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Sensitivity Analysis of Optimal Operation of an Activated Sludge Process Model for Economic Controlled Variable Selection

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ABSTRACT: This paper describes a systematic sensitivity analysis of optimal operation conducted on an activated sludge process model based on the test-bed benchmark simulation model no. 1 (BSM1) and the activated sludge model no. 1 (ASM1). The objective is to search for a control structure that leads to optimal economic operation, while promptly rejecting disturbances at lower layers in the control hierarchy avoiding thus violation of the more important regulation constraints on effluent discharge. We start by optimizing a steady-state nonlinear model of the process. Here, a new steady-state secondary settler mathematical model is developed based on the theory of partial differential equations applied to the conservation law with discontinuous fluxes. The resulting active constraints must be chosen as economic controlled variables. These are the effluent ammonia from the bioreaction section and the final effluent total suspended solids at their respective upper limits, in addition to the internal recycle flow rate at its lower bound. The remaining degrees of freedom need to be fulfilled, and we use several local (linear) sensitivity methods to find a set of unconstrained controlled variables that minimizes the loss between actual and optimal operation; particularly we choose to control linear combinations of readily available measurements so to minimize the effect of disturbances and implementation errors on the optimal static performance of the plant. It is expected that the proposed methodology and results obtained therein can be used in practice as general rules-of-thumb to be tested in actual wastewater treatment plants of the kind discussed in this paper.

1. INTRODUCTION

Operation of wastewater treatment plants (WWTP) has been the focus of intense research for at least the past 20 years as seen from the myriad of paper contributions to the field (see, for example, Olsson and Newel,[1] Olsson et al.,[2] and Olsson[3]). These facilities, working as highly complex processes, should be designed and operated in a way to mitigate the negative impact of nuisance influent to the environment in order to conform to increasingly stricter discharge regulations and pollutant limits and at the same time meet tight operational budget restrictions.

Although optimization of wastewater treatment plants has gained interest in both scientific and industrial communities, surprisingly only few articles discuss the subject either from a heuristic economic point of view[4−6] or by formal optimization using an explicit mathematical model of the process[7−11] for optimal design and operation. However, none of the publications define an optimal operation policy from a systematic viewpoint. Araujo et al.[12] applied a systematic procedure for control structure design of an activated sludge process in which optimization for various operational conditions were carried out using a mathematical model of the process, where they imposed additional operational constraints to the process following heuristics found in the WWTP literature, for example, bounds restricting residual oxygen in the anoxic and aerobic reactors, sludge retention time (SRT) being constrained, and nitrate concentration lying within specified limits. In fact, these variables should be let to vary freely so that their optimal values constitute the result of the optimization.

One important outcome of a systematic optimization procedure is the definition of variables that should be controlled to ensure optimal economic operation, namely, the active constraints, and, if there are still degrees of freedom left, the unconstrained variables that when kept constant at their optimal nominal set points lead to near-optimal operation avoiding the need for reoptimizing the process when disturbances occur (the so-called self-optimizing control technology).[13] Except for Cadet et al.[14] and Araujo et al.,[12] no other reference was found that explored the selection of output controlled variables for wastewater treatment processes. However, Cadet et al.[14] proposed a selection methodology based on a sensitivity analysis (steady-state gain calculation) and did not consider the more important issue related to the economics of the system. On the other hand, although Araujo et al.[12] used a systematic procedure for the selection of controlled variables, the limitations previously discussed about their work gave incomplete information on the truly optimal operation policy for the kind of activated sludge process object of their analysis.

In this paper, a systematic sensitivity analysis of optimal operation of an activated sludge process model based on the benchmark simulation model no. 1 (BSM1)[15] is conducted. It must be clear that all analysis, and hence all conclusions, from this work are based on the underlying mathematical model of

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Table 1. List of Symbols

symbol	description	unit	symbol	description	unit
BOD_5	5 day biological oxygen demand	gBOD/m^3	Q_f	flow rate to settler	m^3/d
c	set of controlled variables		Q_r	sludge recirculation flow rate	m^3/d
c^{opt}	set of optimal values of controlled variables		Q_u	sludge flow rate from settler bottom	m^3/d
d	disturbances (disturbance set)		Q_w	excess sludge flow rate (wastage)	m^3/d
C_D	sludge disposal production	gSS/d	r_h	particle behavior for increasing particle density	
COD	chemical oxygen demand	gCOD/m^3	r_p	particle behavior at weak concentration values	
eff	effluent superscript		$S_{NH}^{(j)}$	ammonia concentration in basin j	gN/m^3
E_A	aeration energy	kWh/d	$S_{NO}^{(j)}$	nitrate concentration in basin j	gN/m^3
E_M	mixing energy	kWh/d	$S_O^{(j)}$	oxygen concentration in basin j	gO$_2$/m^3
E_P	pumping energy	kWh/d	S_O^{sat}	oxygen saturation concentration	gO$_2$/m^3
$\mathbf{F}$	flux function		SRT	sludge retention time	d
$\mathbf{F}$	optimal measurement sensitivity matrix		t	time	d
$\mathbf{G}^y$	gain matrix from the unconstrained degrees of freedom to the measurements		TN	total nitrogen concentration	gN/m^3
$\mathbf{G}_d^y$	Gain matrix from the disturbances to the measurements		TSS	total suspended solids	gSS/m^3
$\mathbf{H}$	combination (coefficient) matrix		u	unconstrained degrees of freedom	
$\mathbf{J}$	cost function		u'	degrees of freedom used to control active constraints	
$\mathbf{J}_{uu}$	Hessian matrix with respect to the unconstrained degrees of freedom		u^{opt}	optimal values of the unconstrained degrees of freedom	
$\mathbf{J}_{ud}$	Hessian matrix with respect to the unconstrained degrees of freedom and disturbances		u_0	original steady-state degrees of freedom	
$K_La^{(j)}$	oxygen transfer coefficient for basin j	d−^{1}	u_0^{opt}	optimal values of the original steady-state degrees of freedom	
$\mathbf{L}$	economic loss		$V^{(j)}$	volume of basin j	m^3
k_D	sludge disposal price	\$/ton	v_0	theoretical maximum velocity	m/d
k_E	energy price	\$/kWh	v_0'	practical maximum velocity	m/d
K_S	kinetic parameter	gCOD/m^3	v_s	settling velocity	m/d
MLSS	mixed liquor suspended solids	gSS/m^3	w	wastage subscript	
n_d	number of disturbance variables		$\mathbf{W}_d$	disturbance scaling matrix	
n_y	number of available measurements		$\mathbf{W}_{ny}$	measurement scaling matrix	
n_u	number of unconstrained degrees of freedom		X	floculated solids concentration	gSS/m^3
n_u'	number of degrees of freedom used to control active constraints		y	set of measurement variables	
n_{u_0}	number of original degrees of freedom		z	spatial coordinate	m
n^y	measurement errors		ε	excess flux	m^3/(d·m^2)
q	flux	m^3/(d·m^2)	δ	dirac measure	
$Q^{(in)}$	influent flow rate	m^3/d	$\bar{\sigma}$	maximum singular value	
Q_a	internal recirculation flow rate	m^3/d	(eff)	effluent superscript	
			(in)	feedflow rate to the WWT plant superscript	

the process and should not be considered as definite guidelines for actual plant operation since the mathematical model may not be able to reproduce many real plant situations. However, the results can be used in practice as general rules-of-thumb to be tested in actual wastewater treatment plants of the kind discussed here. The paper is organized as follows: In section 2, a short description of the process and relevant modeling issues are discussed. Here, a new steady-state secondary settler mathematical model is developed based on the theory of partial differential equations applied to the conservation law with discontinuous fluxes.[16−19] Section 3 gives an outline of the methodology used for sensitivity analysis, emphasizing the importance of variable selection for optimal operation. Application of these guidelines to a revised BSM1 is given in section 4. Discussion of the results are presented in section 5, and some conclusions are drawn in section 6. The most important notation is summarized in Table 1.

2. PROCESS DESCRIPTION

Wastewater treatment plants are very complex units designed to remove pollutants in the influent wastewater by biological reaction and separation (settling) processes. Depending on the characteristics of the wastewater, the desired effluent quality, and the environmental or social factors, the treatment can be achieved in different ways. In general, traditional wastewater treatment processes include, as a first step, a mechanical removal of floating and settleable solids, followed by a biological treatment for nutrients and organic matter abatement with secondary settling for separation of suspended solids, a sludge processing/disposal unit, and water chemical treatment when applicable. Here the continuous activated sludge process is considered for the biological wastewater treatment with the main purpose of nitrogen and carbon compound removal.

The BSM1[15] represents a fully defined protocol that characterizes the process including the plant layout, influent

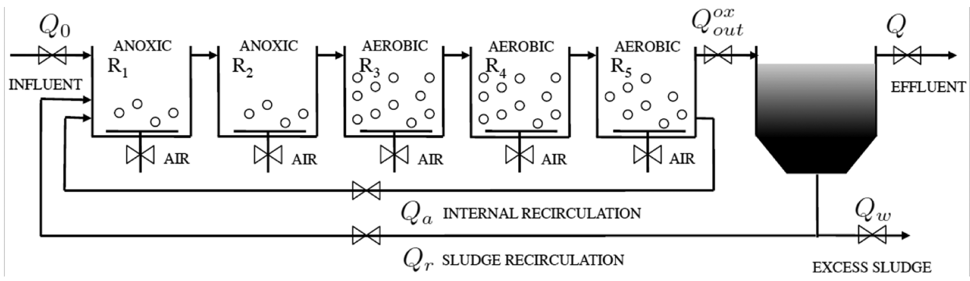

Figure 1. Schematic representation of the BSM1 activated sludge process.

loads, modeling and test procedures, and evaluation criteria. Figure 1 shows a schematic of the process consisting of a bioreaction section divided in five compartments, which can be anoxic or aerobic, and a secondary settling device. In order to maintain the microbiological population, sludge from the settler is recirculated into the reaction section (returned activated sludge, Q_r). Also, part of the mixed liquor leaving the last reactor can be recycled to the inlet of the bioreactor (internal recycle, Q_a) to enhance nitrogen removal. Moreover, excess sludge at a rate Q_w is continuously withdrawn from the settler underflow.

The original BSM1 layout has the following characteristic features: biological treatment reactor with two anoxic zones (1000 m^3 each) followed by three aerobic zones (1333 m^3 each); nonreactive secondary settler with a surface of 1500 m^2 and 4 m depth; recycled flow, Q_r, from the secondary settler to the front end of the plant; nitrate internal recycle, Q_a, from the fifth to the first tank; waste sludge flow rate, Q_w, continuously pumped from the secondary settler underflow.

From a modeling point of view, the original BSM1 is based on two widespread accepted process models: the celebrated activated sludge model no. 1 (ASM1)[20] used to model the biological process and a nonreactive Takacs one-dimensional layer model for the settling process.[21,22] The full model equations, as well as the kinetic and stoichiometric parameters, are given within the benchmark description.[15] In addition, inflow data are provided in terms of flow rates and ASM1 state variables over a period of 14 days with 15 min sampling time. All the information required for the proper implementation of the model in virtually any platform can be found at the COST/IWA 624 Web site (http://www.benchmarkwwtp.org).

Each reactor is modeled as a perfectly mixed, constant-volume tank within which complex biological reactions give rise to component mass balance equations, generating a system of (coupled) ordinary differential equations. The ASM1 is a well-established and reliable model widely used among WWTP modelers, and further discussion on its known capabilities of reproducing with considerable fidelity the behavior of the reaction section of an activated sludge process can be found in the vast wastewater literature.

2.1. Settler Model Development. Unfortunately, the same degree of high reproducibility cannot be attributed to the secondary settler mathematical model because these units display very complex mechanisms that are not still fully understood.[23] Nevertheless, much progress has been made toward building a physically sound model for the secondary settler based on the theory of partial differential equations applied to the conservation law with discontinuous fluxes.[16−19] While these more meaningfully grounded mathematical models satisfying fundamental physical properties[24] still have not found widespread application in the WWT field, it is commonplace to resort to approximate models of the settler, and the one due to Vitasovic[22] later used by Takacs[21] is the most widely used representation of the secondary settler in published studies and commercial software environments. Some authors,[25−27] however, pointed out many setbacks related to this model, among which is the fact that the number of discretization layers is not in agreement with numerical convergence and without distinguishing model formulation and numerical solution, but instead it is used solely as a model parameter in order to match experimental observations.[28] In fact, numerical simulations have shown[24] the failure of Takacs's model to represent the complex behavior of secondary settlers under certain conditions, and this has led researchers to switch to more reliable physically meaningful sedimentation models. One such development is described by Diehl,[16] who formulated and analyzed dynamically the settler model based on the one-dimensional scalar mass conservation law, eq 1,

$$\frac{\partial X(z,\,t)}{\partial t} + \frac{\partial}{\partial z}(F(X(z,\,t),\,z)) = s(t)\delta(z) \tag{1}$$

where X is the flocculated solids concentration, δ is the Dirac measure, s is the source, and $\mathbf{F}$ is the flux function, which is discontinuous at three points in the space coordinate z, namely, at the inlet and the two outlets. Further details are given in the cited references; however it should be emphasized that the model described in Takacs[21,22] is a time discrete version of eq 1 and that the key challenge is the solution method of the partial differential equation described in eq 1.

We here are interested in the sensitivity of the static optimum of the settler coupled with the biological reaction section, and the steady-state solutions of the above equation as given by Diehl[18,19] provide the basis for our analysis. In Table 2 and Figure 2, we partially reproduce the results from ref 18.

Table 2. All the Steady States of the Settler[18]

region in Figure 2	excess flux	X_e	X_u
$\mathcal{U}_1$	$\varepsilon < 0$	0	s/q_u
$\mathcal{U}_2$	$\varepsilon < 0$	0	s/q_u
l_1	$\varepsilon < 0$	0	$f(X_M)/q_u$
l_2	$\varepsilon = 0$	0	$f(X_M)/q_u$
p	$\varepsilon = 0$	0	$f(X_M)/q_u$
l_1	$\varepsilon = 0$	0	$f(X_f)/q_u$
l_4	$\varepsilon = 0$	0	$f(X_f)/q_u$
$\mathcal{O}_1$	$\varepsilon > 0$	$[s - f(X_f)]/q_e$	$f(X_f)/q_u$
l_5	$\varepsilon > 0$	$[s - f(X_M)]/q_e$	$f(X_M)/q_u$
$\mathcal{O}_2$	$\varepsilon > 0$	$[s - f(X_M)]/q_e$	$f(X_M)/q_u$
$\mathcal{O}_3$	$\varepsilon > 0$	$[s - f(X_f)]/q_e$	$f(X_f)/q_u$

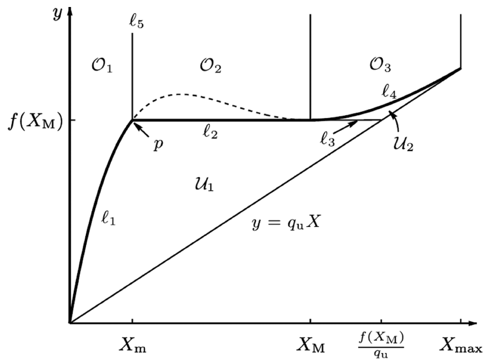

Figure 2. The steady-state chart of the settler.[18]

The development presented next is believed to be new, since no reference thereof has been found in the available literature. A given settler feed condition, represented by the pair (X_f, s), where $s = q_f X_f$ with $q_f = Q_f/\mathbf{A}$ ($\mathbf{A}$ is the cross-sectional area of the settler), can be located anywhere in the 11 regions reported in Table 2. Figure 2 represents those regions and depicts a general flux curve in the thickening zone (i.e., below the feed point), which is given by $f(X) = Xv_s(X) + q_u X$. In this expression, $v_s(X)$ is the settling velocity law, here given by the double exponential, eq 2,[21]

$$v_s(X) = \max(0, \min(v_0', v_0(e^{-r_h(X-X_{\min})} - e^{-r_p(X-X_{\min})}))) \tag{2}$$

which contains five parameters that are usually found experimentally: v_0, the theoretical maximum velocity obtained at the intersection of the v_s vertical axis and the extension of the right exponential curve; v_0', the practical maximum velocity; $X_{\min}$, the minimum concentration below which the settling velocity vanishes (we here consider $X_{\min}$ is a fraction f_{ns} of X_f, that is, $X_{\min} = f_{ns}X_f$);[15] r_h, which determines the particle behavior for increasing particle density; r_p determines the particle behavior at weak concentration values.

Because X_f and s are the input variables to the settler, which are primarily functions of the biological activity in the reaction section, the flow rate through the bottom of the settler, Q_u (or its flux counterpart, $q_u = Q_u/\mathbf{A}$), is the sole degree of freedom (manipulated variable) in the settler and can be used as a decision variable for optimization. It is also the sum of the wastage sludge and the outer recycle, $Q_u = Q_w + Q_r$, as depicted in Figure 1. From an optimum economic operation point of view, the smaller Q_w, the smaller is the cost of wastage treatment and, hence, the smaller is the total cost. Because Q_r is primarily a function of the biological activity in the reaction section, we can presume that minimizing Q_u via Q_w reduces the cost of operation of the entire system. Thus, for a given feed (X_f, s), we can therefore conclude that optimal operation of the settler lies in the overloaded region, up to the point where one of the first of either $X^{(\mathrm{eff})}$, $\mathrm{COD}^{(\mathrm{eff})}$, $\mathrm{BOD5}^{(\mathrm{eff})}$, or $\mathrm{TN}^{(\mathrm{eff})}$ (which are all functions of the suspended solids in the clarification zone) becomes active, as long as the cost of wastage treatment is positive (since anaerobic digestion of sludge can be indeed lucrative if one considers that the resulting biogas can be commercialized).

From Figure 2, the overloaded region spans four distinct subregions. In regions O_1 and l_5, X_f is small, which may not be the case for activated sludge processes due to the large concentration of suspended solids that is usually formed in the biological reactors. We then focus our analysis on the more "concentrated" regions O_2 and O_3 in order to determine the constitutive equations of the settler to be used for optimization. The excess flux, ϵ, is defined as in eq 3[19]

$$\epsilon(X_f, s) \equiv s - f_{\min}(X_f) \tag{3}$$

where the limiting flux, $f_{\min}(X)$, is given by eq 4[29]

$$f_{\min}(X) \equiv \min_{X<\alpha<X_{\max}} f(\alpha) = \begin{cases} f(X_M), X \in (X_m, X_M) \\ f(X), X \in [X_M, X_{\max}] \end{cases} \tag{4}$$

where X_M is a minimizer of $f(X)$, X_m is a value strictly less than X_M satisfying $f(X_m) = f(X_M)$, and $X_{\max}$ is the maximum suspended solids concentration. For regions O_2 and O_3, the excess flux $\epsilon(X_f, s)$ is then eq 5,

$$\epsilon(X_f, s) = \begin{cases} s - f(X_M), X_f \in (X_m, X_M) \\ s - f(X_f), X_f \in [X_M, X_{\max}] \end{cases} \tag{5}$$

In any case eq 6 describes an equation for the solid concentration in the effluent $X^{(\mathrm{eff})}$, where $q_e = Q^{(\mathrm{eff})}/\mathbf{A}$, $Q^{(\mathrm{eff})}$ being the effluent flow rate.

$$X^{(\mathrm{eff})} = \frac{\epsilon(X_f, s)}{q_e} = \frac{\epsilon(X_f, s)}{q_f - q_u} \Rightarrow q_u = q_f - \frac{\epsilon(X_f, s)}{X^{(\mathrm{eff})}} \tag{6}$$

For region O_2, eq 7 applies,

$$q_u = q_f - \frac{s - f(X_M)}{X^{(\mathrm{eff})}} \tag{7}$$

and taking $s = q_f X_f$ and $f(X_M) = X_M v_s(X_M) + q_u X_M$ into eq 7 gives eq 8,

$$q_u = \frac{X^{(\mathrm{eff})} - X_f}{X^{(\mathrm{eff})} - X_M} q_f + \frac{X_M}{X^{(\mathrm{eff})} - X_M} v_s(X_M) \tag{8}$$

Analogously for region O_3, with $f(X_f) = X_f v_s(X_f) + q_u X_f$, eq 9 is found,

$$q_u = q_f + \frac{X_f}{X^{(\mathrm{eff})} - X_f} v_s(X_f) \tag{9}$$

We can reasonably assume that, because X_f and X_M are large, $X_f \gg X^{(\mathrm{eff})}$ and also that $X_M \gg X^{(\mathrm{eff})}$. Hence eq 10 applies.

$$q_u \cong \begin{cases} \dfrac{X_f}{X_M} q_f - v_s(X_M), X_f \in (X_m, X_M) \\ q_f - v_s(X_f), X_f \in [X_M, X_{\max}] \end{cases} \tag{10}$$

Because the pair (X_f, s) is primarily dependent on the biological activity in the reaction section, eq 11 holds.

$$[q_f]_{X_f \in [X_M, X_{\max}]} > \left[\frac{X_f}{X_M} q_f\right]_{X_f \in (X_m, X_M)} \quad \text{and}$$
$$[v_s(X_f)]_{X_f \in [X_M, X_{\max}]} > [v_s(X_M)]_{X_f \in (X_m, X_M)} \tag{11}$$

Therefore, the smallest value of q_u, and hence the minimum wastage disposal cost, is achieved in region O_2 where $X_f \in (X_m, X_M)$. Moreover, having $X_f \in (0, X_m)$ or $X_f \in (X_M, X_{\max})$ depends on the reaction section being able to produce such X_f, which may not be feasible. This is indeed the case for the activated sludge process considered in this paper as shown later in the optimization section. However, for large throughputs, that is, high loads during long periods, it may be the case where $X_f \in (X_M, X_{max})$, and we have to switch to region O_3 where q_u is higher.

As a consequence of the previous analysis, the steady-state model of the settler that holds for optimization purposes is given by eq 12,

$$
\begin{aligned}
X^{(\mathrm{eff})} &= \frac{s - f(X_M)}{q_e} \\
X_u &= \frac{f(X_M)}{q_u} \\
X_M &= \mathbf{M}(q_u) \\
X_f &\in (X_m, X_M)
\end{aligned}
\tag{12}
$$

where M is a function that computes the local minimizer of $f(X_M)$. In addition, we can also calculate the steady-state concentration of suspended solids in the clarification (X_{cl}) and thickening zones (X_{th}) as in eq 13[18]

$$
\begin{aligned}
g(X_{cl}) + s &= f(X_M) \\
X_{th} &= X_M
\end{aligned}
\tag{13}
$$

where $g(X_{cl}) = X_{cl}v_s(X_{cl}) - q_e X_{cl}$.

Note that although in this paper a nonreactive settler is considered, we here follow[17] and treat the dissolved oxygen in the settler in a special way. We assume that the oxygen is consumed within the settler and, as a consequence, the oxygen concentration at the settler's outlets is set to zero, which is indeed a realistic assumption. This results in a more conservative computation of the oxygen demand in the reaction section.

In this paper, the BSM1 protocol[15] with the modified secondary settler model proposed above is reimplemented as a Matlab script, and we use the ADMAT[30] package to compute first-order information based on automatic differentiation for explicit optimization. X_M is computed implicitly together with the other model equations as the solution of $\mathrm{d}f(X)/\mathrm{d}X = 0$ with $\mathrm{d}^2 f(X)/\mathrm{d}X^2 > 0$ as a constrained condition for minimum.

3. CONTROLLED VARIABLE SELECTION METHODOLOGY

In this section, a summary of the sensitivity analysis procedure used in this work is discussed. It is not supposed to be an exhaustive discussion on the subject; instead, we give the necessary elements for a proper understanding of the main ideas lying behind the method. Indeed, this plantwide procedure has been successfully applied to other processes as described in various publications in the field.[31−36,12] Indeed, a review of this methodology and others, more heuristics as well as applications thereof can be found in Rangaiah and Kariwala.[37]

The methodology is mainly based on the first four steps, known as "top-down analysis", of the more general procedure described in Skogestad,[38] where economic variable selection is the key issue. The analysis conducted is of local nature, that is, we use linearized models of the process to develop the methodology. In general, one should always, for a final validation, check the linear results against simulations on the nonlinear model of the process.

In this paper, we use optimal measurement combinations[39] for unconstrained variable selection, that is, the ones left after choosing the active constraints as "primary" economic variables. The basic idea is to select combinations, c, of the measurements, y, such that $c = \mathbf{H}y$, where $\mathbf{H}$ is a (static) selection matrix. To determine $\mathbf{H}$, two approaches are developed based on a linearized model of the process and a second-order Taylor series expansion of the cost function used for optimization; two sources of uncertainty are assumed, which are represented by eq 1, external disturbances (d), and eq 2, implementation (measurement) errors (n). The first of the two approaches combines these uncertainties in one single scaled vector to minimize the worst case economic loss ($\mathbf{L}$), defined as the difference between actual operation (with a given control structure in place) and operation under optimal control. In the second approach, we first minimize the loss with respect to external disturbances and then, if there are still available measurements, minimize the loss with respect to implementation (measurement) errors.

Below we give more details on each step of the sensitivity analysis procedure[38] and for that we consider an existing plant and that we have available a steady-state usually nonlinear mathematical model of the process.

1. **Define operational objectives**. We first quantify the operational objectives in terms of a scalar cost function (here denoted $\mathbf{J}$), that should be minimized or, equivalently, a scalar profit function, $P = -\mathbf{J}$, that should be maximized. A typical cost function is given as in eq 14,

$$
\begin{aligned}
\mathbf{J} = {} & \text{cost of feed} + \text{cost of utilities (e.g., energy)} \\
& - \text{revenue from valuable products}
\end{aligned}
\tag{14}
$$

In addition to the definition of an economic objective, in most cases operation takes place under constrained conditions, such as minimum and maximum values on process variables for process safety, environmental regulations, product specifications, and control limitations. These can be included in the above formulation by defining inequality constraints ($g \le 0$).

2. **Determine the steady-state optimal operation**. Using a steady-state model of the process, identify degrees of freedom and expected disturbances and perform optimizations to assess sensitivity for the expected disturbances.

Usually, the economics of the plant are primarily determined by the (pseudo) steady-state behavior,[40] so the steady-state degrees of freedom (u_0) are usually the same as the economic degrees of freedom. Which variables to include in the set u_0 is immaterial, as long as they make up an independent set. One simple way to identify these degrees of freedom is to use a flowsheet of the process and count the number of independent manipulated variables that can be affected.

The important disturbances (d) and their expected range for future operation must then be identified. These are generally related to feed rate and feed composition, as well as external variables such as temperature and pressure of the surroundings. We should also include as disturbances possible changes in specifications and active constraints (such as product specifications or capacity constraints) and changes in parameters (such as equilibrium constants, rate constants, and efficiencies). Finally, we should include as disturbances the expected changes in prices of products, feeds, and energy. Note, however, that some disturbances may have a small effect on the optimal operation of the process. It is therefore desirable to discriminate the important disturbances that should be considered for steady-state analysis. In this paper, we identify important disturbances to calculate the actual loss in the variable selection step using a nonlinear model of the process.

In order to achieve near-optimal operation without the need to reoptimize the process when disturbances occur, one needs to minimize the loss in eq 15,

$$\mathbf{L} = \mathbf{J}_0(c, d) - \mathbf{J}_0(c^{\mathrm{opt}}(d), d) \geq 0 \tag{15}$$

where $\mathbf{J}_0(c, d)$ is the value of the cost for a chosen set of constant set point variables c that fulfill all remaining degrees of freedom and $\mathbf{J}_0(c^{opt}(d), d)$ is the value of the cost after reoptimization. Clearly, the loss in eq 15 depends on the objective function as well as on the measurements through c, since c is a function of the available y. We then need to learn about the sensitivity to disturbances not only of the cost function but also of the measurements.

To optimize the operation, we select the nominal disturbance d and vary the values of the degrees of freedom in an optimal way $(u_0^{\mathrm{opt}}(d))$ so as to minimize the cost $(\mathbf{J}_0(x, u_0, d))$, while satisfying the constraints. Mathematically, this steady-state optimization problem can be formulated as in eq 16,

$$\begin{aligned} &\min_{u_0} \mathbf{J}_0(x, u_0, d) \\ &\text{subject to} \\ &\text{model equations } f(x, u_0, d) = 0 \\ &\text{operational constraints } g(x, u_0, d) \leq 0 \end{aligned} \tag{16}$$

where x are internal variables (states). In $f(x, u_0, d) = 0$, possible operational equality constraints (like a given feed flow) are also included. The main objective is to determine the optimal nominal operating condition to be used in the variable selection step.

3. **Select "economic" (primary) controlled variables**. In this step, the issue is the implementation of the optimal operation point found in the previous step in a robust and, most importantly, simple manner. We need to identify as many economic controlled variables (c) as there are economic degrees of freedom (u_0). For economic optimal operation, active constraints must be selected,[41] which in turn consumes part (u') of the degrees of freedom. For the remaining degrees of freedom (u, where $n_u = n_{u_0} - n_{u'}$), we select variables for which close-to-optimal operation is achieved with constant nominal set points, even when there are disturbances.[13] Because our considerations in this paper are of local nature, we assume that the set of active constraints does not change with changing disturbances, and we consider the problem in reduced space in terms of the remaining unconstrained degrees of freedom, u, which can be expressed as in eq 17,[42]

$$\begin{aligned} &\min_{u} \mathbf{J}_0(x, u, d) \\ &\text{subject to} \\ &\text{model equations } f(x, u, d) = 0 \\ &\text{active constraints } g_{\mathrm{active}}(x, u, d) = 0 \end{aligned} \tag{17}$$

where we consider as active constraints a subset $g_{\mathrm{active}}(x, u, d)$ of $g(x, u_0, d)$ for which optimal values are always at bounds for all disturbances. By elimination of the states using the equality constraints in eq 17, the unconstrained optimization problem can be expressed simply as in eq 18,

$$\min_{u} \mathbf{J}(u, d) \tag{18}$$

Note that although $\mathbf{J}_0$ and $\mathbf{J}$ are numerically the same, they do not share the same mathematical structure. Indeed, $\mathbf{J}$ is generally not a simple function in the variables u and d but rather a functional.

Ensuring active constraint operation consumes part of the degrees of freedom for optimization. The remaining degrees of freedom need to be fulfilled, and we select variables such that when kept at optimal set points lead to near-optimal economic operation despite disturbances, that is, the deviation (loss $\mathbf{L}$ in eq 15) from reoptimization as a function of disturbances should be small. The optimal set points of c are then determined from the optimization at the nominal operating point. This is the celebrated self-optimizing control technology.[13] A quantitative way to determine the set c is based on a quadratic approximation of the cost function $\mathbf{J}$ as given by eq 18. It can be shown[39] that the second-order accurate expansion of the loss function is given by eq 19,

$$\mathbf{L} = \frac{1}{2}(u - u^{\mathrm{opt}})^T \mathbf{J}_{uu}(u - u^{\mathrm{opt}}) = \frac{1}{2} z^T z = \frac{1}{2} \| z \|_2^2 \tag{19}$$

with $z = \mathbf{J}_{uu}{}^{1/2}(u - u^{\mathrm{opt}})$, where $\mathbf{J}_{uu} = (\partial^2 \mathbf{J}/\partial u^2)_{u^{\mathrm{opt}}}$ is the Hessian of $\mathbf{J}$ with respect to u evaluated at u^{opt}, and u^{opt} is the optimal value of the manipulated variables. We consider that c is expressed as a linear combination of the available measurements y as in eq 20,

$$c = \mathbf{H}y \tag{20}$$

where $\mathbf{H}$ is a real constant matrix, the coefficient matrix, and $\dim(c) = \dim(u)$.

Now, assume we have a linearized (local) model of the process in terms of deviation variables as in eq 21,

$$y = \underbrace{[G^y \ G_d^y]}_{\widetilde{G^y}} \begin{bmatrix} u \\ d \end{bmatrix} \tag{21}$$

It can then be shown[39] that z can be expressed as function of the more appropriate uncertainty variables, eq 22,

$$z = \underbrace{[M_d \ M_{n^y}]}_{M} \begin{bmatrix} d' \\ n^{y\prime} \end{bmatrix} \tag{22}$$

where d' and $n^{y'}$ are the scaled disturbance and measurement error variables related by $d = \mathbf{W}_d d'$ and $n^y = \mathbf{W}_{n^y} n^{y'}$ ($\mathbf{W}_d$ and $\mathbf{W}_{n^y}$ are scaling matrices), and M_d and M_{n^y} are given by eqs 23 and 24, respectively

$$\mathbf{M}_d = -\mathbf{M}_n \mathbf{H} F \mathbf{W}_d \tag{23}$$

$$\mathbf{M}_{n^y} = -\mathbf{M}_n \mathbf{H} \mathbf{W}_{n^y} \tag{24}$$

where

$$\mathbf{M}_n = \mathbf{J}_{uu}{}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1} \tag{25}$$

and $\mathbf{F} = \mathrm{i}\partial y^{\mathrm{opt}}/\partial d$ is the optimal measurement (y^{opt}) sensitivity with respect to the disturbances, which can be found explicitly by eq 26,[39]

$$F = -(\mathbf{G}^y \mathbf{J}_{uu}{}^{-1} \mathbf{J}_{ud} - \mathbf{G}_d^y) \tag{26}$$

where $\mathbf{J}_{ud} = [\partial^2 \mathbf{J}/(\partial u \partial d)]_{u^{\mathrm{opt}}, d^{\mathrm{nom}}}$.

Therefore, we choose to compute the worst-case loss ($\mathbf{L}_{\mathrm{wc}}$) for the expected disturbances and measurement noise as given by eq 27,[39]

$$\mathbf{L}_{\mathrm{wc}} = \max_{\left\|\begin{bmatrix} d' \\ n^{y'} \end{bmatrix}\right\|_2 \leq 1} \mathbf{L} = \frac{1}{2}\bar{\sigma}^2(\mathbf{M}) \tag{27}$$

In other words, we need to find $\mathbf{H}$ that minimizes $\bar{\sigma}(M)$, that is, $\mathbf{H}$ = arg $\min_{\mathbf{H}}\ \bar{\sigma}(M)$. There are basically two approaches to solve for this minimization problem.

The first approach solves the minimization problem in eq 27 at once by combining disturbances and measurement errors in one vector, and in this case, an explicit formula for $\mathbf{H}$ is given by eq 28,[39]

$$\mathbf{H}^{\mathrm{T}} = (\tilde{\mathbf{F}}\tilde{\mathbf{F}}^{\mathrm{T}})^{-1}\mathbf{G}^{y}(\mathbf{G}^{y\mathrm{T}}(\tilde{\mathbf{F}}\tilde{\mathbf{F}}^{\mathrm{T}})^{-1}\mathbf{G}^{y})^{-1}\mathbf{J}_{uu}^{1/2} \tag{28}$$

where $\tilde{\mathbf{F}} = [\mathbf{F}\mathbf{W}_d\ \mathbf{W}_{n^y}]$ and $\tilde{\mathbf{F}}\tilde{\mathbf{F}}^{\mathrm{T}}$ must be full rank. *This expression applies to any number n_y of measurements.*

The second approach, called the extended nullspace method,[39] solves the minimization problem in eq 27 in two steps: first minimizing the loss with respect to disturbances and then, if there are still enough measurements left, minimizing the loss with respect to measurement errors. One justification for this methodology is that disturbances are the reason for introducing optimization and feedback in the first place. Another reason is that it may be easier later to reduce measurements errors than to reduce disturbances. It can be shown that the explicit expression for $\mathbf{H}$ in this case is given by eq 29,[39]

$$\mathbf{H} = \mathbf{M}_n^{-1}\tilde{J}(\mathbf{W}_{n^y}^{-1}\tilde{\mathbf{G}}^{y})^{\dagger}\mathbf{W}_{n^y}^{-1} \tag{29}$$

where $\tilde{\mathbf{J}} = [\mathbf{J}_{uu}^{1/2}\ \mathbf{J}_{uu}^{1/2}\ \mathbf{J}_{uu}^{-1}\ \mathbf{J}_{ud}]$. There are four cases where eq 29 can be applied:

Case 1. "Just-enough" measurements are chosen, that is, $n_y = n_u + n_d$. Here, the expression for $\mathbf{H}$ becomes eq 30,

$$\mathbf{H} = \mathbf{M}_n^{-1}\tilde{J}(\tilde{\mathbf{G}}^{y})^{-1} \tag{30}$$

which is the same as having $\mathbf{H}$ in the left null space of $\mathbf{F}$, that is, $\mathbf{H} \in N(\mathbf{F}^T)$.

Case 2. Extra measurements (select just enough measurements) are also included, that is, $n_y > n_u + n_d$, and we want to select a subset of the measurements y such that $n_y = n_u + n_d$. The solution is to find such a subset that maximizes $\underline{\sigma}(\tilde{\mathbf{G}}^{y})$ using, for example, existing efficient branch-and-bound algorithms.[43] The resulting $\tilde{\mathbf{G}}^{y}$ is then used to compute $\mathbf{H}$ in eq 30.

Case 3. Extra measurements (use all available measurements), that is, $n_y > n_u + n_d$. $\mathbf{H}$ is calculated using eq 29, where † denotes the left inverse, calculated as $\mathbf{A}^{\dagger} = (\mathbf{A}^{\mathrm{T}}\ \mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}$ for any given matrix $\mathbf{A}$.

Case 4. "Too few" measurements are available, that is, $n_y < n_u + n_d$. In this case, the optimal $\mathbf{H}$ in eq 29 is not affected by the noise weight and therefore becomes

$$\mathbf{H} = \mathbf{M}_n^{-1}\tilde{\mathbf{J}}(\tilde{\mathbf{G}}^{y})^{\dagger} \tag{31}$$

where † denotes the right inverse, that is, $\mathbf{A}^{\dagger} = \mathbf{A}^{\mathrm{T}}(\mathbf{A}\mathbf{A}^{\mathrm{T}})^{-1}$.

The above procedure boils down to selecting suitable candidate measurements, that is, identify n_y vis-a-vis $n_u + n_d$, and find that linear combination (matrix $\mathbf{H}$) of all, or a given subset of measurements, which results in the smallest loss among every possible solution. One big hurdle to be surmounted is the numerical calculation of $\mathbf{J}_{uu}$ and $\mathbf{J}_{ud}$. For some ill-posed problems, it may become an intractable task, and one solution is to compute $\mathbf{F}$ numerically instead, since $\mathbf{F}$ = $\mathrm{d}y^{\mathrm{opt}}/\mathrm{d}d$. Hopefully, the extended nullspace general formula, eq 29, can, after some matrix algebra, be reformulated as in 32,

$$\mathbf{H} = \mathbf{M}_s(\mathbf{G}^{y})^{\dagger}[\mathbf{G}^{y}(\mathbf{G}_d^{y} - \mathbf{F})](\mathbf{W}_{n^y}^{-1}\tilde{\mathbf{G}}^{y})^{\dagger}\mathbf{W}_{n^y}^{-1} \tag{32}$$

where $\mathbf{M}_s = (\mathbf{J}_{uu}^{-1/2}\mathbf{M}_n)$ can be any nonsingular $n_u \times n_u$ matrix. In this case, we could select $\mathbf{M}_n = \mathbf{J}_{uu}^{-1/2}$ so that eqs 28 and 29 are independent of Hessian information.

It should be clear that the linear method just described is local in nature, so only small variations around the optimal values can be considered. Many large disturbances will certainly move the operating conditions significantly, and only a nonlinear model of the process could represent such a case.

4. RESULTS

In this section, we focus on the application of the aforementioned procedure to the mathematical model described in section 2, starting with the definition of optimal operation. It is worth mentioning that a nonlinear steady-state model of the process is the main requirement and that the analysis is based on steady-state considerations only.

4.1. Step 1. Operational Objectives. The operational costs in a wastewater treatment plant depend on the wastewater system itself and can be divided into manpower, energy, maintenance, chemical usage, chemical sludge treatment, and disposal costs. However, in this work, the objective is to reduce the cost of energy and sludge disposal as much as possible. Therefore, the following costs are considered: required pumping energy, E_{P}, expressed in kWh/d; required aeration energy, E_{A}, expressed in kWh/d; required mixing energy when aeration need is too low to provide adequate mixing, E_{M}, expressed in kWh/d; sludge disposal, C_{D}, expressed in \$/d.

To express the partial costs over a certain range of time, Θ, we adopt the expressions proposed in Alex et al.[15] The total energy due to the required *pumping energy* depends directly on the recycle flow (Q_r), on the internal recycle (Q_a), and on the waste sludge flow rate (Q_w) through eq 33:

$$E_{\mathrm{P}} = \frac{1}{\Theta}\int_{t_0}^{t_0+\Theta}(0.004Q_a(t) + 0.008Q_r(t) + 0.05Q_w(t))\,\mathrm{d}t \quad [\mathrm{kWh/d}] \tag{33}$$

with the flow rates in m^3/d. The *aeration energy* can be calculated from eq 34, which is a function of the oxygen saturation concentration, $S_{\mathrm{O}}^{\mathrm{sat}}$, in each bioreactor volume, V, and $K_{\mathrm{L}}a$, the combined mass transfer coefficient for oxygen:

$$E_{\mathrm{A}} = \frac{S_{\mathrm{O}}^{\mathrm{sat}}}{\Theta \times 1.8 \times 1000}\int_{t_0}^{t_0+\Theta}\sum_{i=1}^{n} V_i K_{\mathrm{L}}a^{(i)}(t)\,\mathrm{d}t,\ n = 5 \quad [\mathrm{kWh/d}] \tag{34}$$

with $K_{\mathrm{L}}a$ expressed in d^{-1} and i referring to the reactor zone number. In addition to aeration, mechanical mixing might also be supplied to avoid settling. The *mixing energy* is then a function of the compartment volume and can be computed by eq 35:

$$E_{\mathrm{M}} = \frac{24}{\Theta}\int_{t_0}^{t_0+\Theta}\sum_{i=1}^{n}\begin{cases}0.005V_i\,\mathrm{d}t, & \text{if } K_{\mathrm{L}}a^{(i)}(t) < 20\\ 0, & \text{otherwise}\end{cases},\ n = 5 \quad [\mathrm{kWh/d}] \tag{35}$$

The *sludge disposal production* per day is expressed as in eq 36

$$C_D = \frac{1}{\Theta}\int_{t_0}^{t_0+\Theta} (\mathrm{TSS_w}(t)Q_w(t))\,dt \qquad [\mathrm{gSS/d}] \tag{36}$$

where $\mathrm{TSS_w}$ represents the total suspended solids wasted with Q_w. Assuming a constant energy price, k_E = \$0.09/kWh, and a sludge disposal cost of k_D = \$80/ton, the total cost in \$/d can be calculated as in eq 37:

$$\mathrm{cost} = k_E(E_P + E_A + E_M) + k_D C_D \qquad [\$/\mathrm{d}] \tag{37}$$

The overall cost function in eq 37 is then averaged over time for steady-state purposes and minimized subject to environment regulations for the effluent and some constraints related to process operability. These constraints are listed in Table 3.

Table 3. Constraints to the Process

constraint	unit	status
$\mathrm{COD^{(eff)}} \le 100$	$\mathrm{gCOD/m^3}$	regulation constraint
$\mathrm{TSS^{(eff)}} \le 30$	$\mathrm{gSS/m^3}$	regulation constraint
$\mathrm{TN^{(eff)}} \le 18$	$\mathrm{gN/m^3}$	regulation constraint
$\mathrm{BOD_5^{(eff)}} \le 10$	$\mathrm{gBOD/m^3}$	regulation constraint
$S_{NH}^{(eff)} \le 4$	$\mathrm{gN/m^3}$	regulation constraint
$Q_w \le 1845$	$\mathrm{m^3/d}$	manipulation constraint
$Q_r \le 36892$	$\mathrm{m^3/d}$	manipulation constraint
$Q_a \le 92230$	$\mathrm{m^3/d}$	manipulation constraint
$K_La^{(1-5)} \le 360$	$\mathrm{d^{-1}}$	manipulation constraint

The effluent environmental regulation constraints on COD, TSS, TN, $\mathrm{BOD_5}$, and S_{NH} and the values for the manipulation constraints are taken from Alex et al.[15]

4.2. Step 2. Steady-State Optimal Operation. Using the information given in the process flowsheet in Figure 1, we find that there are eight manipulated variables that correspond to eight steady-state degrees of freedom (u), namely, Q_w (excess sludge flow rate), Q_r (external recirculation flow rate), Q_a (internal recirculation flow rate), and $K_La^{(1-5)}$ (mass transfer coefficient of oxygen in each basin). These are the last four entries in Table 3. The liquid levels in the reactor tanks are assumed to be constant at maximum capacity due to the overflow layout considered for the plant. Note that from the 11 valves in Figure 1, the feed valve is not an available degree of freedom since it is a disturbance to the process; the valve at the outlet of the last basin is only used to possibly adjust this basin level; and the valve at the effluent line has indeed no steady-state effect.

4.2.1. Remark 1. We here consider K_La as a manipulated variable to avoid including details of basin and aeration systems geometry into the model because the actual manipulated variable, namely, the flow of compressed air, is generally a function of the type $q_{air} = F(K_La, d_b, h, L_a, f, B, \alpha, \gamma, \nu, A, D)$, where d_b is the diameter of bubbles, h is the submergence of aerators, L_a is the liquid depth in the aeration basin, f is the width of the aeration band, B is the width of the aeration basin, α is the correction factor relating the overall mass-transfer coefficient (K_La) of the wastewater to that of tap water, γ is the temperature correction factor, ν is the water viscosity, A is the sectional area of the basin, and D is the coefficient of molecular diffusion. One such relation given in Khudenko and Shpirt[44] is reproduced in eq 38.

$$K_La = 0.041\alpha\gamma\left(\frac{h}{d_b}\right)^{0.67}\left(\frac{f}{B}\right)^{0.18}\left(\frac{q_{air}}{L_aA}\right) \tag{38}$$

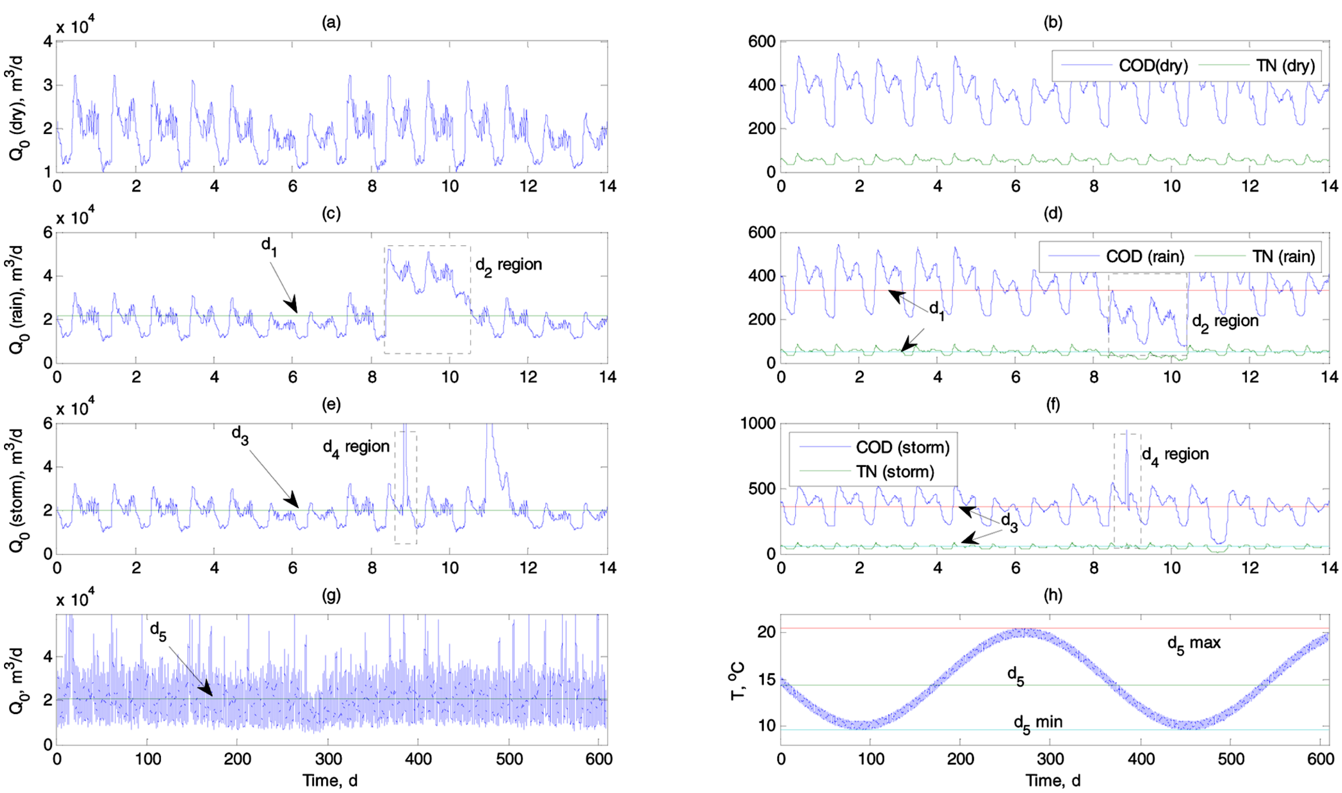

Figure 3. Influent flow rate and organic and nutrient compounds for the given weather events and long-term data[1] (the considered steady-state optimization disturbances are highlighted).

Since our unconstrained variable selection analysis is local (linear) in nature, we here choose as disturbances for this purpose the most important inputs in the influent,[15] which are the flow rate, $Q^{(in)}$, the chemical oxygen demand, COD^{in}, the total suspended solids concentration, TSS^{in}, the total nitrogen concentration, TN^{in}, and the surrounding temperature, T. Obviously, each of these are considered acting upon the process one at the time.

On the other hand, for nonlinear loss evaluation, we must define more realistic disturbance scenarios. Compared with other process industries, a wastewater treatment plant is subject to very distinct operation modes because of daily, weekly, and seasonal variation in the incoming wastewater. In this paper, we consider the influent load data as given by the IWA Task Group in the benchmark Web site. The data are presented in terms of ASM1 state variables and influent flow rates. In general, these data reflect expected diurnal trend variations in weekdays, which are typical for normal load behavior at a municipality treatment facility. Four different weather/influent conditions are considered in four different data sets and from those, different events are deduced for our purposes: (1) *The dry weather file* (Figure 3a,b) gives what is considered to be normal diurnal variations in flow and organic pollutant loads. In the following, the average input compositions and flow rate are considered as *nominal* conditions for the BSM1 plant. (2) *The rain weather file* (Figure 3c,d) represents a long rain event. (3) *The storm weather file* (Figure 3e,f) is a variation of the dry weather file incorporating storms. The first storm event in this file is of high intensity and short duration. The second storm event assumes the sewers were cleared of particulate matter during the first storm event; hence, only a modest increase in COD load is noted during the second storm. (4) *The long-term weather file* (Figure 3g,h) represents 1.5 year data where the first 6 months, starting in winter time, give training data and the last 12 months, starting in summer time, correspond to the monitoring period. Variation in temperature during one year time are also considered. This overcomes one of the recognized limitations[45] of the BSM1 model: the availability of short time data sequences, which in turn results in a long-term benchmark model no. 1 (BSM1_LT). It focuses on long-term process performances and considers temperature variations during one year.

As step change disturbances from the nominal operation for steady-state optimizations, we consider different conditions from the different data sets. Starting from the *nominal* conditions (Figure 3a,b), average values of influent during dry weather, Table 4 summarizes the given disturbances to be used for nonlinear computations in terms of influent flow rate and load. The average composition and flow rate, d_1, and the average values for the process inputs during the rain period, marked as d_2 region, are taken from the rain weather depicted in Figure 3c,d. From Figure 3e,f, we can identify the given disturbance as d_3 representing the average condition during the whole period and d_4 as the average during the storm time. Variations in temperature during one year time are reported in Figure 3g,h, and we consider the average (d_5), minimum ($d_{5,min}$) and maximum ($d_{5,max}$) values for the temperature. In fact, one particular advantage of studying this process is the availability of the weather event profiles for different weather conditions (as well as the long-term data) because it definitely aids the sensitivity analysis with the actual upsets to the plant. The importance of this sort of discrimination is well documented in Gernaey et al.[45]

Table 4. Weather Profiles Events and Derived Disturbances

	$Q^{(in)}$ [m^3/d]	$COD^{(in)}$ [gCOD/m^3]	$TSS^{(in)}$ [gSS/m^3]	$TN^{(in)}$ [gN/m^3]	T [°C]
d_0 (nominal)	18446	381	211	54	15
d_1	21320	333	183	48	15
d_2	40817	204	116	28	15
d_3	19746	353	195	50	15
d_4	34286	281	101	37	15
d_5	20850	347	199	41	15
$d_{5,min}$	20850	347	199	41	9
$d_{5,max}$	20850	347	199	41	21
expected range					
$\max(\lvert d_0 - d_{i,max}\rvert, \lvert d_0 - d_{i,min}\rvert)$	22371	100	110	26	6

To achieve optimal operation, we select the active constraints as variables to be monitored,[41] whereas the difficult issue of deciding which unconstrained variables to select is resolved by recurring to the concepts of step 3 of the procedure described in the preceding section. The starting point for the selection of primary (economic) variables is the optimization of the process. To this end, the BSM1 model plus the proposed model of the secondary settler is reimplemented as a script in MatLab and the nominal optimization is performed subjected to the constraints given in Table 3. The in-built MatLab subroutine "fmincon.m" is the optimizer of choice, and in order to make the optimization run more robustly, we used an automatic differentiation software[30] to compute first-order (sparse) information, that is, Jacobians and gradients.

4.3. Step 3. Controlled Variable Selection.

The results of the optimization can be seen in Table 5, which gives the values of relevant variables involved in the process. Three constraints are active, namely, $TSS^{(eff)}$ (upper limit), $S_{NH}^{(eff)}$ (upper limit), and Q_a (lower limit). As expected (see discussion in section 2), $TSS^{(eff)}$ is at its maximum to make Q_w small. In general, the reason free ammonia ($S_{NH}^{(eff)}$) is active at its upper bound is that because nitrification is an oxygen-demanding process and because the transfer efficiency of oxygen from gas to liquid is relatively low so that only a small amount of oxygen supplied is used by the microorganisms, the aeration demand (E_A), which is the major cost contributor in a wastewater treatment plant, is high. The fact that $Q_a = 0$ is somehow surprising. However, from a practical point of view, $Q_a = 0$ is possible. In fact, the internal recirculation is needed in the pre-denitrification configuration of the activated sludge process as carbon source (in this way, no external carbon source, like methanol, is added into anoxic zones) and to enhance denitrification in the system. In our case, the return sludge from the secondary settler returns quite sufficient organic matter and nitrate for denitrification; for this reason, Q_a might be avoided in a more economically convenient way. The optimization results show that at the given steady-state conditions the original pre-denitrification configuration could be beneficially replaced by a different configuration with lower oxygen concentration profile along the bioreactor. Of course, Q_a would be certainly needed dynamically together with higher dissolved oxygen concentrations to enhance the capabilities of the control system in terms of reductions of the effluent peaks and disturbance rejection as long as some reset is programmed to always send it back to its steady-state optimal values, that is, $Q_a = 0$. Another interesting fact is that the process is optimally operated aerobically, that is to say, with no anoxic zone. The

Table 5. Effect of Disturbances on Optimal Values of Selected Variables in the System

variable	unit	nominal[a]	original[a]	status	measurement range	measurement noise
cost	\$/d	428.294	460.641			
E_P	\$/d	17.365	20.278			
E_A	\$/d	250.815	259.612			
E_M	\$/d	0.000	21.600			
C_D	\$/d	160.114	159.151			
$S_O^{(1)}$	gO_2/m^3	0.1	0.0	measurement #1	0–10	0.250
$S_{NO}^{(1)}$	gN/m^3	1.4	0.2	measurement # 2	0–20	0.500
$S_{NH}^{(1)}$	gN/m^3	14.9	16.1	measurement #3	0–50	1.250
$S_O^{(2)}$	gO_2/m^3	0.2	0.0	measurement #4	0–10	0.250
$S_{NO}^{(2)}$	gN/m^3	2.4	0.0	measurement #5	0–20	0.500
$S_{NH}^{(2)}$	gN/m^3	12.5	16.8	measurement #6	0–50	1.250
$S_O^{(3)}$	gN/m^3	0.2	0.3	measurement #7	0–10	0.250
$S_{NO}^{(3)}$	gN/m^3	3.4	2.5	measurement #8	0–20	0.500
$S_{NH}^{(3)}$	gN/m^3	9.6	11.7	measurement #9	0–50	1.250
$S_O^{(4)}$	gO_2/m^3	0.2	0.3	measurement #10	0–10	0.250
$S_{NO}^{(4)}$	gN/m^3	4.8	5.0	measurement #11	0–20	0.500
$S_{NH}^{(4)}$	gN/m^3	6.7	7.6	measurement #12	0–50	1.250
$S_O^{(4)}$	gO_2/m^3	0.2	0.3	measurement #13	0–10	0.250
$S_{NO}^{(5)}$	gN/m^3	6.2	7.7	measurement #14	0–20	0.500
$S_{NH}^{(5)}$	gN/m^3	4.0	4.0			
MLSS	gSS/m^3	5856.5	5983.8	measurement #15	0–10000	250.000
SRT	d	13.83	14.20			
FM	gCOD/gSS/d	0.2	0.2			
$COD^{(eff)}$	$gCOL/m^3$	67.0	67.3			
$TESS^{(eff)}$	gSS/m^3	30.0	30.0			
$TN^{(eff)}$	gN/m^3	13.3	15.0			
$S_{NH}^{(eff)}$	gN/m^3	4.0	4.0			
$BOD5^{(eff)}$	$gBOD/m^3$	4.6	4.7			
TSS^w	gSS/m^3	10458.0	10238.0	measurement #16	0–10000	250.000
S_{NO}^w	gN/m^3	6.2	7.7			
Q_w	m^3/d	191.4	194.3	measurement #17	0–100000	2500.000
Q_r	m^3/d	22922.0	25349.2	measurement #18	0–100000	2500.000
Q_a	m^3/d	0.0	3199.9			
$Q_w/Q^{(in)}$		0.01	0.01			
$Q_r/Q^{(in)}$		1.24	1.37			
$K_La^{(1)}$	d^{-1}	122.77	0.00	measurement #19[b]	0–360	9.000
$K_La^{(2)}$	d^{-1}	123.03	0.00	measurement #20[b]	0–360	9.000
$K_La^{(3)}$	d^{-1}	100.44	184.13	measurement #21[b]	0–360	9.000
$K_La^{(4)}$		97.18	159.98	measurement #22[b]	0–360	9.000
$K_La^{(5)}$	d^{-1}	88.28	142.67	measurement #23[b]	0–360	9.000
$Q^{(in)}$	m^3/d	18446.0	18446.0	measurement #24	0–100000	2500.000
$S_{NH}{}^{(in)}$	gN/m^3	31.6	31.6	measurement #25	0–50	1.250
$COD^{(in)}$	$gCOD/m^3$	381.2	381.2	measurement #26	0–1000	25.000
$TSS^{(in)}$	gSS/m^3	211.3	211.3	measurement #27	0–10000	250.000
$TN^{(in)}$	gN/m^3	54.4	54.4			
$T^{(in)}$	°C	15.0	15.0	measurement #28	5–25	0.625

[a]We here assume that measurement accuracy for concentration is 15% of the range. For the other measurements, the accuracy is given by the range of the measurement noise. [b]These measurements can be inferred from, for example, eq 38.

possible reason is due to the attempt to minimize the high aeration costs, and to the fact that the effluent total nitrogen and ammonia constraints are quite easily attained for the given influent loads. Optimization of the process assuming the original configuration of the BSM1 model where the first two tanks are operated anoxically, that is, with $K_La^{(1)} = K_La^{(2)} = 0$, was also conducted (see column dubbed "original" in Table 5), resulting in a higher cost of operation.

It is worth notice at this point that since the settler is modeled as a nonreactive process, the ammonia concentration in the effluent matches, at least at steady-state, the one in the last aerobic tank, and this also applies for all other soluble components. In practice, however, there is an anoxic condition in the settler that favors denitrification with an improved final total nitrogen of about 15% smaller compared with the nonreactive model assumed in this paper.[46]

Because those three active constraints must be implemented to ensure optimal operation,[41] we are left with five degrees of freedom, and we use the local methods described in step 3 of the procedure to decide for the best (optimal) set of unconstrained self-optimizing control variables to fulfill the available degrees of freedom. We consider the measurements

Table 6. Nonlinear loss calculation for various disturbances

	unit	d_1	d_2	d_3	d_4	d_5	$d_{5,\min}$	$d_{5,\max}$
$\mathrm{Cost}^{\mathrm{opt}}$	\$/d	426.783	490.086	420.555	599.359	419.829	491.283	357.955
$\mathrm{Cost}^{\mathbf{H}}{}_1$	\$/d	427.088	507.184	420.615	602.525	420.361	494.371	Inf
$\mathrm{Loss}^{\mathbf{H}}{}_1$	%	0.072	3.489	0.014	0.528	0.127	0.629	Inf
$\mathrm{Cost}^{\mathbf{H}}{}_2$	\$/d	427.067	Inf	420.601	Inf	419.937	507.737	359.401
$\mathrm{Loss}^{\mathbf{H}}{}_2$	%	0.067	Inf	0.011	Inf	0.026	3.349	0.404
$\mathrm{Cost}^{\mathbf{H}}{}_3$	\$/d	426.970	495.860	420.597	608.948	420.368	492.817	358.711
$\mathrm{Loss}^{\mathbf{H}}{}_3$	%	0.044	1.178	0.010	1.600	0.128	0.312	0.211

indicated as such in Table 5, which according to Alex et al.[15] are readily available for the process. Moreover, the range and noise level for each measurement variable are also provided,[15] where the measurement noise corresponds to 0.25% of the maximum value of the measurement interval. Overall, there are $n_y = 28$ measurements, $n_u = 5$ manipulated variables, and $n_d = 5$ disturbances, and clearly with $n_y > n_u + n_d$ one can expect to substantially reduce the loss for both disturbances and measurement errors.

Because there are as many measurements as there are manipulated variables and disturbances, one can compute various **H** matrices. The methods considered in this paper are (1) the combined disturbances and measurement errors using all available measurements, where **H** is computed by eq 28, in which case, $\mathbf{H}_1$ is a 5 × 28 combination matrix, (2) the extended nullspace using all measurements, with **H** computed by eq 32, in which case, $\mathbf{H}_2$ is also a 5 × 28 combination matrix, and (3) the extended nullspace using just enough measurements, where $\tilde{\mathbf{G}}^y$ in eq 32 is found by a branch and bound algorithm,[43] in which case, $\mathbf{H}_3$ is a 5 × 10 combination matrix.

Note that we here normalize the magnitude of the elements in each matrix **H** such that $\|\mathbf{H}\|_F = 1$, where $\|\cdot\|_F$ is the Frobenius norm.

4.3.1. Remark 2: Ranking of the Losses. The losses as computed by eq 27 must satisfy $\mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_1} < \mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_2} < \mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_3}$ since one of the options for $\mathbf{H}_1$ is to use only the measurements selected by $\mathbf{H}_3$, hence $\mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_1} < \mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_3}$. In addition, $\mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_1} < \mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_2}$ because the computation of $\mathbf{H}_1$ includes both disturbances and measurement errors simultaneously. Finally, because $\mathbf{H}_2$ uses all measurements, the resulting loss for $\mathbf{H}_3$ must be larger than that for $\mathbf{H}_2$, that is $\mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_2} < \mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_3}$.

4.3.2. Remark 3: Scaling of H before Computing the Loss. Scaling of **H** does not change the loss as given in eq 27, with $\mathbf{M}_{\mathrm{n}}$ computed via eq 25 with second-order information ($\mathbf{J}_{uu}$) available, since

$$\begin{aligned}\mathbf{M} &= -\mathbf{J}_{uu}{}^{1/2}\left(\frac{\mathbf{H}}{\|\mathbf{H}\|}\mathbf{G}^y\right)^{-1}\frac{\mathbf{H}}{\|\mathbf{H}\|}[\mathbf{F}\mathbf{W}_d\mathbf{W}_n^y] \\ &= -\mathbf{J}_{uu}{}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}\mathbf{H}[\mathbf{F}\mathbf{W}_d\mathbf{W}_n^y] \\ &= [\mathbf{M}_d\mathbf{M}_{n^y}]\end{aligned} \tag{39}$$

The above derivations are local in nature since we have assumed a linear process model and a second-order Taylor series expansion of the objective function in the inputs and the disturbances. Thus, the proposed controlled variables are only globally optimal for the case with a linear model and a quadratic objective. However, in this Article, for a final validation, the sensitivity of the proposed control structure at steady state through the actual losses is checked using the nonlinear model of the process as given in Table 6. This table shows that the losses are about the same order of magnitude for a given disturbance. Although $\mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_1} < \mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_2} < \mathbf{L}_{\mathrm{wc}}^{\mathbf{H}_3}$ is true in a linear fashion, the extended nullspace method, like any other local method, does not guarantee that the rank of linear and nonlinear losses, that is, those calculated from the nonlinear model of the process, is the same.

Also from Table 6, we can see that feasibility is not always guaranteed, and indeed only the alternative where **H** was computed using the extended nullspace method with "just-enough" measurements is feasible for all disturbance spectra. In this particular case, the variables (to be combined) chosen by the branch-and-bound algorithm that maximized the minimum singular value of $\tilde{\mathbf{G}}^y$ were $y = [S_{\mathrm{O}}^{(3)}\ S_{\mathrm{O}}^{(4)}\ S_{\mathrm{NO}}^{(3)}\ \mathrm{MLSS}\ K_{\mathrm{L}}a^{(1)}\ K_{\mathrm{L}}a^{(2)}\ K_{\mathrm{L}}a^{(3)}\ K_{\mathrm{L}}a^{(4)}\ \mathrm{COD}^{(\mathrm{in})}\ T^{(\mathrm{in})}]$, and their respective linear combinations are given by eq 40

$$\begin{aligned}
c_1 &= (5.91570)S_{\mathrm{O}}^{(3)} + (-3.05028)S_{\mathrm{O}}^{(4)} + (2.15592)S_{\mathrm{NO}}^{(4)} \\
&\quad + (-3.60985)\mathrm{MLSS} + (-5.75283)K_{\mathrm{L}}a^{(1)} + (3.35123)K_{\mathrm{L}}a^{(2)} + (3.42391)K_{\mathrm{L}}a^{(3)} + (3.39584)K_{\mathrm{L}}a^{(4)} \\
&\quad + (52.61097)\mathrm{COD}^{(\mathrm{in})} + (-4.40483)T^{(\mathrm{in})} \\
c_2 &= (2.93476)S_{\mathrm{O}}^{(3)} + (-0.52902)S_{\mathrm{O}}^{(4)} + (5.35700)S_{\mathrm{NO}}^{(4)} \\
&\quad + (11.63321)\mathrm{MLSS} + (0.45551)K_{\mathrm{L}}a^{(1)} + (1.28712)K_{\mathrm{L}}a^{(2)} \\
&\quad + (1.31741)K_{\mathrm{L}}a^{(3)} + (1.32573)K_{\mathrm{L}}a^{(4)} + (-209.25538)\mathrm{COD}^{(\mathrm{in})} + (3.21371)T^{(\mathrm{in})} \\
c_3 &= (-0.74280)S_{\mathrm{O}}^{(3)} + (0.57466)S_{\mathrm{O}}^{(4)} + (0.28840)S_{\mathrm{NO}}^{(4)} \\
&\quad + (2.44229)\mathrm{MLSS} + (0.02816)K_{\mathrm{L}}a^{(1)} + (2.15399)K_{\mathrm{L}}a^{(2)} \\
&\quad + (-1.37556)K_{\mathrm{L}}a^{(3)} + (-1.36647)K_{\mathrm{L}}a^{(4)} \\
&\quad + (-26.47753)\mathrm{COD}^{(\mathrm{in})} + (1.25175)T^{(\mathrm{in})} \\
c_4 &= (-2.88048)S_{\mathrm{O}}^{(3)} + (1.06803)S_{\mathrm{O}}^{(4)} + (-2.96165)S_{\mathrm{NO}}^{(4)} \\
&\quad + (-4.10911)\mathrm{MLSS} + (1.95871)K_{\mathrm{L}}a^{(1)} + (-2.71534)K_{\mathrm{L}}a^{(2)} + (0.77048)K_{\mathrm{L}}a^{(3)} + (-2.74441)K_{\mathrm{L}}a^{(4)} \\
&\quad + (73.52450)\mathrm{COD}^{(\mathrm{in})} + (-0.27567)T^{(\mathrm{in})} \\
c_5 &= (-2.99251)S_{\mathrm{O}}^{(3)} + (1.04006)S_{\mathrm{O}}^{(4)} + (-2.97401)S_{\mathrm{NO}}^{(4)} \\
&\quad + (-4.24283)\mathrm{MLSS} + (1.98108)K_{\mathrm{L}}a^{(1)} + (-2.88617)K_{\mathrm{L}}a^{(2)} + (-2.92184)K_{\mathrm{L}}a^{(3)} + (0.59870)K_{\mathrm{L}}a^{(4)} \\
&\quad + (69.65180)\mathrm{COD}^{(\mathrm{in})} + (-0.05839)T^{(\mathrm{in})}
\end{aligned} \tag{40}$$

In the above expressions, the matrix **H** is scaled with respect to the measurements such that the new matrix $\mathbf{H}_y = \mathbf{H}\mathbf{D}_y$, where $\mathbf{D}_y = \mathrm{diag}[\mathrm{span}(y)]$ and span(y) is given as the measurement range in Table 5. Note that the measurements that most affect the selected controlled variables are related to the COD at the plant inlet. The most sensitive variable to measurement change is c_2 as $\|\mathbf{H}_y(2,:)\|_2 = 210$, and c_3 is the less sensitive one with $\|\mathbf{H}_y(3,:)\|_2 = 27$. All in all, not much physical information can be inferred from the above expressions since the extend nullspace method is purely mathematical in nature.

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Table 7. Optimal Constraint Values for the Set of Disturbances in Table 4

constraint	unit	nominal	d_1	d_2	d_3	d_4	d_5	$d_{5,min}$	$d_{5,max}$
$COD^{eff} < 125$	$gCOD/m^3$	67.0	64.6	51.7	66.1	56.6	64.7	64.0	66.7
$TSS^{eff} < 30$	gSS/m^3	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0
$TN^{eff} < 18$	gN/m^3	13.3	13.0	12.7	12.8	14.8	10.3	15.8	7.3
S_{NH}^{eff}	gN/m^3	4.0	4.0	4.0	4.0	4.0	4.0	4.0	4.0
$BOD5^{eff} < 10$	$gBOD/m^3$	4.6	4.8	5.3	4.7	5.3	4.8	5.5	4.2
$Q_w < 1844.6$	m^3/d	191.4	189.0	250.9	185.7	342.0	205.1	262.3	146.2
$K_La^{(1)} < 360$	d^{-1}	122.8	117.7	83.7	123.6	67.8	145.5	51.5	148.6
$K_La^{(2)} < 360$	d^{-1}	123.0	124.4	135.8	122.2	160.7	111.3	124.2	118.3
$K_La^{(3)} < 360$	d^{-1}	100.4	102.6	124.7	99.8	148.9	91.7	110.8	102.7
$K_La^{(4)} < 360$	d^{-1}	97.2	99.7	121.0	95.4	143.8	79.8	102.5	84.7
$K_La^{(5)} < 360$	d^{-1}	88.3	89.7	103.4	85.9	125.5	62.4	87.6	56.3
$Q_a < 92230$	m^3/d	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$Q_r < 36892$	m^3/d	22922.0	24910.9	36892.0	23552.7	36892.0	22704.0	28157.0	14424.1

One can argue whether to include all five measured disturbances in the extended nullspace method using "just-enough" measurements since then there would be no need to infer the effect of disturbances from the other process measurements, which is a good "feedforward" strategy that could improve control quality. We tested this option and found that the best set of variables (to be combined) chosen by the branch-and-bound algorithm that maximized the minimum singular value of $\tilde{\mathbf{G}}^y$ were $y = [Q_r\ K_La^{(1)}\ K_La^{(2)}\ K_La^{(3)}\ K_La^{(4)}\ Q^{(in)}\ S_{NH}{}^{(in)}\ TSS^{(in)}\ COD^{(in)}\ T^{(in)}]$. Nonetheless, the nonlinear loss calculations (not detailed this time) showed this choice gives infeasible operation for disturbances d_4, d_7, and d_8 and was therefore not selected.

5. DISCUSSION

This paper focused on the application of a sensitivity analysis procedure to the BSM1/ASM1 wastewater treatment process. The work is based upon a steady-state analysis of a rigorous nonlinear model of the plant where the settler was modeled by the static one-dimension scalar mass conservation law with discontinuous fluxes, since the more traditional Takacs's model fails to represent the complex behavior of secondary settlers. The resulting mathematical representation of the settler operation under steady-state conditions brings about a smoother function that may help convergence of the computational routine used to numerically optimize the model. The goal was to minimize operational costs subject to the most important requirement of delivering effluent within the regulation constraints given in Table 3. However, some aspects of the application of the aforementioned procedure to the WWTP need to be addressed.

The nominal optimization results showed that it is economically optimal to keep effluent suspended solids and ammonia concentrations at their respective upper bounds and that no internal recirculation of sludge should be used, at least under the steady-state assumption. Indeed, optimizations based on the nonlinear model of the process for the given set of disturbances confirm that these variables are always active (see Table 7). When operating the process dynamically, one may consider using Q_a to control some internal variable so as to improve the disturbance rejection capability of the process. If these variables are controlled at their respective optimal set points (active constraint control), a choice had to be made on the selection of the remaining five degrees of freedom, and we use the sensitivity analysis based on a plantwide procedure to decide on which five variables to fixor control at their respective nominal optimum values. The exact local (linear) method and the extended nullspace method based on the concept of self-optimizing control were used to systematically select those variables such that the cumbersome combinatorial curse of choosing and testing 5 out of 28 possible variable combinations, resulting in 98 280 possible control structures, is avoided. The combination matrices **H** were easily computed using elementary matrix algebra, as described by formulas 28, 29, and 30. The only burden with those calculations lies in the computation of the optimal matrices $\mathbf{J}_{uu}$, $\mathbf{J}_{ud}$, and **F**. Since accuracy of second-order information found numerically is known to be difficult to guarantee, in addition to assuring positive definiteness of $\mathbf{J}_{uu}$, calculation of **F** might become more attractive, and a replacement formula for eq 29 was derived as in eq 32. $\mathbf{M}_n$ in this equation can be freely selected, as long as it is a nonsingular matrix, and we chose $\mathbf{M}_n = \mathbf{J}_{uu}{}^{1/2}$ so to avoid the need to compute $\mathbf{J}_{uu}$. Moreover, since the solution for **H** in eq 28 is not unique,[39] we can also find a nonsingular $n_u \times n_u$ **D** matrix such that $\mathbf{H}_{new} = \mathbf{DH}$ is another yet solution, and we can select **D** as a function of $\mathbf{J}_{uu}{}^{1/2}$; in this paper, we assumed $\mathbf{D} = \mathbf{J}_{uu}{}^{-1/2}$.

6. CONCLUSION

This paper discussed the application of a sensitivity analysis procedure for selection of economic controlled variables for optimal operation of a wastewater treatment plant. For the given modified mathematical model of the process where a new model of the settler was developed based upon the static one-dimension scalar mass conservation law with discontinuous fluxes theory, keeping the active constraints ($S_{NH}{}^{(eff)}$, $TSS^{(eff)}$, and Q_a) at their optimal values and using linear combinations of the measurements as the five remaining unconstrained degrees of freedom can guarantee near-optimal operation with minimum economic loss when operating at the nominal optimal mode despite the severe disturbances that affect the process. Future work will focus on the design of a control system for the wastewater treatment process discussed in this contribution along with the dynamic performance assessment of proposed control configurations.

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Notes

The authors declare no competing financial interest.

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