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Databank transfer-of-information, shortcut and exact estimators used in the wastewater biological treatment process identification

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Abstract

The biological treatment is the most complex step in removing organic and inorganic pollutants from wastewaters, being very sensitive to input-flow oscillations, operating conditions, and biomass evolution. Sudden increases in substrate concentration or some inhibitory substances, deterioration of the biomass, or few observed species, all of these lead to a difficult process modelling and need repeated biokinetics identification for each waste and biomass type. However, the bioprocess numerical analysis is crucial for obtaining significant improvements in the wastewater treatment (WWT) plant performances and safety indices even under imperfect data. The paper exemplifies an advanced route to quickly on-line identify the biodegradation characteristics of new substrates processed by a series of perfectly mixed aeration basins with biomass recycle. The Monod kinetics is recursively identified by using the available collection of plant previous transient operating data and a robust shortcut estimator (MIP). The approximate solution is periodically refined with an exact nonlinear estimator (NLS), checked for consistency and significance versus prior information, and stored in databanks. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: Shortcut and exact estimators; Kinetic estimation; Kinetic databank; Wastewater biological treatment

1. Introduction

Industrial wastewaters contain a large variety of contaminants. In most cases, the wastewater streams are coming from a variety of sources. An important problem to be solved is the rapid identification of the biodegradation characteristics in order to determine the optimal operating conditions and the maximum amounts of wastes that can be processed by an existing wastewater treatment (WWT) plant. Although difficult, model-based analysis, optimisation and control of the WWT process was reconsidered over the last decades (Beck, 1986).

A classical WWT plant consists in a series of sections, primary (mechanical and chemical); secondary (biological); and tertiary (advanced) pollutant removal. The biological WWT is very sensitive to input-flow oscillations, operating conditions and biomass evolution. Process characterisation via detailed dynamic

plant and kinetic process models require extensive off-/on-line process investigations under a wide range of operating conditions at different scales. The obtained set of ordinary differential equations (ODE) and parameters are of complexity which depends on the amount of available information and on the utilisation scope, knowledge of process kinetics and transport phenomena, process design and optimisation, or real-time process monitoring, safety analysis and control. For plant optimisation and risk analyses reduced mechanistic models are preferred because of diminished development costs. The physical meaning of the parameters offers the possibility to better interpret the estimate quality and to store the results in databanks ready for further use. Monod kinetic expressions for the micro-organism growth can be satisfactory if the model is up-dated on-line according to the new information from the process sampled with an appropriate frequency (Maria & Maria, 1998; 'tendency modelling' Fotopoulos, 1996). Parameter sensitivity, physical restrictions, principal component and ridge selection, all

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can allow a model reduction in terms of reactions or variables (Maria & Ognean, 1989; Maria & Rippin, 1993; Tomlin, Turanyi & Pilling, 1995). Starting from filtered, reconciled, and smoothed experimental data, the WWT process biokinetics is derived by means of several techniques. Direct methods (based on model transformation and approximate problem solution in one step), indirect methods (objective function iterative minimisation with repeated model evaluation), or classical on-line state-parameter recursive estimators (extended Kalman filters, EKF, Goodwin & Sin, 1984). Problem multimodality, highly interrelated model parameters, variable observability of various species, particular model form or incomplete data, all these can cause serious convergence or solution reliability problems when an incomplete numerical analysis is applied. Moreover, the biological processes are characterised by an excess of degrees of freedom in adjustable parameters over the observed and manipulated variables. Key-parameter subset selection and reduced model updating have to compensate the plant data and model mismatch and to predict the plant optimum operating conditions by taking into account the estimate uncertainty (Friedman & Reklaitis, 1975). To invest a minimum of experimental and computational effort, prior information about analogous pollutant biodegradation kinetics is helpful. Maria and Rippin (1997) proposed an effective shortcut estimator for ODE sets (e.g. the MIP) with the possibility of including prior information in generating a quick and reliable approximate solution.

The scope of this paper is to exemplify an advanced route for a rapid WWT process kinetic identification when new substrates are present in the system or biomass characteristics change. Consistent data concerning plant past transient evolution in removing various pollutants can be used by the rapid MIP in an approximate identification of the current process if some similarities are pointed-out. Periodic solution NLS refinements and checks vs. databank information increase the solution reliability. This rule is exemplified in the case of Monod kinetics and a series of perfectly mixed (CSTR) aeration basins with ideal settling and partial biomass recycle.

2. Biological WWT plant data storage and analysis

Classical biological WWT consists in a series of mechanically aerated basins, with a continuous wastewater flow over an activated sludge and operated in transitory or quasi-steady-state conditions. The clarified water is separated and part of the settled activated sludge is recycled to the aeration tank in order to maintain a quasi-constant sludge bioactivity. The series of basins presents some advantages, the air supplied uniformly can exceed the oxygen demand; the biologi-

cal solids can withstand shock pollutant loads; more flexibility in adjusting the operating conditions; and a favourable economic operation and maintenance. The organic pollutants (usually expressed as the biochemical oxygen demand, BOD) must be related with the active sludge volatile suspended solids (VSS). The dynamic evolution of the pollutant (substrate) and biomass concentrations in the bioreactor includes kinetic information about the biodegradation process. However, this dynamical behaviour is characterised by a wide range of time constants, non-linearity, imprecision and some irreproducibility of data, substantial stability punctuated by abrupt failures, and a sensitive, readily adaptable community of micro-organisms. Frequent fluctuations in influent loads, biomass characteristics, operation and mixing conditions make a systematic process identification difficult. However, portions of the recorded kinetic trajectories, mass balance equilibrated (Maquin & Ragot, 1989), separated from mass transport limitations, and regularised by using smoothing spline functions (Maria & Muntean, 1987), can be stored and used for process kinetic identification. As an example, Maria, Constantinescu and Ozil (2000) used smoothed transitory evolutions of a WWT plant of a moderate noise level to identify new pollutant biodegradation characteristics via the MIP rapid shortcut estimator. A complete kinetic model up-dating methodology was presented by Maria and Rippin (1996). Oriented software can be used in developing biokinetic models (Seressiotis & Bailey, 1988, review of Gilles & Reuss, 1999) based on recorded data and stored information about WWT and pollutants: physico-chemical and biodegradability properties (Pedersen, Tyle, Niemela, Guttmann, Lander & Wedeband, 1994), pollutant removal data (Hoigne & Bader, 1983; Buxton, Greenstock, Helman & Ross, 1988; Xu & Nirmalakhandan, 1998). While general software allow chemical plant simulation and prediction of waste effluents, oriented software allow WWT plant simulation (Patry & Chapman, 1989; Aelion & Petrides, 1994; ENVITEC, 1995), design (Fels, Pinter & Lycon, 1997), optimisation (Petrides, Cruz & Calandranis, 1998; Low & Chase, 1999), control and risk analysis (Beck, 1986; Jenkins, Richard & Daigger, 1993; Waldraff, Biener, Oswald, Sippel, King & Gilles, 1993; Bastin & Van Impe, 1995; Szafnicki, Bourgois & Graillot, 1998).

3. Shortcut and exact biokinetics identification

The WWT process dynamics and the few observed species need a repeated biokinetic study according to each waste and biomass type. In order to derive and check a consistent model, the biological WWT process is analysed both at an industrial and lab level. Because of the high noise and frequent industrial process fluctu-

ations, the process is preferably checked at a bench-scale similarly operated (influent, hydraulic residence time HRT, biomass recycle ratio, pH, dissolved oxygen DO, temperature, biomass characteristics) to fulfil simplifying hypotheses which make transport limitations negligible or easy to evaluate. After data pre-treatment and reconciliation, the next step is to propose a kinetic model according with the process evolution and with the stored biodegradation information. Although more costly, the mechanistic models are preferred because of the better quality predictions, and the physical meaning of the parameters. Overparameterised models require extensive experiments to check intermediate species and steps, and an increased computational effort to estimate and check the parameters (Daiger & Leslie, 1982). Monod expressions for the micro-organism growth can be satisfactory if they are up-dated on-line according to the new process information via combined chemometric and estimation techniques (Maria & Rippin, 1993). Kinetic parameters are estimated by minimising the residual differences between data and model predictions in terms of output variables, by means of several techniques, indirect methods (NLS), or direct methods (shortcuts). Classical shortcut estimators, i.e. the discretisation procedure (DP, Glowinski & Stocki, 1981), and the integral transformation procedure (IP, Hosten, 1979), offer an approximate solution by solving a (non-) linear over-determined constrained algebraic set. These simple methods require few model evaluations, but they are very sensitive to the noise level and they do not use the prior information about the process and model parameters. The shortcut estimate is further refined with a NLS, thus increasing the convergence rate and the solution reliability (Edgar & Himmelblau, 1989; Maria, 1998). Combinations of direct and indirect methods provide reliable estimates, MIP and MMA (Maria, Terwiesch & Rippin, 1996; Maria, 1998); DP, IP and ARS (Maria & Muntean, 1987); factor analysis and ARS (Maria & Rippin, 1993); IP and Marquardt's method (Vajda, Valko & Yermakova, 1986). The MIP of Maria and Rippin (1997) can also replace the classical state-parameter recursive estimators (EKF) which are very sensitive to the chosen model structure, data noise level, variation in species/reaction observability, model linearisations, tuning factors, and prior information (de Valliere & Bonvin, 1990; Maria et al., 1996). Final model discrimination has to be coupled with physical meaning checks of the estimate.

Starting from the observed data, the MIP shortcut kinetic estimator transforms the ODE set into an algebraic one but also considering the prior information about an analogous process, from which kinetic data and parameters are known. The similarity analysis is applied to the pair of similar species (scaled in a common time domain by means of a factor $\varphi > 0$) by identifying portions where the current/historic process rate ratio is quasi-constant. In this interval, the integral rate ratios of the similar species are decomposed, by estimating first the dominant reaction term parameters. The rule is repeated in several time sub-intervals, avoiding poor conditioning by using the same relative parameter ratios as in the previous process. As proven (Maria & Rippin, 1997) the MIP is superior to other shortcut estimators because of its simplicity, reliability, no tuning factor or model linearisations required, and the possibility of including databank information.

To exemplify the MIP estimation, an ideal WWT aeration basin coupled with a settler for recycling the sludge are considered (Snape, Dunn, Ingham & Prenosil, 1995, Fig. 1). If the biomass is sufficiently aerated, with no resistance on the substrate diffusion to the flocks, and the clarified water contains no biomass, the isothermal bioreactor and settler dynamic model is:

$$\begin{aligned} \frac{dX_J}{dt} &= \frac{Q_r}{V} X_{J,r} - \frac{Q_{in} + Q_r}{V} X_J + r_{X_J}; & X_J \Big|_{t=0} &= X_{J,o}; \\ X_{J,r} &= X_J \frac{Q_{in} + Q_r}{Q_w + Q_r}; & S_{J,r} &= S_J; \\ \frac{dS_J}{dt} &= \frac{Q_{in}}{V} (S_{J,in} - S_J) - \frac{r_{X_J}}{Y_J} + \frac{\Phi_J}{C_J}; & S_J \Big|_{t=0} &= 0, \end{aligned} \quad (1)$$

(X_J , S_J , biomass, substrate J concentrations (g/m³); V , reactor volume, (m³); Q_{in} , Q_w , Q_r , input, waste sludge, and recycled volumetric flow rates (m³/day); r_{X_J} , Φ_J species J growing rates (g/m³/day); Y_J , stoichiometric coefficients (g/g); C_J , ratios of Y_J (g/g); t , time, days). For an adopted Monod kinetics with a first-order death rate:

$$r_X = \frac{dX}{dt} = \frac{\mu SX}{K + S} - bX; \quad r_S = \frac{dS}{dt} = -\frac{1}{Y} \frac{\mu SX}{K + S} \quad (2)$$

the MIP is applied to the pair of similar species [current $S(t)$, $X(t)$, and historic $S'(t')$, $X'(t')$ concentrations], by identifying the common reduced time domains $[t_0, t]$ and $[t'_0, t']$ where the rate ratios are quasi-constant. Thus, the unknown kinetic parameters [μ , K , b , Y] are

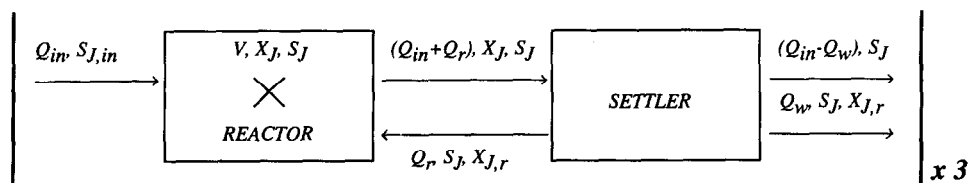


Fig. 1. Series of three biological WWT aerators and settlers with partial sludge recycle.

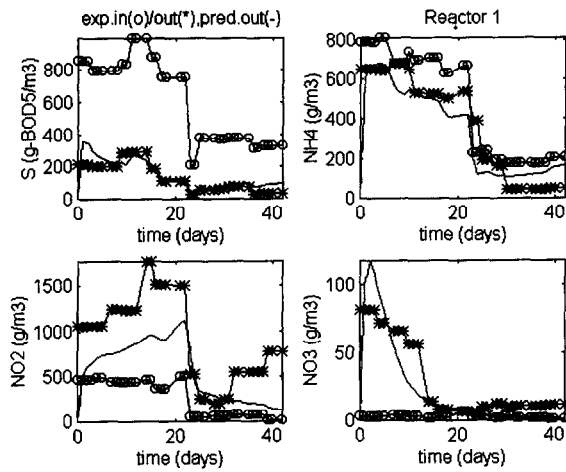


Fig. 2. BOD organics, NH_4^+ , NO_2^- , NO_3^- evolution in R1 (\circ , experimental input; *, experimental output; -, predicted output).

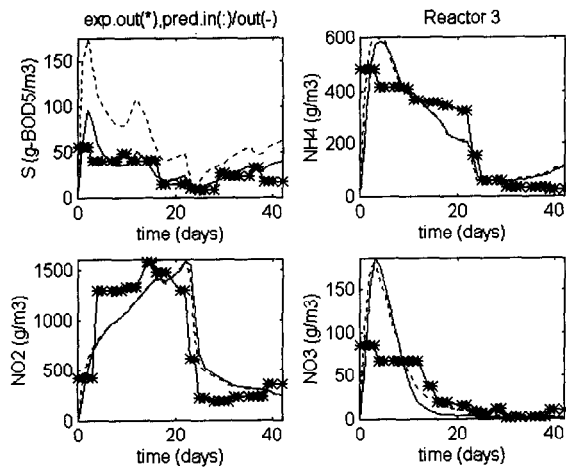


Fig. 3. BOD organics, NH_4^+ , NO_2^- , NO_3^- evolution in R3 (*, experimental output; --, predicted input; -., predicted output).

estimated by using the historic process parameters $[\mu', K', b', Y']$, and the integral form of the rate ratios (Maria & Rippin, 1997). Under the hypothesis of constant bioreactor volumes and flow-rates in the analysed time sub-intervals, and by neglecting the substrate formation Φ_j , one obtains the MIP over-determined linear algebraic set (for every J):

$$\frac{[\Delta X - \alpha \int_{t_0}^t X dt]}{[\Delta X' - \alpha' \int_{t_0}^t X' dt]} \approx \frac{K' \int_{X_0}^X S dX}{K \int_{X_0}^{X'} S' dX'} \approx \frac{b \int_{t_0}^t X dt}{b' \int_{t_0}^t X' dt} \approx;$$

$$\frac{K'(\mu - b) \int_{t_0}^t S X dt}{K(\mu' - b') \int_{t_0}^t S' X' dt} \approx \frac{YK[\Delta S - \beta]}{Y'K'[\Delta S' - \beta']} \approx \frac{\mu \int_{t_0}^t S X dt}{\mu' \int_{t_0}^t S' X' dt} \quad (3)$$

$$\alpha = \frac{Q_r Q_{in} + Q_r}{V Q_w + Q_r} - \frac{Q_{in} + Q_r}{V};$$

$$\beta = \frac{Q_{in}}{V} \left[\int_{t_0}^t S_{in} dt - \int_{t_0}^t S dt \right]$$

By applying the MIP algebraic set (Eq. (3)) to various transient WWT plant data of moderate noise, Maria et al. (2000) obtained an up-dated kinetic model of good quality, close to the exact NLS solution.

4. Case study: bioprocess identification in a series of three WWT aeration basins

4.1. Plant operation and model

A WWT plant processes wastewaters from an organic synthesis/synthetic fibres production section of complex composition: solids in suspension, organic pollutants, cyanides, chlorides, sulphates, ammonium, nitrates, nitrites, heavy metals. The biological WWT section consists of a series of three aerated basins (R1–R3) with continuous activated sludge settling, partial recycle and excess discharge (Fig. 1). In order to quickly predict the optimum plant operating conditions and risk limits, the biodegradation kinetics of the main lumped substrates (BOD organics, compounds with NH_4^+ , NO_2^- , NO_3^-) is necessary.

Consistent data are collected from a bench-scale plant built-up and operated similarly with the industrial one (the same HRT, pH, DO, temperature and nutrient additives) and using the same acclimatised sludge and wastewater quality. The experiments were carried out over 42 days, by recording the four lumped substrates, overall biomass content (VSS), pH, temperature, DO, inorganic phosphorous, a.o. on a daily basis (Figs. 2 and 3).

A compromise among the model complexity and the amount of experimental information can be realised by adopting the following simplifying hypotheses and operating conditions, (i) continuous aerated CSTR for mainly removing organics in R1 (2 g/m³ DO), nitrification in R2 (1.5 g/m³ DO), and denitrification in R3 (1 g/m³ DO), thus ensuring biomass maintenance (DO > 0.3 g/m³); (ii) quasi-isothermal conditions (18°C), constant fed flow-rates of $Q_{in} = 5$ l/day and volumes of $V = 2.5$ l; the average food-to-micro-organism (F/M) loading is 0.3 gBOD/(gVSS day) in R1, 0.13 (g/g day) in R2, and 0.1 (g/g day) in R3; (iii) constant pH, 7.5 in R1, pH, 8 in R2 (by continuous addition of Na_2CO_3 in a ratio of $C/\text{NH}_4^+ = 0.39\text{--}0.65$ g/g, Gray, 1990), and pH, 7 in R3 (Glass & Siverstein, 1998); (iv) continuous addition of nutrients (BOD5/N/P = 100/5/1–100/6/1 g/g per g, Gray, 1990) to prevent bulking, thinner sludge, increased water turbidity and biomass diminishment; (v) continuous biomass recirculation with a diminished ra-

tio (Q_r/Q_{in} of 0.24 in R1, 0.15 in R2, and 0.09 in R3) to ensure an increased sludge residence time (> 4 days) for nitrification–denitrification; (vi) reduced biomass recycle ratios and aeration in R2 and R3 which lead to a more aged and less active sludge (4–6 gVSS/L in R1, average 2 gVSS/l in R2, and 1–1.5 gVSS/l in R3), requiring $F/M < 0.1–0.15$ (gBOD/gVSS day); (vii) purged sludge diminished flows of $Q_w/Q_{in} = 1.695E-2$ in R1, $8.928E-3$ in R2, and $3.436E-3$ in R3, ensuring an increasingly sludge age [e.g. $V\bar{X}/(Q_w X_w)$ of 6.1 days in R1, 7.7 days in R2, and 12.5 days in R3]; (viii) addition of activated carbon powder in R2 to prevent settling problems due to $F/M < 0.2$ (g/g day), and bulking, foaming and sludge rising because of the nitrification–denitrification; (ix) added methanol in R3 for maintaining the sludge growth ($C/N = 1.7–1.8$ g/g, Gray, 1990); (x) ideal settling and negligible biomass concentration in the clarified water.

Model (1) was successively applied for the each WWT reaction-separation unit allowing prediction of the biomass (X), BOD, NH_4^+ , NO_2^- , NO_3^- concentration dynamic evolution, under a serial fluid circulation, $(S_J)_{R1} = (S_{J,in})_{R2}$; $(S_J)_{R2} = (S_{J,in})_{R3}$. Substrates are produced with the rates $\Phi_J = 0$ for $J = \text{BOD}, NH_4^+$; $\Phi_J = r_{X_{NH_4}}/Y_{NH_3}$ for $J = NO_2^-$, and $\Phi_J = r_{X_{NO_2}}/Y_{NO_2}$ for $J = NO_3^-$, with stoichiometric ratios of $C_{NO_2} = 0.39$ (g NH_4 /g NO_2), $C_{NO_3} = 0.74$ (g NO_2 /g NO_3).

4.2. Process kinetics

Monod kinetics (Eq. (2)) is adopted, the biomass and oxygen inhibition terms being neglected because of the moderate X -values and $DO > 0.3$ g/m³. The BOD is removed with an approximately $Y_{BOD} = 0.5$ (gVSS/gBOD) (Gray, 1990), and Monod parameters of $\mu_{X_{BOD}} < 2.5$ 1/day, $K_{BOD} \sim 100$ g/m³. Most of the organic nitrogen is transformed to ammonium that is assimilated into the cell material and ca. 15–50% is released to the water. Produced ammonium is negligible when large influent loads are present.

The nitrification consists of a two-step $NH_3-NH_4^+$ oxidation, with the average stoichiometry of $Y_{NH_4} = Y_{NO_2} = 0.2$ (gVSS/g NH_4^+-N), with the Monod constants of (Tchobanoglous & Burton, 1991):

$$\mu_{X_J} = \mu_{X_{j,m}} [1 - 0.833(7.2 - pH)] \exp[0.098(T - 15)] \times \frac{DO}{1.3 + DO}, \text{ (1/day),}$$

$$J = NH_4^+, NO_2^- \text{ (T in } ^\circ\text{C); } \mu_{X_{NH_4m}} \in [0.3, 2]; \mu_{X_{NO_2m}} \in [0.4-3], \text{ (1/day);}$$

$$\log K_{NH_4} = 0.05T - 1.158; K_{NO_2} 1.4(\text{g/m}^3). \text{ (4)}$$

The denitrification reactions in the presence of a source of carbon in excess transform the nitrates in N_2 removed to the atmosphere. Combined nitrification–denitrification removes ca. 70–95% of the total nitrogen with an avg. $Y_{NO_3} = 0.8$ (gVSS/g NO_3^-) and:

$$\mu_{X_{NO_3m}} < 0.3-0.9(\text{1/day}), K_{NO_3} = 0.1 \text{ (g/m}^3\text{);}$$

$$\mu_{X_{NO_3}} = \mu_{X_{NO_3m}} (T/20)^2, \text{ (1/day). (5)}$$

4.3. MIP shortcut and NLS exact kinetic estimate

The MIP Eq. (3) was applied to each substrate trajectory of Fig. 2 in the experimental time domains where the terms Φ_J are not dominant.

The prior knowledge corresponds to a similar industrial WWT plant evolution (Maria et al., 2000, not displayed here), with the known kinetics of $[\mu', K', b', Y] = [1 \text{ 1/day}, 300 \text{ g/m}^3, 0, 0.4 \text{ g/g}]$. By adopting the stoichiometric coefficients Y_J , the MIP estimates of μ_{X_J} , K_J and $X_{J,0}$ are thus obtained. As only the overall biomass concentration ($X_t = \sum X_J$) can be measured, each biomass culture is derived indirectly by matching the corresponding substrate evolution during the process. The MIP solution of Table 1 is of very good quality, fulfilling the statistical tests for model adequacy and parameter significance (not presented here). The MIP estimate of $p = 11$ parameters was refined with an exact NLS estimator in respect to all the $n = 42$ data points and the five observed species $S = [S_{BOD}, S_{NH_4}, S_{NO_2}, S_{NO_3}]$, X_t , in each reactor (e.g. a total of $r = 3 \times 5 = 15$ observations). Because the noise level depends on the observation, a weighted least squares criterion was used in the presence of explicit parameter constraints related with their physical significance. A highly effective adaptive random search (MMA of Maria, 1998), implemented in the Matlab environment, leads to the local solution (A) of Table 1. The estimated

Table 1
Estimated kinetic parameters [average noise level of $\hat{\sigma} = 10$ g/m³; $s_e^2 = \|[S, X_t]_{exp} - [\hat{S}, \hat{X}_t]\|_2^2 / (nr - p)$; $\alpha = X_{BOD}/X_t$, $\beta = X_{NH_4}/X_t$, $\gamma = X_{NO_2}/X_t$; n, r, p , number of runs, observations, parameters]

Method	α	β	γ	$\mu_{X_{BOD}}$ (1/day)	$\mu_{X_{NH_4m}}$ (1/day)	$\mu_{X_{NO_2m}}$ (1/day)	$\mu_{X_{NO_3m}}$ (1/day)	K_{BOD} (g/m ³)	K_{NH_4} (g/m ³)	K_{NO_2} (g/m ³)	K_{NO_3} (g/m ³)	s_e^2
MIP	0.52	0.05	0.3	0.3	0.33	0.095	0.21	112	338	311	13.7	37.4
NLS (A)	0.60	0.05	0.3	0.3	0.35	0.080	0.30	112	338	311	14	35.9
NLS (B)	0.70	0.01	0.15	0.3	0.35	0.10	0.20	100 ^a	0.55 ^a	1.4 ^a	0.1 ^a	36.3

^a Adopted value.

μ_x are in agreement with the parameters reported by Tchobanoglous & Burton (1991), Gernaey, Vanrolleghem & Verstraete (1998), Kornaros & Lyberatos (1998), while the estimated K_J are in agreement only with Kornaros & Lyberatos (1998). The model predictions are displayed together with the experimental values in Fig. 2 (R1) and Fig. 3 (R3). By adopting the K_J -values of Tchobanoglous & Burton (1991), the local solution (B) was derived (Table 1). Although estimate (A) seems to be superior in predictions, supplementary model checks in different operating regions will be necessary for final conclusions.

5. Concluding remarks

Quick estimation of the WWT biokinetics by combining databank information, modern shortcut techniques for transferring prior information and effective exact estimators allows a rapid reduced model updating in on-line process identification and monitoring. Consistent information concerning the WWT plant past dynamic evolutions together with regularised kinetic curves and parameters characterising various pollutants' removal can be successfully used to identify the current process characteristics if some similarities occur. The effective and simple MIP kinetic model up-dating does not require tuning factors or model linearisations leading to an estimate of good quality for moderately noised data. On-line up-dated reduced models can be used for plant optimisation and risk analyses.

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