} + S_{O_2}} \frac{S_{NH_X}}{K_{NH_X,ANO} + S_{NH_X}} \tag{2c}$$

This simplified model utilizes the half-saturation constants K, which can be compared to physical values from literature, while a range of newly introduced constants k cannot be translate to physically interpretable parameters but can still be calcutated by using the equations listed in 6.2. The simplified model has only three state variables (which can be measured online): oxygen S_{O_2}, nitrate and nitrite S_{NO}, and ammonia S_{NH} concentrations.
The dynamics of the dissolved oxygen S_{O_2} are very fast and often a local control loop regulates the oxygen concentration to a setpoint. [30, 31, 32, 33] model this control loop by including K_{La} in the S_{O_2} equation. We assume a PID controller follows a setpoint and controls S_{O_2} directly. This reduces the model (1) to only two states.

If we insert typical ASM1 values for all these parameters we see that k^{NH}_{NH} and k^{NH}_{NO} are much bigger than the other terms and dominate the equations. Consequently, we end up with

$$\dot{S}_{NH} = -k^{NH}_{NH}\rho_{NH} \tag{3a}$$

$$\dot{S}_{NO} = k^{NH}_{NO}\rho_{NH} \tag{3b}$$

$$\rho_{NH} = \frac{S_{O_2}}{K_{O_2,ANO} + S_{O_2}} \frac{S_{NH_X}}{K_{NH_X,ANO} + S_{NH_X}} \tag{3c}$$

We use this reduced model for estimation in the remaining part of the paper.

2.2. Adding transport flows

The nitrogen removal process takes place in a tank reactor with constant volume V, which is assumed to be a Continuously Stirred Tank Reactor (CSTR). Under these common assumptions the mass balance for S_j with process reaction rate ρ_j is

$$\dot{S}_j = \frac{Q}{V}(S^{in}_j - S_j) + \rho_j \tag{4}$$

With no reaction, $\rho_j = 0$, and constant flow Q this is simply a first order low pass filter smoothing the inlet concentration. The time constant or hydraulic retention time of the tank is $\tau = \frac{V}{Q}$. Obviously, a higher flow yields a faster response towards a steady state where $S_j = S^{in}_j$. For a given treatment process the transport flows can be added to each state variable in the reduced ASM1 model (3).

3. Stochastic greybox model likelihood parameter estimation

The developed dynamical model (3) of the activated sludge process is time-varying and nonlinear. We wish to estimate the model parameters online from data and evaluate the model uncertainty, so we can use it for prediction and control. The model fits the general model structure for continuous-discrete stochastic state space models, i.e. a model of the state variables in continuous time and discrete time samples measurements of some of the states.

$$\mathrm{d}x_t = f(x_t, u_t, t, \theta)\,\mathrm{d}t + \sigma(u_t, t, \theta)\,\mathrm{d}\omega_t \tag{5a}$$

$$y_k = h(x_k, u_k, t_k, \theta) + e_k \tag{5b}$$

where $t \in \mathbb{R}$ is time and $k \in \mathbb{Z}$ is the discrete time index of the sampled time instants t_k spaced with sampling period T_s. $x_t \in \mathbb{R}^n$ contains the n state variables, $u_t \in \mathbb{R}^m$ is the m input variables, $y_k \in \mathbb{R}^l$ is the l output variables while $\theta \in \mathbb{R}^p$ contains the p model parameters to be estimated. $f(\cdot) \in \mathbb{R}^n$, $\sigma(\cdot) \in \mathbb{R}^{n\times n}$, and $h(\cdot) \in \mathbb{R}^l$ are nonlinear functions. When these functions are linear (5) reduce to linear state space models. ω_t is an n-dimensional standard Wiener process and e_k is an l-dimensional white noise process with $e_k \in N(0, S(u_k, t_k, \theta))$ characterizing the measurement noise.

Given a model structure and a set of $N + 1$ measurements $\mathcal{Y}_N = [y_N, y_{N-1}, \ldots, y_1, y_0]$ we wish to find the parameters θ that maximizes the likelihood function

$$L(\theta, \mathcal{Y}_N) = p(\mathcal{Y}_N|\theta) = p(y_0|\theta) \prod_{k=1}^{N} p(y_k|\mathcal{Y}_{k-1}, \theta) \tag{6}$$

$p(y_k|\mathcal{Y}_{k-1}, \theta)$ is a conditional density denoting the probability of observing y_k given the previous observation set $\mathcal{Y}_{k-1}$ and parameters θ. For sufficiently fast sampled measurements we approximate this conditional density with a Gaussian distribution such that

$$p\left(y_k|\mathcal{Y}_{k-1}, \theta\right) = \frac{\exp\left(-\frac{1}{2}\epsilon_k^T R_{k|k-1}^{-1}\epsilon_k\right)}{\sqrt{|R_{k|k-1}|}\sqrt{2\pi}^l} \tag{7}$$

where

$$\epsilon_k = y_k - \hat{y}_{k|k-1} \tag{8a}$$
$$\hat{y}_{k|k-1} = E[y_k|\mathcal{Y}_{k-1}, \theta] \tag{8b}$$
$$R_{k|k-1} = V[y_k|\mathcal{Y}_{k-1}, \theta] \tag{8c}$$

defines the output residual ϵ and estimated mean output $\hat{y}$ with covariance R. A Kalman filter provides exactly these estimates for Gaussian noise densities, even for nonlinear models in the extended linearizing version the Extended Kalman Filter (EKF) [34].

If we assume the initial probability density $p(y_0|\theta)$ to be known and put (7) into the likelihood function (6), then we can find a set of parameters $\hat{\theta}$ that maximizes the likelihood function by solving the following nonlinear optimization problem

$$\underset{\hat{\theta}\in\Theta}{\text{maximize}}\ \log[L(\hat{\theta}, \mathcal{Y}_N|x_0)] \tag{9}$$

Including the logarithm decomposes the likelihood function into sums instead of products that is easier to handle when solving the optimization problem. We assume each parameter to take values within predefined bounds with equal probability, so the parameters are constrained to the set Θ. The problem can also be extended to maximum a posteriori (MAP) estimation, where instead of giving simple parameter bounds, a prior probability density function limits the parameter value. This is useful if some prior knowledge about the probability density is available.

3.1. Software

We use R and the package `CTSM-R`[1] [35, 36, 37] to model and estimate the parameters using Maximum Likelihood Estimation. `CTSM-R` solves the optimization problem (9) and provides estimates of the parameters and their uncertainty. It also includes outlier detection, handles irregular sampling and can combine multiple independent data sets into the same estimation procedure. Finally, the implemented Extended Kalman Filter estimates any missing observations caused by calibrating sensors or communication faults.

[1] `www.ctsm.info`

4. Case study: Kolding WWTP

Kolding WWTP in Denmark runs a BioDenitro™ process with a treatment capacity of 125,000 PE and a load of 75,000 PE. We use data from this plant as a case study for validating our greybox model and running the state estimation. We wish to estimate the NH_4 concentration in both tanks. Estimating unmeasured states accurately leads to better control performance without adding costly additional sensors.

4.1. BioDenitro operation

The BioDenitro process involves two hydraulically connected tank reactors that are operated with equal loading in counter phase. The continuous influent wastewater is divided between the reactors while the operating conditions alternates between aerobic or anoxic conditions. The influent primarily flows to the anoxic reactor to utilize its organic carbon content for denitrification. The reactor role is toggled as soon as the NH_4 and NO_3 concentrations in the anoxic reactor reach a set point or if a process time limit is exceeded. Each reactor is equipped with actuators for aeration and propellers for mixing. The BioDenitro process approaches a batch process, because the phases are short relative to the hydraulic retention time and the inlet wastewater volume is small compared to the total tank volume. Figure 2 shows the operation cycle of a typical BioDenitro plant with indication of flow patterns and phases. A RBC strategy that changes the cycle lengths depending on online measurements [38] is the commercially available control system STAR for the BioDenitro process developed by Krüger A/S. After its development in the early 1990s [39, 40, 41] approximately 400 plants primarily in Denmark run the BioDenitro process (or BioDenipho if Phosphorus is treated as well). The process is very flexible and can adapt to different waste water compositions. The periodically higher concentrations yields faster reaction times and the continuous alternating excitation of the dynamics makes it easier to estimate the process rates through mathematical system identification. However, the phase control design is quite complex where nitrification and denitrification are performed sequentially in a semi-batch manner by cyclically switching flow and aeration pattern.

Kolding WWTP has four aeration tanks, i.e. two BioDenitro tank sets, equipped with two O_2 sensors each. Figure 1 shows the plant layout from above. Figure 2 shows the flow directions and sensors in one BioDenitro tank set at Kolding. All possible flow combinations and aeration on/off patterns are described in [39]. At Kolding only one tank, i.e. the master tank A, has a NH_4 and a NO_3 sensor, and in this case study we estimate the NH_4 in tank B. Estimating the concentration in tank B will increase the control performance in terms of better effluent quality and lower power consumption without an expensive physical sensor. As the two tanks sets are disconnected and only one tank set have NH_4 and NO_3 sensors we can not estimate the concentrations in the second tank set. So the other tank set simply copy the control action from tank A and B in an open loop manner.

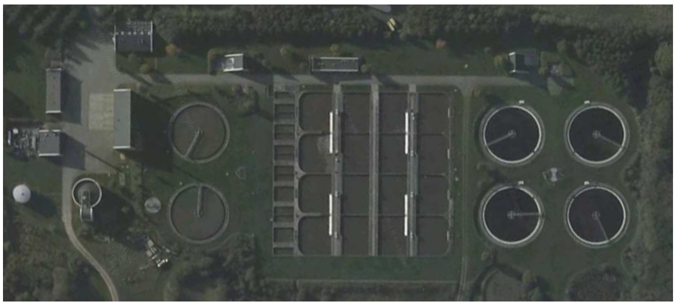

Figure 1: Kolding WWTP with two BioDenitro lines including four aeration tanks.

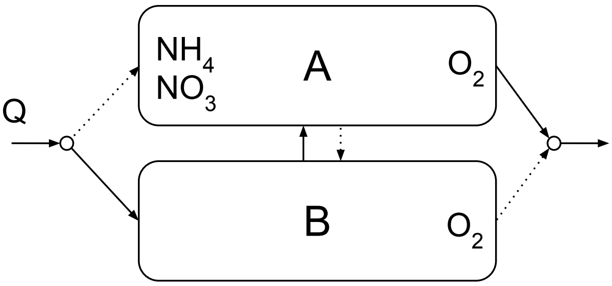

Figure 2: BioDenitro aeration tank pair and flow directions. The weir at the input and at the output have two possible flow directions, while the middle connection allows a flow between the tanks. Only tank A has an NH_4 and an NO_3 sensor.

4.2. Data

We have measurements of NH_4, NO_3, O_2 and flows between the tanks from Kolding WWTP. In total we use a 48 hour data set for the greybox model estimation. The sensors sample every 5 min while the process control system samples every 2 min. So the individual sensor measurements are collected multiple times and repeated in the data either two or three times. Consequently, to pick out the actual observations, we excluded all points as missing observations when their finite difference was very low, ideally zero. `CTSM-R` easily handles these missing observations and non-equidistant samples.

The sensors also calibrate automatically 3-4 times per day leaving the control with no measurements up to 1 hour.

For the given data set we time shifted the observations 8 samples to account for sensor and actuation delays. The delay might vary over time and can be included in the model or estimated independently.

4.3. Reduced greybox model of BioDenitro process

We build a model of the NH_4 concetrations in tank A and B using (3). We assume that the incoming waste water contains no NO_3 or O_2 such that $S_{NO}^{in} = 0$ and $S_O^{in} = 0$.

$$\dot{S}_{NH}^A = \theta_1 Q\left[S_{NH}^{in} w_i + S_{NH}^B \tilde{w}_i - S_{NH}^A\right] - \theta_2 \frac{S_{NH}^A}{K_{NH}^A + S_{NH}^A} \frac{S_O^A}{K_O^A + S_O^A} \tag{10a}$$

$$\dot{S}_{NH}^B = \theta_3 Q\left[S_{NH}^{in} \tilde{w}_i + S_{NH}^A w_i - S_{NH}^B\right] - \theta_4 \frac{S_{NH}^B}{K_{NH}^B + S_{NH}^B} \frac{S_O^B}{K_O^B + S_O^B} \tag{10b}$$

The states are $x = [S_{NH}^A, S_{NH}^B]^T$ with inputs $u = [w_i, S_O, Q, S_{NH}^{in}]^T$. The parameters θ contain the tank volume and we have the unknown parameters: $\theta = (\theta_1, \theta_2, \theta_3, \theta_4, K_O^A, K_O^B, K_{NH}^A, K_{NH}^B, \sigma_3)$. w_i is a binary variable equal to 1 when the inlet weir is open to tank A and 0 for tank B. $\tilde{w}_i$ is the boolean inverse of w_i. Q is the inlet flow that we assume is also equal to the outlet flow. We neglect the very short time periods where a tank has neither inlet or outlet. S_{NH}^{in} is the NH_4 concentration in the inlet.

4.4. Estimating unmeasured NH_4 concentrations

Unlike the inlet flow input, the other important part of the waste water load, namely the NH_4 inlet concentration, is not measured. We know that this concentration follows the inlet flow with a diurnal profile. We estimate it using the EKF and the greybox model by writing the model equations (10) as a set of stochastic differential equations on the form (5). In order to estimate the inlet concentration we add S_{NH}^{in} as a third state driven by noise such that

$$dS_{NH}^{in} = 0\,dt + \sigma_3 d\omega_3, \quad \sigma_3 > 0. \tag{11}$$

This is a random walk model for S_{NH}^{in} that allows S_{NH}^{in} to vary in a flexible manner. Any model discrepancies will be transferred to this state and might disrupt the physical interpretation of the concentration. Since the NH_4 concentration in tank B, S_{NH}^B, is also not measured, we also get an estimate of this concentration.

Figure 3 shows the model fit on the estimation data set. The one-step ahead predictions fit the data very well with low residuals. All missing observations and unmeasured states are estimated by the EKF. As expected the NH_4 concentration in tank B is similar to tank A but time-shifted due to the alternating pattern. The diurnal pattern of the NH_4 inlet concentration is also clearly evident but not completely smooth. This is mainly due to the sensor placement and practical non-ideal mixing conditions. Also the NH_4 concentrations are controlled to low values due to the treatment process, so consequently we see only short periods of mixing where the load goes towards the higher NH_4 inlet concentration.

The parameter estimation for 48 hours of data using `CTSMR` took around 10 seconds on a laptop but is running online on a server every 2 minutes as part of the plant control software.

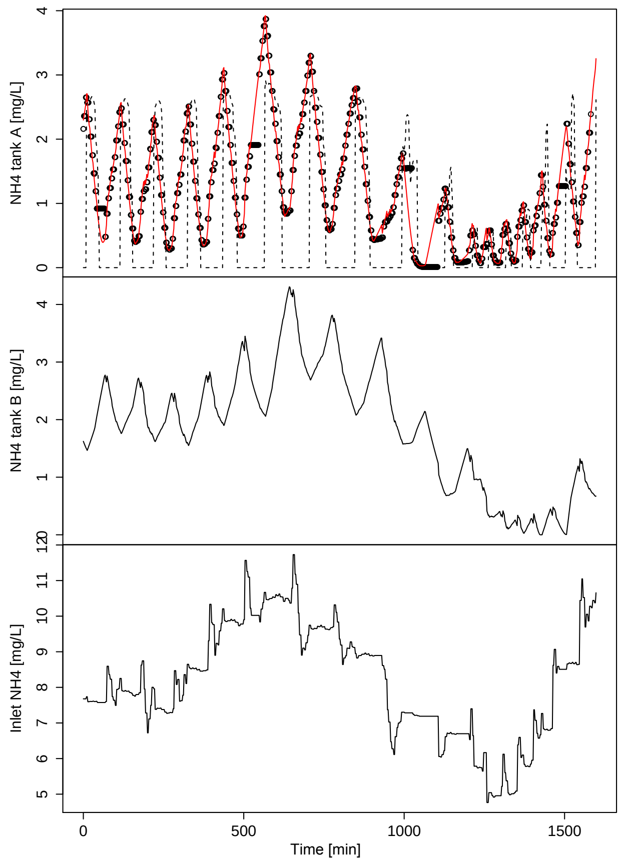

Figure 3: Estimated one-step predictions of NH_4 concentrations in both tanks and the inlet. The dotted line in the upper plot is the intermittent aeration pattern.

Parameter	Value	Std.
$S^{A}_{NH,0}$	2.29e+00	6.99e-02
$S^{B}_{NH,0}$	5.35e-01	1.25e+00
$S^{in}_{NH,0}$	9.66e+00	2.96e+00
K^{A}_{NH}	3.49e-01	9.06e-02
K^{B}_{NH}	1.44e+00	9.26e-01
K^{A}_{OA}	1.79e-01	8.39e-02
K^{B}_{OA}	1.74e+00	1.17e+00
σ_{MsNH}	3.78e-04	3.21e-04
σ_{A}	3.38e-02	2.37e-03
σ_{B}	7.09e-07	2.25e-05
σ_{NHin}	2.07e-01	7.82e-02
θ_1	5.96e-02	2.05e-02
θ_2	7.32e-02	7.16e-03
θ_3	6.39e-02	1.52e-02
θ_4	9.34e-01	8.09e-01

Figure 4: Parameter estimates.

5. Conclusion

The method provides a greybox model for the process which describes the uncertainty, and state estimation which are critical for Model Predictive Control purposes. We built a stochastic greybox model of a BioDenitro process aiming for a time horizon below 24 hours. An R-package, `CTSMR`, estimates the model parameters using maximum likelihood optimization and the Extended Kalman FIlter. If run repeatedly, e.g. in moving 48 hours windows, the algorithm adaptively fits the model parameters to the current operating conditions and fills in missing sensor measurements. This is particular important in the frequent and long periods where the sensors are calibrating and not providing measurements to the control system. Since we estimate missing observations, the inlet load, and the concentrations in the sensorless tank, we could obtain a more accurate control performance. The model is an important piece in predicting the process and applying Model Predictive Control.

References

[1] G. Olsson, B. Carlsson, J. Comas, J. Copp, K. V. Gernaey, P. Ingildsen, U. Jeppsson, C. Kim, L. Rieger, I. Rodríguez-Roda, J.-P. Steyer, I. Takács, P. a. Vanrolleghem, A. Vargas, Z. Yuan, L. Åmand, Instrumentation, control and automation in wastewater - from London 1973 to Narbonne 2013., Water Science & Technology 69 (7) (2014) 1373–85. doi:10.2166/wst.2014.057.
URL http://www.ncbi.nlm.nih.gov/pubmed/24718326

[2] H. Gao, Y. D. Scherson, G. F. Wells, Towards energy neutral wastewater treatment: methodology and state of the art., Environmental science. Processes & impacts 16 (6) (2014) 1223–46. doi:10.1039/c4em00069b.
URL http://www.ncbi.nlm.nih.gov/pubmed/24777396

[3] W. Mo, Q. Zhang, Energy-nutrients-water nexus: integrated resource recovery in municipal wastewater treatment plants., Journal of environmental management 127 (2013) 255–67. doi:10.1016/j.jenvman.2013.05.007.
URL http://www.ncbi.nlm.nih.gov/pubmed/23764477

[4] C. Sweetapple, G. Fu, D. Butler, Does carbon reduction increase sustainability? A study in wastewater treatment., Water research 87 (2015) 522–530. doi:10.1016/j.watres.2015.06.047.
URL http://www.sciencedirect.com/science/article/pii/S0043135415300956

[5] K. V. Gernaey, M. C. van Loosdrecht, M. Henze, M. Lind, S. B. Jørgensen, Activated sludge wastewater treatment plant modelling and simulation: state of the art, Environmental Modelling & Software 19 (9) (2004) 763–783. doi:10.1016/j.envsoft.2003.03.005.
URL http://linkinghub.elsevier.com/retrieve/pii/S1364815203002044

[6] M. Henze, W. Gujer, M. Takashi, M. C. M. van Loosdrecht, Activated Sludge Models ASM1, ASM2, ASM2d and ASM3, Tech. rep. (2000).

[7] K. V. Gernaey, U. Jeppsson, P. A. Vanrolleghem, J. B. Copp (Eds.), Benchmarking of Control Strategies for Wastewater Treatment Plants, IWA Publishing Company, 2014.

[8] H. Zhao, S. H. Isaacs, H. Søeberg, M. Kümmel, A novel control strategy for improved nitrogen removal in an alternating activated sludge process – Part I. Process Analysis, Water Research 28 (3) (1994) 521–534.

[9] S. H. Isaacs, H. Zhao, H. Soeberg, M. Kummel, Modeling the nitrogen dynamics in an alternating activated sludge process, Mathematics and Computers in Simulation 39 (1995) 617–626.

[10] H. Zhao, S. Isaacs, H. Søeberg, M. Kümmel, A novel control strategy for improved nitrogen removal in an alternating activated sludge process – Part II. Control development, Water Research 28 (3) (1994) 535–542. doi:10.1016/0043-1354(94)90004-3.
URL http://linkinghub.elsevier.com/retrieve/pii/0043135494900043

[11] S. H. Isaacs, Short Horizon Control Strategies for an Alternating ASP, Water Science and Technology 34 (1-2) (1996) 203–212.

[12] T. G. Potter, B. Koopman, S. A. Svoronos, Optimization of a periodic biological process for nitrogen removal from waste water, Water Research 30 (1) (1996) 142–152.
[13] S. H. Isaacs, Cycle length aeration time N removal alternating ASP, Water Science and Technology 35 (1) (1997) 225–232.
[14] S. H. Isaacs, D. Thornberg, A comparison between model and rule based control of a periodic activated sludge process, Water Science and Technology 37 (12) (1998) 343–351.
[15] J. S. Anderson, T. J. McAvoy, O. J. Hao, Use of Hybrid Models in Wastewater Systems, Industrial & Engineering Chemistry Research 39 (6) (2000) 1694–1704. doi:10.1021/ie990557r.
URL http://pubs.acs.org/doi/abs/10.1021/ie990557r
[16] L. J. S. Lukasse, Control and Identification in Activated Sludge Processes, Ph.D. thesis, Wageningen Agricultural University (1999).
[17] L. J. S. Lukasse, K. J. Keesman, Optimized operation and design of alternating activated sludge processes for N-removal, Water Practice & Technology 33 (11) (1999) 2651–2659.
[18] I. Manaa, F. M'Sahli, Unknown inputs observer applied to an alternating activated sludge process, 21st Mediterranean Conference on Control and Automation (2013) 634–639doi:10.1109/MED.2013.6608789.
URL http://ieeexplore.ieee.org/lpdocs/epic03/wrapper.htm?arnumber=6608789
[19] M. Mulas, Modelling and Control of Activated Sludge Processes, Ph.D. thesis (2006).
[20] B. Holenda, Development of modelling, control and optimization tools for the activated sludge process, Ph.D. thesis (2007).
[21] S. R. Weijers, Modelling , Identification and Control of Activated Sludge Plants for Nitrogen Removal, Ph.D. thesis, Technische Universiteit Eindhoven (2000).
[22] J. Alferes, A. Lynggaard-Jensen, T. Munk-Nielsen, S. Tik, L. Vezzaro, A. K. Sharma, P. S. Mikkelsen, P. A. Vanrolleghem, Validating data quality during wet weather monitoring of wastewater treatment plant influents, in: Proceedings of WEFTEC2013, 2013.
[23] F. Baggiani, S. Marsili-Libelli, Real-time fault detection and isolation in biological wastewater treatment plants., Water science and technology : a journal of the International Association on Water Pollution Research 60 (11) (2009) 2949–61. doi:10.2166/wst.2009.723.
URL http://www.ncbi.nlm.nih.gov/pubmed/19934517
[24] Y. Liu, Y. Pan, Z. Sun, D. Huang, Statistical Monitoring of Wastewater Treatment Plants Using Variational Bayesian PCA, Industrial & Engineering Chemistry Research 53 (8) (2014) 3272–3282. doi:10.1021/ie403788v.
URL http://pubs.acs.org/doi/abs/10.1021/ie403788v
[25] C. Rosen, J. A. Lennox, Multivariate and multiscale monitoring of wastewater treatment operation, Water Research, Water Res 35 (14) (2001) 3402–3410.
[26] J. Alferes, S. Tik, J. Copp, P. A. Vanrolleghem, Advanced monitoring of water systems using in situ measurement stations: data validation and fault detection, Water Science and Technology 68 (5) (2013) 1022–1030.
[27] J. Carstensen, Identification of Wastewater Processes, Phd thesis, Technical University of Denmark (1996).
[28] M. K. Nielsen, H. Madsen, J. Carstensen, Identification and control of nutrient removing processes in wastewater treatment plants, in: IEEE International Conference on Control and Applications (CCA), Ieee, 1994, pp. 1005–1010. doi:10.1109/CCA.1994.381196.
URL http://ieeexplore.ieee.org/lpdocs/epic03/wrapper.htm?arnumber=381196
[29] M. Henze, C. P. L. Grady Jr, W. Gujer, G. v. R. Marais, T. Matsuo, Activated Sludge Model no. 1, Tech. rep., IAWPRC (1987).
[30] B. Holenda, E. Domokos, Á. Rédey, J. Fazakas, Dissolved oxygen control of the activated sludge wastewater treatment process using model predictive control, Computers & Chemical Engineering 32 (6) (2008) 1270–1278. doi:10.1016/j.compchemeng.2007.06.008.
URL http://linkinghub.elsevier.com/retrieve/pii/S009813540700155X
[31] C. Vlad, M. Sbarciog, M. Barbu, S. Caraman, A. V. Wouwer, Indirect Control of Substrate Concentration for a Wastewater Treatment Process by Dissolved Oxygen Tracking, CEAI 14 (1) (2012) 37–47.
[32] M. Fikar, B. Chachuat, M. A. Latifi, Optimal operation of alternating activated sludge processes, Control Engineering Practice 13 (7) (2005) 853–861. doi:10.1016/j.conengprac.2004.10.003.
URL http://linkinghub.elsevier.com/retrieve/pii/S0967066104002126
[33] A. Stare, D. Vrecko, N. Hvala, S. Strmcnik, Comparison of control strategies for nitrogen removal in an activated sludge process in terms of operating costs: A simulation study, Water Research 41 (9) (2007) 2004–14. doi:10.1016/j.watres.2007.01.029.
URL http://www.ncbi.nlm.nih.gov/pubmed/17346768
[34] T. Kailath, A. H. Sayed, B. Hassibi, Linear Estimation, Prentice Hall, 2000.
[35] R. Juhl, N. R. Kristensen, P. Bacher, J. K. Møller, H. Madsen, CTSM-R User Guide, Tech. rep., Technical University of Denmark (2013).
[36] N. R. Kristensen, H. Madsen, Continuous Time Stochastic Modelling – CTSM 2.3 Mathematics Guide, Tech. rep., Technical University of Denmark (2003).
[37] N. R. Kristensen, H. Madsen, S. B. Jørgensen, Parameter estimation in stochastic grey-box models, Automatica 40 (2) (2004) 225–237. doi:10.1016/j.automatica.2003.10.001.
URL http://linkinghub.elsevier.com/retrieve/pii/S000510980300298X
[38] H. Zhao, A. J. Freed, R. W. Dimassimo, S.-N. Hong, E. Bundgaard, H. A. Thomsen, Demonstration of Phase Length Control of BioDenipho Process Using On-line Ammonia and Nitrate Analyzers at Three Full-Scale Wastewater Treatment Plants, WEFTEC.
[39] E. Bundgaard, K. L. Andersen, G. Pedersen, BioDenitro and BioDenipho systems – Experiences and Advanced Model Development: The Danish Systems for Biological N and P Removal, Water Science and Technology 21 (1989) 1727–1730.
[40] J. Sorensen, D. E. Thornberg, M. K. Nielsen, Optimization of a Nitrogen-Removing Biological Wastewater Treatment Plant Using On-Line Measurements, Water Environment Research 66 (3) (1994) 236–242.
[41] M. K. Nielsen, T. B. Önnerth, Improvement of a recirculating plant by introducing STAR control, Water Science & Technology 31 (2) (1995) 171–180.
[42] J. Huang, O. J. Hao, Alternating aerobic-anoxic process for nitrogen removal: Dynamic modeling, Water Environment Research 68 (1) (1996) 94–104.
[43] H. Kim, H. Lim, J. Wie, I. Lee, M. F. Colosimo, Optimization of modified ABA2 process using linearized ASM2 for saving aeration energy, Chemical Engineering Journal 251 (2014) 337–342. doi:10.1016/j.cej.2014.04.076.
URL http://linkinghub.elsevier.com/retrieve/pii/S1385894714005087
[44] C.-S. Gomez-Quintero, I. Queinnec, Robust estimation for an uncertain linear model of an activated sludge process, in: IEEE International Conference on Control and Applications (CCA), Vol. 2, 2002.
[45] I. Y. Smets, J. V. Haegebaert, R. Carrette, J. F. Van Impe, Linearization of the activated sludge model ASM1 for fast and reliable predictions., Water Research 37 (8) (2003) 1831–51. doi:10.1016/S0043-1354(02)00580-8.
URL http://www.ncbi.nlm.nih.gov/pubmed/12697227
[46] B. Chachuat, N. Rouche, M. A. Latifi, Reduction of the ASM1 model for optimal control of small-size activated sludge treatment plants.
[47] S. Xie, L. Zhou, A. Ma, L. Zhao, Model Reduction Based on Time-Scale Decomposition for Wastewater Treatment Process, in: 4th International Conference on Natural Computation, Ieee, 2008, pp. 567–572. doi:10.1109/ICNC.2008.501.
URL http://ieeexplore.ieee.org/lpdocs/epic03/wrapper.htm?arnumber=4667499
[48] I. Queinnec, C.-S. Gómez-Quintero, Reduced modeling and state observation of an activated sludge process., Biotechnology progress 25 (3) (2009) 654–66. doi:10.1002/btpr.178.
URL http://www.ncbi.nlm.nih.gov/pubmed/19496181
[49] J. S. Anderson, H. Kim, T. J. McAvoy, O. J. Hao, Control of an alternating aerobic-anoxic activated sludge system – Part 1: development of a linearization-based modeling approach, Control Engineering Practice 8 (3) (2000) 271–278. doi:10.1016/S0967-0661(99)00174-4.
URL http://linkinghub.elsevier.com/retrieve/pii/S0967066199001744
[50] S. Julien, J. P. Babary, P. Lessard, Theoretical and Practical Identifiability of a Reduced Order Model in an Activated Sludge Process doing Nitrification and Denitrification, Water Science and Technology 37 (12) (1998)

309–316.

[51] H. Zhao, S. Isaacs, H. Søeberg, M. Kümmel, An analysis of nitrogen removal and control strategies in an alternating activated sludge process, Water Research 29 (2) (1995) 535–544. doi:10.1016/0043-1354(94)00174-6.
URL http://linkinghub.elsevier.com/retrieve/pii/0043135494001746

[52] M. Mulas, S. Tronci, R. Baratti, Development of a 4-measurable states activated sludge process model deduced from the ASM1, in: 8th International IFAC Symposium on Dynamics and Control of Process Systems (DYCOPS), Vol. 1, 2007, pp. 213–218.

[53] P. Vega, S. Revollar, J. M. Martin, M. Francisco, Static and dynamic set point optimization techniques for optimal operation of wastewater treatment plants, in: European Control Conference (ECC), 2013, pp. 3415–3420.

6. Appendix

In the following sections we firstly introduce the ASM1 model and then we simplify it based on several assumption that are met when looking at predictive control and probabilistic forecasting up to 24 hours ahead.

6.1. *Activated Sludge Model no. 1 (ASM1)*

For practical purposes, the ASM models are commonly presented by using the Gujer matrix representation (see Table 1), where the state variable are presented in columns, while processes are in the rows. The mass balance for the modelled system is simply calculated as

$$Input - Output + Reaction - Accumulation \qquad (12)$$

The reaction rate r_i $[gm^{-3}d^{-1}]$ for each *i-th* state variable is then calculated as

$$r_i = \sum_j \nu_{ij}\rho_j \qquad (13)$$

where ν_{ij} are the stoichiometric coefficients and ρ_j are the rates for the *j-th* process. By using this framework, the ASM1 model can be described by 9 variables and 8 processes (see Table 1).
The biological processes are described by using the Monod kinetics, which in practice operates as continuous concentration-dependent switching functions for the different process rates, mainly to distinguish between aerobic ($S_{O_2} > 0$) and anoxic ($S_O = 0, S_{NO_x} > 0$) conditions.

6.1.1. *ASM1 differential equations*

Baed on the tables provided in the previous section, we can write up the set of first order ordinary differential equations de-

Table 1: Guyer matrix for ASM1 (from [6], adapted with the new notation from [?])

j	Component → *i* Process ↓	S_B	X_U	X_{OHO}	X_{ANO}	S_{O_2}	S_{NO_x}	S_{NH_x}	$S_{NB,org}$	$X_{NB,org}$	Process rate $\rho_j[gm^{-3}d^{-1}]$
1	Aerobic Growth of heterotrophs	$-\frac{1}{Y_{OHO}}$		1		$-\frac{1-Y_{OHO}}{Y_{OHO}}$		$-i_{N\_Bio}$			$\hat{\mu}_{OHO,max}\left(\frac{S_B}{K_{S_B}+S_B}\right)\left(\frac{S_{O_2}}{K_{O_2,OHO}+S_{O_2}}\right)X_{OHO}$
2	Anoxic Growth of heterotrophs	$-\frac{1}{Y_{OHO}}$		1			$-\frac{1-Y_{OHO}}{2.86Y_{OHO}}$	$-i_{N\_Bio}$			$\hat{\mu}_{OHO,max}\left(\frac{S_B}{K_{S_B}+S_B}\right)\left(\frac{S_{O_2}}{K_{O_2,OHO}+S_{O_2}}\right) \times\left(\frac{S_{NO_x}}{K_{NO_x,OHO}+S_{NO_x}}\right)\eta_{\mu,OHO}X_{OHO}$
3	Aerobic Growth of autotrophs				1	$-\frac{4.57-Y_{ANO}}{Y_{ANO}}$	$-\frac{1}{Y_{ANO}}$	$-i_{N\_Bio}-\frac{1}{Y_{ANO}}$			$\hat{\mu}_{ANO,max}\left(\frac{S_{NH_x}}{K_{NH_x,ANO}+S_{NH_x}}\right)\left(\frac{S_{O_2}}{K_{O_2,ANO}+S_{O_2}}\right)X_{OHO}$
4	Decay of of heterotrophs		$1-f_{Bio\_X}$	-1		f_{Bio_X}				$i_{N\_Bio}-f_{Bio\_X}i_{N\_Bio,E}$	$b_{OHO}X_{OHO}$
5	Decay of of autotrophs		$1-f_{Bio\_X}$		-1	f_{Bio_X}				$i_{N\_Bio}-f_{Bio\_X}i_{N\_Bio,E}$	$b_{ANO}X_{ANO}$
6	Ammonification of soluble organic nitrogen							1	-1		$q_{am}S_{NB,org}X_{OHO}$
7	Hydrolysis of entrapped organics	1	-1								$q_{hyd}\frac{X_U/X_{OHO}}{K_{hyd+(X_U/X_{OHO})}}\left[\left(\frac{S_{O_2}}{K_{O_2,OHO}+S_{O_2}}\right) +\eta_{hyd}\left(\frac{S_{O_2}}{K_{O_2,OHO}+S_{O_2}}\right)\left(\frac{S_{NO_x}}{K_{NO_x,OHO}+S_{NO_x}}\right)\right]X_{OHO}$
8	Hydrolysis of entrapped organic nitrogen								1	-1	$\rho_7\left(X_{NB,org}/X_U\right)$

Table 2: List of state variables for ASM1 (from [6])

State Variable	Units	Description
S_B	$gCODm^{-3}$	Readily biodegradable substrate
X_U	$gCODm^{-3}$	Slowly biodegradable substrate
X_{OHO}	$gCODm^{-3}$	Ordinary heterotrophic organisms
X_{ANO}	$gCODm^{-3}$	Autotrophic nitryfing organisms
S_{O_2}	$gCODm^{-3}$	Oxygen (negative COD)
S_{NO_x}	gNm^{-3}	Nitrate and nitrite nitrogen
S_{NH_x}	gNm^{-3}	Ammonium plus ammonia nitrogen
$S_{NB,org}$	gNm^{-3}	Soluble biodegradable organic nitrogen
$X_{NB,org}$	gNm^{-3}	Particulate biodegradable organic nitrogen

Table 3: List of stoichiometric parameters for ASM1 (from [6])

Parameter	Units	Description
f_{Bio_X}	$-$	Fraction of biomass yielding particulate products
i_{N_Bio}	$gN(gCOD)^{-1}$	Mass N / Mass COD in biomass
$i_{N\_Bio,E}$	$gN(gCOD)^{-1}$	Mass N / Mass COD in products from biomass
Y_{ANO}	$gX_{ANO}(gN)^{-1}$	Autotrophic yield
Y_{OHO}	$gX_{OHO}(gN)^{-1}$	Heterotrophic yield

Table 4: List of kinetic parameters for ASM1 (from [6])

Parameter	Units	Description
b_{ANO}	d^{-1}	Decay coefficient for autotrophic biomass
b_{OHO}	d^{-1}	Decay coefficient for heterotrophic biomass
K_{hyd}	$g\ slowly\ biodeg.\ COD$ $\cdot(g\ cell\ COD)^{-1}$	Half-saturation coeff. for hydrolysis of slowly biodegradable substrate
$K_{NH_x,ANO}$	gNO_xm^{-3}	Ammonium and ammonia half-saturation coeff. for of autotrophs
$K_{NO_x,OHO}$	gNO_xm^{-3}	Nitrate and nitrite half-saturation coeff. for of heterotrophic
$K_{O_2,ANO}$	gO_2m^{-3}	Oxygen half-saturation coeff. for of autotrophic biomass
$K_{O_2,OHO}$	gO_2m^{-3}	Oxygen half-saturation coeff. for of heterotrophic biomass
K_{S_B}	$gCODm^{-3}$	Half-saturation coeff. for heterotrophic biomass
$\eta_{\mu,OHO}$	-	Correction factor for anoxic growth of heterotrophs
η_{hyd}	-	Correction factor for hydrolysis under anoxic conditions
$\hat{\mu}_{ANO,max}$	d^{-1}	Autotrophic nitryifiers growth rate
$\hat{\mu}_{OHO,max}$	d^{-1}	Heterotrophic growth rate
q_{am}	$m^3COD(gd^{-1})$	Ammonification rate
q_{hyd}	$g\ slowly\ biodeg.\ COD$ $\cdot(g\ cell\ COD\ d)^{-1}$	Hydrolysis rate

scribing the ASM1 dynamics

$$\dot{S}_{NH} = -i_{XB}\left(\rho_1 + \rho_2\right) - \left(i_{XB} + \frac{1}{Y_A}\right)\rho_3 + k_a S_{ND} X_{B,H} \tag{14a}$$

$$\dot{S}_{NO} = -\frac{1-Y_H}{2.68Y_H}\rho_2 + \frac{1}{Y_A}\rho_3 \tag{14b}$$

$$\dot{S}_O = -\frac{1-Y_H}{Y_H}\rho_1 - \frac{4.57-Y_A}{Y_A}\rho_3 \tag{14c}$$

$$\dot{S}_S = \rho_7 - \frac{1}{Y_H}\left(\rho_1 + \rho_2\right) \tag{14d}$$

$$\dot{X}_S = (1-f_p)(b_H X_{B,H} + b_A X_{B,A}) - \rho_7 \tag{14e}$$

$$\dot{X}_{B,H} = \rho_1 + \rho_2 - b_H X_{B,H} \tag{14f}$$

$$\dot{X}_{B,A} = \rho_3 - b_A X_{B,A} \tag{14g}$$

$$\dot{S}_{ND} = \rho_8 - k_a S_{ND} X_{B,H} \tag{14h}$$

$$\dot{X}_{ND} = (i_{XB} - f_p i_{XP})(b_H X_{B,H} + b_A X_{B,A}) - \rho_8 \tag{14i}$$

The four remaining original ASM1 variables S_I, X_I, X_P, and S_{ALK} do not affect any other state variables in (14) and were left out. [29] provides details about all the variables and parameters and these will not be repeated here. The state variables are influenced by the nonlinear process rates

$$\rho_1 = \hat{\mu}_H \frac{S_S}{K_S + S_S}\frac{S_O}{K_{O,H} + S_O} X_{B,H} \tag{15a}$$

$$\rho_2 = \hat{\mu}_H \frac{S_S}{K_S + S_S}\frac{K_{O,H}}{K_{O,H} + S_O}\frac{S_{NO}}{K_{NO} + S_{NO}}\eta_g X_{B,H} \tag{15b}$$

$$\rho_3 = \hat{\mu}_A \frac{S_{NH}}{K_{NH} + S_{NH}}\frac{S_O}{K_{O,A} + S_O} X_{B,A} \tag{15c}$$

$$\rho_7 = k_h \frac{X_S/X_{B,H}}{K_X + X_S/X_{B,H}}\left(\frac{S_O}{K_{O,H} + S_O} + \eta_h \frac{K_{O,H}}{K_{O,H} + S_O}\frac{S_{NO}}{K_{NO} + S_{NO}}\right) X_{B,H} \tag{15d}$$

$$\rho_8 = \rho_7\left(X_{ND}/X_S\right) \tag{15e}$$

The Monod-expressions serve as continuous concentration-dependent switching functions for the different process rates. Mainly to distinguish between aerobic ($S_O > 0$) and anoxic ($S_O = 0$, $S_{NO} > 0$) conditions. If the variable in the Monod-expression is rarely in the nonlinear switching region, i.e. near the half-saturation constant K, the Monod-expression can be approximated by a binary signal.

6.2. Short time horizon ASM1 assumptions

The Monod kinetics operate as switching functions, and if the variable in the Monod-expression is rarely in the nonlinear switching region, i.e. near the half-saturation constant K, then the Monod-expression can be approximated by a binary signal.

A great number of variables in the ASM1 change very little on a daily basis. [42, 43] manually estimate and tune the parameters while [43, 44] use a linear model. In this paper, we aim to build a model that is accurate on an hourly timescale in dry weather operation and we assume that

$$X_{OHO} \simeq 0 \qquad X_{ANO} \simeq 0 \qquad S_B \simeq 0 \qquad X_U \simeq 0$$

i.e., we assume that the biomass (X_{OHO} and X_{ANO}) could be replaced by simple functions of measured SS concentration. This slowly varying parameter could be added to model longer term prediction or rain weather operation.
The substrate (S_B and X_U) can be lumped into ones state variable, assuming that measurements of chemical oxygen demand COD cannot distinguish between soluble and particulate components, i.e. COD is measured as total concentration and then subdivided into the two components by assuming a fraction f. The two variables accounting for substrate can therefore be expressed as

$$S_B = f_{S_B\_COD_{tot}} COD_{tot} \qquad X_U = f_{X_U\_COD_{tot}} COD_{tot}$$

We further assume that there is no ammonium production from organic bound nitrogen. Consequently,

$$S_{NB,org} \simeq 0.$$

This eliminates $X_{NB,org}$ as well, leaving only the three most important and often measured state variables S_{NH_x}, S_{NO_x}, and S_{O_2}. Most control-oriented models contain only these three states [45, 46, 47, 48, 49], some also S_B [50, 51].
The model complexity reduces significantly when the slowly varying states are assumed locally constant and is routinely done for real-time control-oriented ASP models [52, 53]. The reduced model is then only valid for shorter prediction horizons. However, if the model parameters are re-calibrated frequently the model will adapt to the slowly changing processes. We re-calibrate the model by estimating all parameters and states using the latest measurement window.

Based on these assumptions, the ASM1 model (Table 1) becomes a model with only three variables and three removal processes (Table 5)

where we can define new constants related to the original ASM1 parameters:

$$\begin{aligned}
k^{O}_{NH} &= i_{OHO} k_{NH_x} \\
k_{NH} &= \hat{\mu}_{OHO,max}\left(\frac{S_B}{K_{S_B} + S_B}\right) X_{OHO} \\
k^{NO}_{NH} &= i_{OHO} k_{NO} \\
k_{NO} &= \eta_{\mu,OHO} k_{NH} \\
k^{NH}_{NH} &= \left(i_{OHO} + \frac{1}{Y_{ANO}}\right) k_O \\
k_O &= \hat{\mu}_{ANO,max} X_{ANO} \\
k^{NO}_{NO} &= \frac{1 - Y_{OJO}}{2.68 Y_{OHO}} k_{NO} \\
k^{O}_{O} &= \frac{1 - Y_{OHO}}{Y_{OHO}} k_{NH} \\
k^{NH}_{NO} &= \frac{1}{Y_{ANO}} k_O \\
k^{NO}_{O} &= \frac{4.57 - Y_{ANO}}{Y_{ANO}} k_O
\end{aligned}$$

Table 5: Guyer matrix for the reduced model of the BioDenitro process

j	Component → i Process ↓	S_{O_2}	S_{NO_x}	S_{NH_x}	Process rate $\rho_j [gm^{-3}d^{-1}]$
1	Aerobic Growth of heterotrophs	$-\frac{1 - Y_{OHO}}{Y_{OHO}}$		$-i_{N\_Bio}$	$\hat{\mu}_{OHO,max}\left(\frac{S_B}{K_{S_B} + S_B}\right)\left(\frac{S_{O_2}}{K_{O_2,OHO} + S_{O_2}}\right) X_{OHO}$
2	Anoxic Growth of heterotrophs		$-\frac{1 - Y_{OHO}}{2.86 Y_{OHO}}$	$-i_{N\_Bio}$	$\hat{\mu}_{OHO,max}\left(\frac{S_B}{K_{S_B} + S_B}\right)\left(\frac{S_{O_2}}{K_{O_2,OHO} + S_{O_2}}\right)$ $\times\left(\frac{S_{NO_x}}{K_{NO_x,OHO} + S_{NO_x}}\right)\eta_{\mu,OHO} X_{OHO}$
3	Aerobic Growth of autotrophs	$-\frac{4.57 - Y_{ANO}}{Y_{ANO}}$	$-\frac{1}{Y_{ANO}}$	$-i_{N\_Bio} - \frac{1}{Y_{ANO}}$	$\hat{\mu}_{ANO,max}\left(\frac{S_{NH_x}}{K_{NH_x,ANO} + S_{NH_x}}\right)\left(\frac{S_{O_2}}{K_{O_2,ANO} + S_{O_2}}\right) X_{OHO}$