# Wastewater Treatment Plant Synthesis and Design: Combined Biological Nitrogen and Phosphorus Removal

**Noelia Alasino, Miguel C. Mussati,* Nicolás J. Scenna, and Pio Aguirre**

*INGAR Instituto de Desarrollo y Diseño (CONICET-UTN), Avellaneda 3657, S3002GJC Santa Fe, Argentina*

In the present work, a previous superstructure model developed for simultaneous optimization of the process configuration and equipment dimensions, i.e., optimal process synthesis and design and the operation conditions of activated sludge wastewater treatment plants, is extended to account for phosphorus as well as nitrogen removal. Along the activated sludge treatment process, the wastewater stream is exposed to different environmental conditions (anaerobic, anoxic, and aerated zones) in order to facilitate the different microbiological processes such as the release and uptake of phosphorus and the nitrification/denitrification processes. The Activated Sludge Model No. 3 extended with the Bio-P module for computing biological phosphorus removal is used to model the reaction compartments and the Takàcs model for representing the secondary settler. The performance criterion selected is the minimization of the net present value that includes investment and operating costs while verifying compliance with the effluent permitted limits. The problem is posed as a NLP problem, specifically a nonlinear programming problem with discontinuous derivatives DNLP. The optimization model is implemented and solved using a General Algebraic Modeling System, GAMS. Optimal configurations and designs obtained for several case studies are reported and discussed. The model itself and the resolution methodology prove to be robust and flexible enough to solve efficiently scenarios with a wide range of operation conditions, embedding conventional and nonconventional process configurations.

## 1. Introduction

In Alasino et al.[1] the optimal process synthesis and design of activated sludge wastewater treatment plants for nitrogen (N) removal based on a superstructure model was presented. Rigorous models for biochemical and settling processes aiming at plant costs minimization were considered. The natural approach to solve superstructure models is the mixed-integer nonlinear programming, MINLP, methodology. At the first developing stages of the model, this optimization problem has been posed as MINLP. However, only a small percentage of optimization runs ended up successfully verifying convergence and feasibility when applying the multiple starting point strategy. As the characteristics of this specific process allowed setting negligible lower bound values in flows and volumes, thus avoiding integer variables, the optimization problem was finally formulated as a NLP model. In addition, the cost functions found in the literature for a wastewater treatment plant design (Gillot et al.,[2] Espirito Santo et al.[3]) do not normally include fixed costs, thus avoiding integer variables in the cost model. Specifically, the problem was posed as a nonlinear programming problem with discontinuous derivatives, DNLP, due to the nonlinearities and nonsmooth functions. It was shown that the mathematical model proposed is a robust and flexible tool able to achieve quasi-optimal practical solutions.

Pontes and Pinto[4] developed a mathematical model for the synthesis of anaerobic digester networks based on the optimization of a superstructure that also relies on a nonlinear programming NLP formulation. The model contains the rigorous kinetic and hydraulic equations for up-flow anaerobic sludge blanket (UASB) and expanded granular sludge bed (EGSB) digesters. Superstructures of a single and multiple anaerobic digester networks are developed. It is also shown how complex a network becomes once the number of reactors increases and how an understanding of the wastewater treatment process is decisive to the success of the synthesis strategy. The model was implemented and optimized in GAMS using the solver BARON for global optimization and CONOPT for local optimization. In that work the global optimality of the smaller problems provides the initial points for the larger problems.

Phosphorus (P) removal is nowadays one of the key issues in many full-scale wastewater treatment plants (WWTPs). Indeed, biological P removal is often proposed in European treatment plants as an alternative to chemical P removal based on P precipitation with metal salts such as $FeCl_3$.[5] In this context, new mathematical models considering P and N removal were implemented. In a first work considering P removal (Alasino et al.[6]), optimal operation conditions for a superstructure embedding most widely used configurations for combined N and P removal aiming at minimizing operating annual costs was investigated for given wastewater specifications. In that work the plant was supposed given, and no investments costs were computed. The Activated Sludge Model No. 3 (ASM3)[7] extended with the Bio-P module[8] of EAWAG (Swiss Federal Institute for Environmental Science and Technology) was used for the description of the biological processes. As P removal is considered in these new models, more variables for components and new equations are incorporated. The superstructure is also enlarged to 7 reaction compartments, instead of 5 as in the previous work, for embedding most widely used configurations for combined N and P removal (Figure 1), because P removal processes require anaerobic conditions as well as anoxic and aerobic ones. Consequently, the mathematical models are more complex and difficult to solve.

In the present work a superstructure model developed for simultaneous optimization of the process configuration and equipment dimensions, i.e., process synthesis and design, and the operation conditions of activated sludge wastewater treatment plants in continuous operation and for given wastewater specifications and flow rate is developed to account for

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* To whom correspondence should be addressed. Tel.: +54-342-4534451. Fax: +54-342-4553439. E-mail: mmussati@santafe-conicet.gov.ar.

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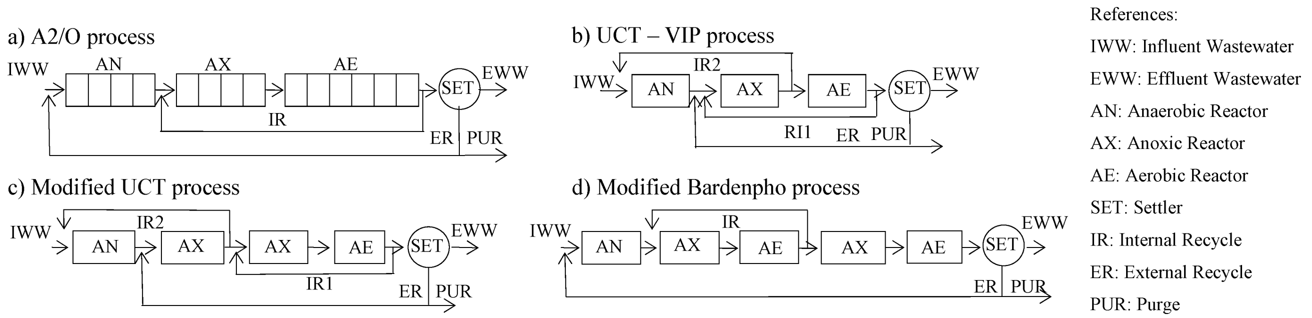

**Figure 1.** Most widely used ASWWTP configurations for combined nutrient removal.

phosphorus as well as nitrogen removal. Here, the model embeds a chain of up to seven reaction compartments in series followed by a secondary settler. It allows for flow distribution of the main process streams, i.e., bypasses and recycles among reaction compartments, sludge recycles from the sedimentation zone to any reactor, and fresh feed distribution and external carbon source dosage along the reaction zone. The settler is supposed to have fixed dimensions, as is later explained, but the reaction compartment volumes are to be optimized. Each compartment will operate in aerobic, anoxic, or anaerobic conditions according to its aeration flow rate selected and the streams fed to it. As explained in the previous work,[1] all decision variables are modeled as continuous variables and some negligible lower bounds were used when necessary to avoid numerical problems. When a reaction compartment volume and/or a streamflow rate take a zero value at a solution point, the corresponding unit and/or stream is removed from the superstructure. The objective function is to minimize the net present value, NPV, considering investment and operating costs.

## 2. Process Description

In activated sludge processes (ASPs), the influent wastewater stream is exposed to different environmental conditions (anaerobic, anoxic, and aerated zones) to facilitate the different microbiological processes such as the release or uptake of phosphorus, nitrification, and denitrification. Reduction of carbonaceous matter and nitrification (ammonium is converted to nitrate by autotrophs) are favored by aerobic conditions, while denitrification (nitrate is converted to $N_2$ gas by heterotrophs) is favored by anoxic conditions, if readily biodegradable organic matter (a C source) is available. Biological P removal relies on P uptake by aerobic heterotrophs (known as phosphate-accumulating organisms PAOs) capable of storing orthophosphate in excess of their biological growth requirements. Under anaerobic conditions, PAOs convert readily available C (e.g., volatile fatty acids) to C compounds called polyhydroxyalkanoates PHAs. PAOs use energy generated through the breakdown of polyphosphate molecules to create PHAs. This breakdown results in P release. Under subsequent aerobic or anoxic conditions, PAOs use the stored PHAs as energy to take up the P that was released in the anaerobic zone as well as any additional phosphate present in the wastewater.

Figure 1 presents the most widely used activated sludge wastewater treatment plant (ASWWTP) configurations for combined N and P removal. The A2/O process presents a sequence of anaerobic reactors to promote the growth of PAOs, followed by a sequence of anoxic ones to promote denitrification, and finally aerobic reactors. It has one internal and one external recycle stream. The internal recycle stream conducts a fraction of the nitrified liquor from the last aerobic to the first anoxic compartment, and the external recycle conducts a fraction of the sludge from the underflow of the sedimentation tank to the first compartment. In the process developed by the University of Cape Town (known as the UCT process), both recycle streams are feed to the anoxic zone and a second internal recycle stream is present from the anoxic to the anaerobic compartment. The modified UCT process has two internal recycles and one external recycle as in the original UCT process, but the anoxic zone is divided into two zones. The external recycle is directed from the underflow of the decanter to the first anoxic zone. The first internal recycle stream conducts a fraction of the nitrified liquor from the aerobic to the second anoxic zone. Finally, the second internal recycle pumps a fraction of the mixed liquor from the first anoxic back to the anaerobic compartment. The modified Bardenpho process configuration also has an external recycle from the sedimentation tank to the anaerobic zone and an internal recycle from the first aerobic zone to the first anoxic zone.

In general, addition of external C to the anoxic zone could be detrimental to P removal in an enhanced biological P removal (EBPR) plant, as the ordinary heterotrophs have competing advantages for nitrate over the denitrifying PAOs, resulting in poor anoxic P uptake. It is recommendable that the external C to be added to the anaerobic zone of an EBPR plant short of COD. The C source is taken up by PAOs to form intracellular C storage compounds, whose utilization improves both P and N removal under anoxic conditions.

## 3. Problem Definition

The problem addressed in this paper is the simultaneous optimization of the system structure (process configuration), design (equipment dimensions, i.e., reaction compartment volumes), and operating conditions (e.g., flow rate of aeration, recycles, bypasses, and external carbon source to each reaction compartment) of ASWWTPs for combined biological N and P removal and C oxidation, aiming at minimizing the NPV, given (1) defined influent wastewater specifications (composition and flow rate), (2) effluent permitted limits, (3) a process superstructure model with a maximum of seven reaction compartments and one secondary settler, and (4) a defined cost model computing operation and investment costs.

A NLP (strictly a DNLP) problem is proposed and solved for different case studies.

## 4. Models

**4.1. Proposed Superstructure Model.** The considered process superstructure is shown in Figure 2.

The superstructure embeds up to seven reaction compartments, whose volumes are to be optimized, followed by a secondary settler of fixed dimensions (cross area $A_{\mathrm{sett}}$ and height $h_{\mathrm{sett}}$). Pumps and stream mixers and splitters complete the

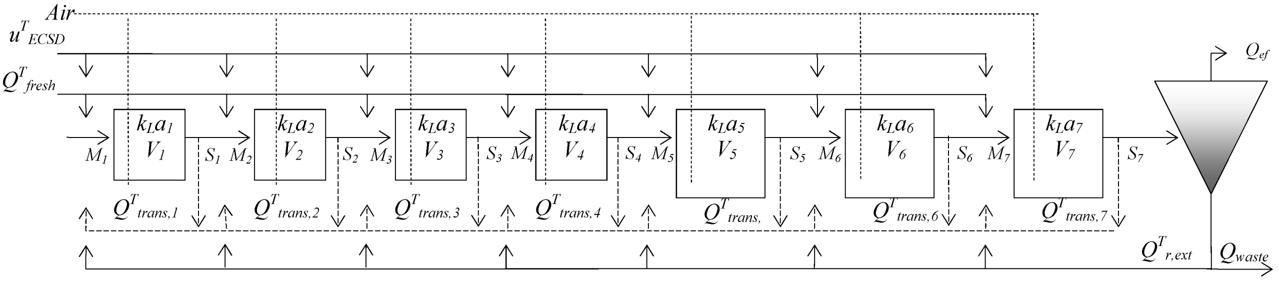

**Figure 2.** Representation of the WWTP superstructure.

superstructure and allow for flow distribution of the process streams, i.e., sludge recycles and fresh feed, and all possible connections among compartments as well as external carbon source dosage along the reaction zone. All reaction compartments are supposed to be continuous stirred tank reactor (CSTR) type.

The design variables (volume of each compartment $V_i$) are to be optimized simultaneously with the operation variables (aeration and process streams flow rates). The flow rate of the fresh feed ($Q^{T}_{\text{fresh}}$), recycle and bypass streams among compartments ($Q^{T}_{\text{trans},i}$), external (sludge) recycle stream ($Q^{T}_{r,\text{ext}}$), and external carbon source dosage ($u^{T}_{\text{ECSD}}$) can be distributed into one or more of the seven reaction compartments. The external recycle stream pumps a fraction of sludge from the secondary settler underflow back to the reaction zone. The recycle and bypass streams among compartments are indicated by $Q_{\text{trans},i}$. For example, the outcoming flow rate from reactor 2 is split in two streams: one is directed to reactor 3 (called $Q_{2,3}$) and the other called the “transverse” stream ($Q^{T}_{\text{trans},2}$). This stream ($Q^{T}_{\text{trans},2} = Q_{\text{trans},2,1} + Q_{\text{trans},2,4} + Q_{\text{trans},2,5} + Q_{\text{trans},2,6} + Q_{\text{trans},2,7}$) recycles liquor from the second to the preceding compartment ($Q_{\text{trans},2,1}$) or bypasses liquor from the second to reactors forth to seventh ($Q_{\text{trans},2,4}$, $Q_{\text{trans},2,5}$, $Q_{\text{trans},2,6}$ and $Q_{\text{trans},2,7}$) as shown in Figure 2.

The reaction compartment volumes can range from ‘zero’ to a given arbitrary maximum value. A ‘zero’ reaction compartment volume indicates that it is eliminated from the superstructure, as explained in the previous work.[1] Finally, reaction compartments can operate under anoxic, aerobic, or anaerobic conditions, depending on the optimal value computed for the oxygen transfer coefficient $k_{\text{L}}a$, and the conditions developed in each compartment. If the $k_{\text{L}}a$ value for a given compartment is zero, an anoxic or anaerobic reactor is selected, depending on the nitrate and nitrite concentration ($S_{\text{NO}}$) reached.

When a decision variable (such as a compartment reaction volume and/or a process streamflow rate) takes at the solution point zero value or the (negligible) lower bound value set for numerical convenience, the corresponding unit and/or stream is not included as part of the resultant final process configuration (flow sheet). It should be noted that this process component is “physically removed” from the flow sheet but not in the sense that its equations (mathematical representation) are eliminated from the mathematical model of the superstructure.

The preference for a given plant configuration over the others depends on the influent wastewater flow rate and composition, the cost functions used, and several economical and technological aspects and trade offs. It is clear that the conventional processes described in section 2 are embedded in the superstructure and, hence, are candidates for the optimal flow sheet resulting from the assumed hypotheses.

**4.2. Process Units Models.** For the aeration tanks, steady-state continuous stirred tank reactors (CSTR) are considered. The Activated Sludge Model No. 3 (ASM3)[7] extended with the Bio-P module[8] is chosen as the biological process model. This model considers removal of the carbonaceous matter and nitrogen and phosphorus compounds. The ASM3 model extended with the Bio-P module considers 17 compounds ($C_x$), which are divided into soluble compounds and particulate compounds, whose concentrations are indicated by $S$ and $X$, respectively, and involves 23 transformation processes. The kinetic constants used are those calculated to 15 °C based on the calibrated EAWAG BioP module parameter values at 20 °C and their temperature coefficient values $\theta_{\text{T}}$, using the function given by Gujer et al.[7] A summary of the reactor model equations is presented in Appendix A.1.

As explained above, to avoid numerical problems (e.g., division by zero) very small (negligible) lower bound values are set for reaction compartment volumes ($V_{i,\min} = 0.01$ m$^3$) and oxygen mass transfer coefficients ($k_{\text{L}}a_{i,\min} = 0.0001$ day$^{-1}$). If a $k_{\text{L}}a_i$ value reaches its lower bound value in the optimal solution, it is considered zero and, consequently, the corresponding reaction compartment is assumed to be anoxic or anaerobic.

The secondary settler is modeled as a nonreactive settling tank subdivided into 10 layers of equal thickness using the double-exponential settling velocity model.[9] A more detailed description of the settler model can be found in the previous work.[1] A fixed settler depth $h_{\text{sett}}$ of 4 m, a feed point allocation at the sixth layer from the bottom, and a cross area $A_{\text{sett}}$ of 1500 m$^2$ are adopted. These assumptions are justified considering the recommended design criteria in practice and a few difficulties found in the settler modeling. Specifically, considering the 10-layer one-dimensional settler model of Takàcs with a 0.4 m thick each layer, a 4 m deep settler results. From a modeling point of view, it would be impossible to have a converged model of the whole plant by defining the thickness of each settler layer as a decision variable. Then, at first, the settler height was fixed, but the settler cross area was defined as a decision variable fixing an upper bound of 1500 m$^2$ in order to keep the height-to-diameter ratios to recommended practical values. In almost all optimal solutions found for the case studies analyzed, the computed settler area was at its upper bound value. For higher upper bound values, a small percentage of initial points led to numerical convergence and/or kept feasibility. Therefore, in order to gain robustness and simplify the model, both settler dimensions were fixed based on a practical design criterion i.e., keeping the height-to-diameter ratio at the recommended value. It should be noted that this assumption is valid since the process scale is the same order as the considered benchmarks, in which those settler dimensions are adopted. The remaining process units and equipment model equations such as stream mixer and splitter are also summarized in Appendix A.1.

**4.3. Optimization Model. 4.3.1. Objective Function.** Here, the net present value (NPV) is adopted as the objective function

**Table 1. Influent Wastewater Specifications for Case Study I.A**

| component | value | component | value |
|---|---|---|---|
| $S_I$ (g of COD m$^{-3}$) | 30.00 | $S_{NOX}$ (g of N m$^{-3}$) | 0.00 |
| $S_S$ (g of COD m$^{-3}$) | 69.50 | $S_{N2}$ (g of N m$^{-3}$) | 0.00 |
| $X_I$ (g of COD m$^{-3}$) | 51.20 | $S_{NH}$ (g of N m$^{-3}$) | 40.60 |
| $X_S$ (g of COD m$^{-3}$) | 202.3 | $S_{ALK}$ (g of COD m$^{-3}$) | 7.00 |
| $X_H$ (g of COD m$^{-3}$) | 28.17 | $S_{PO4}$ (g of P m$^{-3}$) | 9.01 |
| $X_A$ (g of COD m$^{-3}$) | 0.00 | $X_{PAO}$ (g of COD m$^{-3}$) | 0.00 |
| $X_{STO}$ (g of COD m$^{-3}$) | 0.00 | $X_{PHA}$ (g of COD m$^{-3}$) | 0.00 |
| $X_{SS}$ (g of SS m$^{-3}$) | 215.5 | $X_{PP}$ (g of P m$^{-3}$) | 0.00 |
| $S_O$ (g of COD m$^{-3}$) | 0.00 | $Q^T{}_{fresh}$ (m$^3$ day$^{-1}$) | 18446 |

to be minimized. An equations summary of the cost and performance models is presented in Appendix A.2.

**4.3.2. Specification Constraints.** The effluent threshold values used as specification constraints are as follows:[1,5] $S_{NH,ef} = 4$ g of N m$^{-3}$, $P_{TOT,ef} = 1.5$ g of P m$^{-3}$, $N_{TOT,ef} = 18$ g of N m$^{-3}$, $BOD_{ef} = 10$ g of COD m$^{-3}$, $COD_{ef} = 100$ g of COD m$^{-3}$, $X_{SS,ef} = 30$ g of SS m$^{-3}$. These values are the same as those used in Alasino et al.,[1] except for $P_{TOT,ef}$, which is proposed by Gernaey and Jorgensen[5] based on the Danish effluent standard for P.

**4.3.3. Maximum Values for Operation Variables.** The maximum values of operation variables have been chosen according to the limit values recommended in practice:[5,10] $Q^T{}_{r,ext} = 36\,892$ $(=2Q^T{}_{fresh})$ m$^3$ day$^{-1}$, $Q^T{}_{trans,i} = 92\,230$ $(=5Q^T{}_{fresh})$ m$^3$ day$^{-1}$, $Q_{waste} = 1844.6$ $(=0.1Q^T{}_{fresh})$ m$^3$ day$^{-1}$, $u_{ECSD} = 2000$ kg of COD day$^{-1}$, $k_La_i = 360$ day$^{-1}$.

## 5. Case Studies

Two different scenarios are selected (I and II), which differ in the optimization problem to be solved. Each scenario is solved in turn for a variety of cases, which differ in the influent wastewater specifications. The considered case studies allow showing the model capacities, mainly its robustness and flexibility.

In case study I, the superstructure model described above is used for simultaneous optimization of the process configuration and equipment dimensions, i.e., process synthesis and design, and the operation conditions for three given wastewater flow rate levels.

The influent wastewater components concentrations used in case I.A are the original flow-weighted average dry weather influent concentrations proposed in the COST (European Cooperation in the Field of Scientific and Technical Research) benchmark[10] for the ASM1 model, modified here to make them compatible with the ASM3+BioP model in order to have the same biodegradable total N $(= TKN - i_{N,SI}\,S_I - i_{N,XI}\,X_I)$

$$\begin{aligned}(S_{NH})_{ASM3+BioP} = {} & (S_{NH} + S_{ND} + X_{ND})_{ASM1} - \\ & (i_{N,SS}S_S + i_{N,XS}X_S)_{ASM3+BioP} + \\ & ((i_{N,BM})_{ASM1} - (i_{N,BM})_{ASM3+BioP})(X_H + X_A + X_{PAO})\end{aligned} \tag{1}$$

The influent $PO_4{}^{=}$ concentration ($S_{PO}$) has been taken from Gernaey and Jorgensen.[5] On the basis of the COST benchmark,[5,10] the influent wastewater flow rate for case I.A is set at 18 446 m$^3$ day$^{-1}$. Table 1 shows the influent wastewater specifications for case study I.A.

A sensitivity analysis of some selected model parameters was made for the locally optimal solution obtained for case I.A (results discussed in section 7.1). The most relevant model parameter was the influent wastewater flow rate. On this basis, case studies I.B and I.C are defined by decreasing and increasing the influent flow rate 25% with respect to case I.A, respectively. Optimal solutions resulting from each case are then compared and analyzed.

In case study II, the WWTP configuration is given and the equipment size is fixed; consequently, the investment cost $IC^T$ is fixed. The model is used for optimization of the operation conditions aiming to minimize the $OC^T$ using different influent wastewater compositions. Specifically, the optimal plant configuration previously obtained in case I.A is here supposed given, and some relevant influent wastewater component concentrations (detected from the sensitivity analysis) are decreased and increased up to 25%, keeping the influent wastewater flow rate at 18 446 m$^3$ day$^{-1}$ as in case I.A.

A multiple starting points strategy for model initialization was adopted for each case, and as in the previous work,[1] several locally optimal solutions were found depending on the initial values set. Moreover, networks with two or more reactors of the same type could present solutions with the same objective function value and different combinations of reactors.[1,4] Here, this characteristic has also been found in most of the analyzed examples, as expected.

The WWTP configurations that result from the proposed superstructure model showing the minimal NPV values, using a multiple starting points strategy for problem initialization, are represented and shown in the respective figures and tables. The optimal values of the main variables and costs are included for each case.

## 6. Computational Aspects

The optimization models were implemented in GAMS[11] and solved with the code CONOPT,[12] which is a local optimization solver. As previously discussed, a multiple starting points strategy for model initialization was adopted for each case.

The GAMS model statistics resulted in 293 blocks of equations, 874 single equations, 258 blocks of variables, 963 single variables, 6445 nonzero elements, 4460 nonlinear N-Z, 25 derivative pool, and 65 constant pool. The total time needed to solve the models was around 80 s on an Intel Pentium IV of 2.40 GHz CPU with 248 MB of RAM.

## 7. Results and Discussion

**7.1. Case Study I.** The DNLP model presented in section 4 is solved for WWTP synthesis and design considering the influent wastewater component concentrations listed in Table 1 and an influent wastewater flow rate of 18 446, 13 834.5, and 23 057.5 m$^3$ day$^{-1}$ for subcases I.A, I.B, and I.C, respectively. The WWTP configurations showing the minimal NPV values for cases I.A, I.B, and I.C are represented in Figure 3a, 3b, and 3c, respectively, while Table 2 shows the effluent concentrations, main variables optimal values, and costs. A detailed list of computed costs for the optimal solution for each subcase is presented in Table 3.

**Analysis of Case I.A.** As shown in Figure 3a, optimization of case I.A results in a configuration with six reaction compartments with volumes of 3941, 1237, 2994, 776, 609, and 5117 m$^3$, that is, the optimal configuration includes six of the seven available reaction compartments. The last compartment volume achieves the negligible lower bound value, then "eliminated" from the process superstructure, and then not included in the figure that represents the final flow sheet. The second, fourth, and fifth compartments were aerated. Hereafter, the aerobic zones are considered as those that were aerated, i.e., $k_La > 0$; as such, the terms "aerated" and "aerobic" are used indistinctly in this work. By evaluating the environmental conditions of the

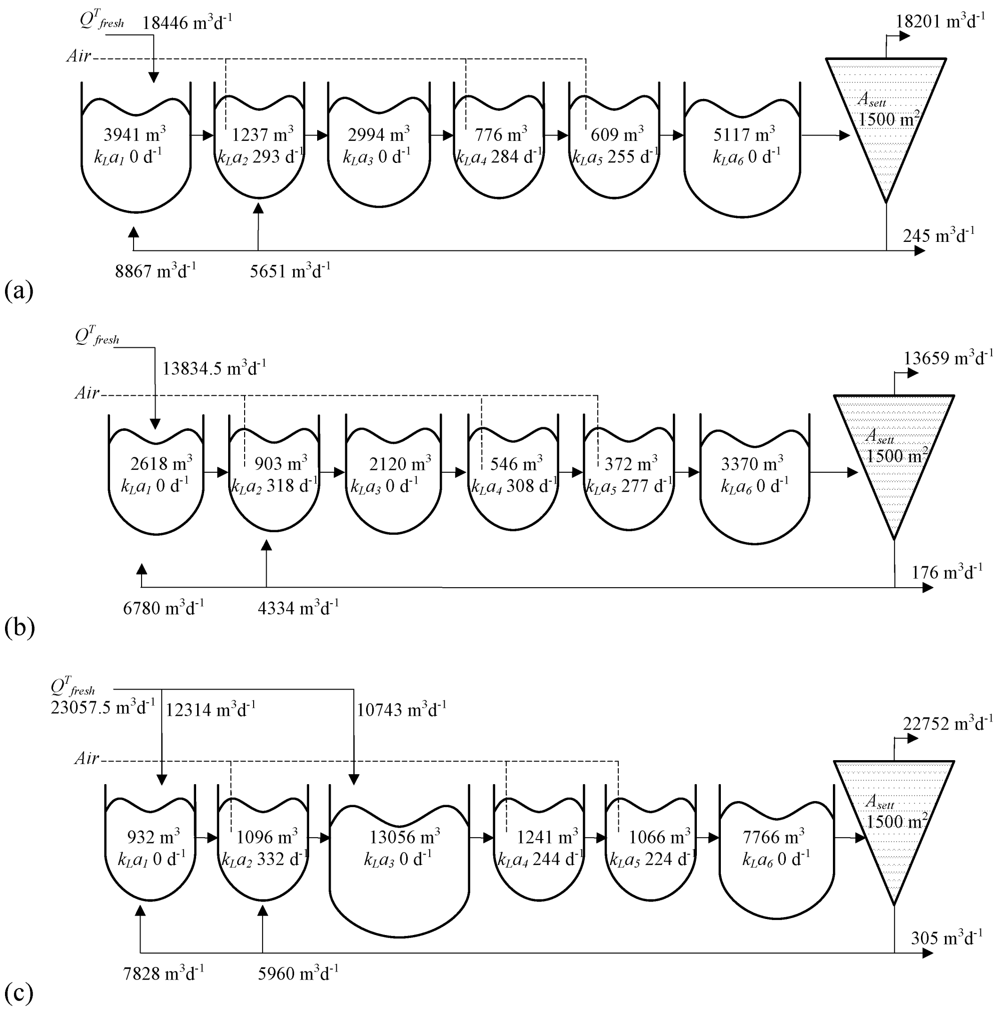

**Figure 3.** Optimal configuration and main process variable values for (a) case I.A (solution I.A), (b) case I.B (solution I.B), and (c) case I.C (solution I.C).

**Table 2. Main Variables Optimal Values for (a) Case I.A (solution I.A), (b) Case I.B (solution I.B), and (c) Case I.C (solution I.C)**

| | a | b | c |
|---|---|---|---|
| effluent contaminant | solution I.A | solution I.B | solution I.C |
| $S_{\mathrm{NH,ef}}$, g of N m$^{-3}$ | 3.34 | 3.09 | 3.94 |
| $N_{\mathrm{TOT,ef}}$, g of N m$^{-3}$ | 5.37 | 5.07 | 5.93 |
| $P_{\mathrm{TOT,ef}}$, g of P m$^{-3}$ | 1.50 | 1.50 | 1.50 |
| BOD$_{\mathrm{ef}}$, g m$^{-3}$ | 1.67 | 1.55 | 1.75 |
| COD$_{\mathrm{ef}}$, g of COD m$^{-3}$ | 45.00 | 43.91 | 45.62 |
| $X_{\mathrm{SS,ef}}$, g of SS m$^{-3}$ | 15.05 | 13.90 | 15.68 |
| costs (Euros) | | | |
| OC$^{\mathrm{T,Annual}}$ | 561 979 | 409 576 | 718 557 |
| IC$^{\mathrm{T}}$ | 3 311 404 | 2 853 878 | 3 836 174 |
| NPV | 10 313 672 | 7 957 202 | 12 789 395 |

other compartments, the WWTP consists of a sequence of compartments with the following characteristics: *Ana-Ae-Anox-Ae-Ae-Anox*. It should be noted that there is not any kind of indicator defined in the model that defines clearly the anaerobic from the anoxic zones. In this work, it is assumed that anaerobic conditions prevail over anoxic conditions in a particular reaction zone with respect to another one in the same configuration by inspecting the $S_{\mathrm{NO}}$, the variation of $S_{\mathrm{NH}}$, $S_{\mathrm{NO}}$, and $S_{\mathrm{PO}}$ entering and leaving the reactor, and the relative reaction rates of the biological stages in that zone: denitrification or anoxic growth ($\rho_5$), nitrification or anoxic growth of autotrophs ($\rho_{10}$), anaerobic storage of polyhydroxyalkanoates $X_{\mathrm{PHA}}$ or phosphate release ($\rho_{\mathrm{p1}}$), aerobic storage of poliphosphate $\mathrm{X_{PP}}$ or phosphate uptake ($\rho_{\mathrm{p2}}$), and anoxic storage of poliphosphate $X_{\mathrm{PP}}$ or phosphate uptake ($\rho_{\mathrm{p3}}$). The optimal solution considers the flow distribution of the external recycle stream directing around 61% of the flow rate (8867 m$^3$ day$^{-1}$) to the first compartment and the rest to the second one. No feed distribution is necessary, and no external carbon source is dosed. As shown in Table 2a, only the $P_{\mathrm{TOT,ef}}$ concentration achieves the effluent threshold value.

In the previous work,[1] the synthesis and design for nitrogen removal processes, i.e., without considering P compounds, for similar wastewater concentration specifications and flow rate, and optimizing a superstructure of only 5 reaction compartments, resulted in three reaction compartments with volumes of 1083 (moderately aerated, $k_{\mathrm{L}}a = 218$ day$^{-1}$), 9096 (slightly aerated, $k_{\mathrm{L}}a = 36$ day$^{-1}$), and 6099 m$^3$ (slightly aerated, $k_{\mathrm{L}}a = 27$ day$^{-1}$), respectively. The flow distribution of the influent feed stream

**Table 3. Costs Computed for Case Studies I.A, I.B, and I.C (in Euros)**

| | OC$^{\mathrm{T}}_{\mathrm{EQ}}$ | OC$^{\mathrm{T}}_{\mathrm{pump}}$ | OC$^{\mathrm{T}}_{\mathrm{a}}$ | OC$^{\mathrm{T}}_{\mathrm{SLDGD}}$ | OC$^{\mathrm{T}}_{\mathrm{ECSD}}$ | OC$^{\mathrm{T}}$ | IC$_{\mathrm{t}}$ | IC$_{\mathrm{a}}$ | IC$_{\mathrm{set}}$ | IC$_{\mathrm{ips}}$ | IC$_{\mathrm{sr}}$ | IC$^{\mathrm{T}}$ | NPV |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| I.A | 2 447 112 | 183 942 | 1 955 715 | 2 415 500 | 0 | 7 002 268 | 2 382 674 | 181 764 | 442 671 | 268 985 | 35 310 | 3 311 404 | 10 313 672 |
| I.B | 1 754 083 | 140 673 | 1 382 413 | 1 826 155 | 0 | 5 103 324 | 1 990 801 | 159 838 | 442 671 | 228 013 | 32 555 | 2 853 879 | 7 957 203 |
| I.C | 3 247 593 | 175 603 | 2 491 568 | 3 038 457 | 0 | 8 953 221 | 2 850 991 | 201 830 | 442 671 | 305 922 | 34 760 | 3 836 174 | 12 789 395 |

was computed directing 56% of the influent flow rate (10 360 $m^3$ $day^{-1}$) to the first compartment and the rest to the second one, and an external sludge recycle of 11 841 $m^3$ $day^{-1}$ conducted to the first reaction compartment was obtained. It is clear that the total reaction volume (sum of all compartment volumes) there computed is similar to the one obtained here for case I.A. As in that case, P compounds and the microorganisms for P removal ($X_{PAO}$) were not considered; only 3 reaction compartments for facilitating conditions to N removal were needed. As P removal is here targeted, an anaerobic compartment is essential to develop the environmental conditions for the P release stage of the P removal process. As carbonaceous matter is metabolically required for P as well as for N removal processes, i.e., for P release and uptake processes and for the nitrification/denitrification processes, there is a shortage of carbonaceous matter; this fact determinates an effluent quality not so good as in previous work. Since the effluent ammonium concentration $S_{NH}$ is higher for this case and the P compounds are considered, a worse effluent quality index EQ and consequently a higher cost due to fines are computed. In addition, the amount of sludge produced for disposal is higher, thus increasing sludge treatment cost. All this results in an increased NPV for combined N and P removal (10 313 672 Euros) with respect to N removal only (7 473 917 Euros) for the scenario analyzed.

Following, the WWTP configuration and operation conditions for combined N and P removal proposed by Gernaey and Jorgensen[5] is evaluated via simulation for equivalent wastewater specifications using the cost model and effluent permitted limits here considered. The goal is to compare the open-loop steady-state performance of that plant with the optimal configuration obtained for case I.A. Briefly, that plant consists of 7 biological tanks of 500, 750, 750, 750, 1333, 1333, and 1333 $m^3$, with $k_La$ values of 240 $day^{-1}$ for tanks 5 and 6 and 60 $day^{-1}$ for tank 7. The reaction zone is in series with a sedimentation tank with a volume of 6000 $m^3$, an area of 1500 $m^2$, and a depth of 4 m. It presents a nitrate (or internal) recycle from the seventh to the third tank at a flow rate of 300% of the influent flow rate (55 338 $m^3$ $day^{-1}$), a sludge (or external) recycle from the underflow of the sedimentation tank to the first tank at a flow rate of 100% of the influent flow rate (18 446 $m^3$ $day^{-1}$), and a wasted sludge flow rate of 400 $m^3$ $day^{-1}$.

The total *annual* operating cost $OC^{T,Annual}$ computed here by optimization decreases around 31% with respect to the computed by simulation of that plant (561 979.79 vs 818 473.79 Euros/year, results not shown). Moreover, the optimal solution obtained meets the effluent limits while the other one does not ($S_{NH,ef}$ = 4.16 g of N $m^{-3}$ and $P_{TOT,ef}$ = 5.28 g of P $m^{-3}$). As the cost model considered is only valid when the effluent limits are met, the estimated $OC^{T,Annual}$ of 818 473.79 Euros/year should be larger using a cost model considering "extra" fines for violating the effluent quality limits (see Vanrolleghem et al.[13] for details). Taking into account the investment cost, IC, the NPV obtained by optimization (10 313 672.27 Euros) decreases around 21% with respect to the simulated WWTP (12 996 271.59 Euros). It should be noted that the IC itself is higher for the optimized plant (3 311 404.11 vs 2 798 088.22 Euros) as it is related to the process units size.

**Sensitivity Analysis for Solution I.A.** A sensitivity analysis of the optimal solution obtained for case I.A is presented and discussed. Some critical model parameters related to cost functions, influent wastewater specifications (concentration and flow rate), and effluent permitted limits are selected for this analysis. The sensitivity analysis is based on a local sensitivity method.[14] It computes local gradients of the objective function Φ with respect to infinitesimal variations of a parameter $p_i$. The analysis is focused on the marginal values $MV_i$ (eq 2) and relative marginal values $RMV_i$ (eq 4) for each parameter $p_i$. In this case, the objective function Φ is the net present value NPV (eq 3)

$$MV_i = \frac{\partial \Phi}{\partial p_i} \tag{2}$$

$$\Phi = NPV \tag{3}$$

$$RMV_i = \frac{\partial\Phi/_{\Phi}}{\partial p_i/_{p_i}} = MV_i \cdot \frac{p_i}{\Phi} \tag{4}$$

Then, the marginal value $MV_i$ represents the variation in the NPV for a unitary increment in the parameter $p_i$. The $RMV_i$ is the perceptual variation in the NPV for a perceptual increment in the parameter $p_i$. The sign of $RMV_i$ indicates the direction of the change in the NPV. A positive $RMV_i$ indicates an increase in the NPV when increasing the corresponding parameter value. Each marginal value $MV_i$ can be directly obtained from the GAMS output file (filename.LST) by inspecting "parameter_investigated.M" at the solution point. The corresponding relative marginal value $RMV_i$ is then computed by multiplying $MV_i$ by the factor $p_i/\Phi$ (eq 4).

Table 4 lists the values and he RMVs for the model parameters *p* considered. They are ranked according to their descending *absolute* RMVs, reflecting their relative importance.

It can be seen that the fresh wastewater flow rate $Q^T{}_{fresh}$ is the most sensitive parameter for this locally optimal solution (RMV = +0.934). This analysis confirms that a slight increment in the influent concentration of the relevant contaminants, ammonium $S_{NH,fresh}$ (RMV = +0.602) or phosphorus $S_{PO,fresh}$ (RMV = +0.357), would increase the NPV. This is due to the fact that more N or P content has to be removed from a medium where the carbonaceous organic matter necessary to promote the N and P removal processes is scarce. On the other hand, an increment in the influent concentration of slowly biodegradable organic matter $X_{S,fresh}$ (RMV = −0.528) or readily biodegradable organic matter $S_{S,fresh}$ (RMV = −0.117) would paradoxically decrease the NPV since they are also contaminants. Consequently, they deteriorate the influent wastewater quality. In this case, however, they positively contribute with more carbonaceous organic matter required for N and P removal processes.

**Table 4. Sensitivity Analysis Values of Solution I.A**

| parameter | value | RMV | parameter | value | RMV |
|---|---|---|---|---|---|
| $Q^T{}_{fresh}$ | 18 446 | 0.939 | $b_{ips2}$ | 2123 | 0.007 |
| $S_{NH,fresh}$ | 40.601 | 0.602 | $b_{sett2}$ | 6338 | 0.007 |
| $X_{S,fresh}$ | 202.32 | −0.528 | $b_{sr}$ | 5038 | 0.003 |
| $X_{SS,fresh}$ | 215 | 0.378 | $b_{ips3}$ | 3090 | 0.003 |
| $S_{PO,fresh}$ | 9.01 | 0.357 | $X_{A,fresh}$ | 0 | |
| $\alpha_{EQ}$ | 50 | 0.237 | $X_{PHA,fresh}$ | 0 | |
| $\alpha_{PSLDG}$ | 75 | 0.234 | $X_{PAO,fresh}$ | 0 | |
| $b_t$ | 10 304 | 0.231 | $X_{STO,fresh}$ | 0 | |
| $\alpha_E$ | 25 | 0.207 | $S_{O,fresh}$ | 0 | |
| $S_{S,fresh}$ | 69.5 | −0.117 | $S_{NO,fresh}$ | 0 | |
| $S_{HCO,fresh}$ | 7 | −0.071 | $X_{PP,fresh}$ | 0 | |
| $P_{TOT,lim}$ | 1.5 | −0.068 | $\alpha_{ECSD}$ | 109.5 | 0.0 |
| $S_{I,fresh}$ | 30 | 0.040 | $S_{NH,ef,lim}$ | 4 | 0.0 |
| $b_{sett1}$ | 2630 | 0.036 | $DBO_{ef,lim}$ | 10 | 0.0 |
| $b_a$ | 8590 | 0.018 | $DQO_{ef,lim}$ | 100 | 0.0 |
| $b_{ips1}$ | 2334 | 0.016 | $S_{N2,fresh}$ | 0 | |
| $X_{I,fresh}$ | 51.2 | 0.013 | $N_{TOT,lim}$ | 18 | 0.0 |
| $X_{H,fresh}$ | 28.17 | 0.009 | $TSS_{ef,lim}$ | 30 | 0.0 |

The most critical operation cost parameter corresponds to the fines to be paid due to the effluent quality $\alpha_{EQ}$ (RMV = +0.237), followed closely by the cost parameter associated to the sludge treatment $\alpha_{PSLDG}$ (RMV = +0.234) and by that related to the energy demand for pumping and aeration $\alpha_E$ (RMV = +0.207). The RMV of the cost parameter related to the external carbon dosed $\alpha_{ECSD}$ is zero for this local solution, i.e., the objective function is insensitive to its variation, as that resource is not utilized in this solution.

Regarding the investment costs, the parameter $b_t$ related to the reaction compartments volume is the most critical one (RMV = +0.231), followed by the decanter cost parameter $b_{sett,1}$ (RMV = +0.0363). The NPV does not show a significant sensitivity with respect to the other investment cost parameters (RMVs < 0.0178).

The most important permitted limit corresponds to the effluent total phosphorus $P_{TOT,lim}$ (RMV = −0.0678), being the most difficult threshold to meet for this case. Clearly, its negative value indicates that a higher limit value would decrease the NPV, resulting in a less demanding scenario. Indeed, by inspecting the optimal solution values (Table 2), it is observed that the effluent total P concentration $P_{TOT,ef}$ reaches its limit ($P_{TOT,lim}$ = 1.5 g of P m$^{-3}$), being the limiting contaminant. This result agrees with the fact that the RMV of the other permitted limits ($S_{NH,ef,lim}$, $DBO_{ef,lim}$, $DQO_{ef,lim}$, $N_{TOT,lim}$, and $TSS_{ef,lim}$) are zero, meaning that the objective function is not sensitive to their variations around the optimal solution point. From the treatment point of view, it is an indication of how far the system operates from the effluent limits.

Because several model parameters, mainly influent WW specifications such as $X_{A,fresh}$, $X_{PAO,fresh}$, $S_{NO,fresh}$ and $S_{O,fresh}$, are zero, their RMVs cannot be computed as defined above. However, their marginal values MVs (not shown) indicate qualitatively their effect on the NPV. Similarly, a negative MV value for a given parameter indicates an improved NPV around the solution point.

**Analysis of Case I.B.** The fresh flow rate $Q^T_{fresh}$ is set to 13 834.5 m$^3$ day$^{-1}$ instead of 18 446 m$^3$ day$^{-1}$ as in case I.A, i.e., 25% lower. The optimal solution for case I.B is represented in Figure 3b and Table 2 (column b). This solution resulted in six reaction compartments with volumes of 2618, 903, 2120, 546, 372, and 3370 m$^3$. The total influent wastewater flow rate and 61% of the recycle sludge are fed to the first compartment. The remaining recycle streamflow rate is fed to the second compartment. In this configuration, the second, fourth, and fifth compartments are aerated. According to the prevailing conditions, the sequence of compartments was *Ana-Ae-Anox-Ae-Ae-Anox*. No external carbon source is dosed to the process. As shown in Table 2 (column b), the $S_{PO}$ effluent concentration is also at the effluent threshold value.

The NPV is lower than case A, as expected. The operation costs decrease by 27%, the investment costs by 14%, and the NPV by around 23%. However, the solution obtained has some similarities with solution A. The aerated compartments have the smallest volumes and are also located at the second, fourth, and fifth places. The anoxic compartments take the third and last places and the anaerobic the first one. The external recycle sludge (which is the microorganism's source but also a $S_{NO}$ source) is distributed to the first and second compartments. The fresh wastewater is completely fed to the first reactor, making it develop anaerobic conditions and taking advantage of more readily biodegradable matter ($S_S$) available for the phosphorus-accumulating organisms ($X_{PAO}$) and, consequently, more efficiently used for $S_{PO}$ released, improving the P removal process efficiency.

**Analysis of Case I.C.** The influent flow rate is increased 25% with respect to case I.A, i.e., from 18 446 to 23 057.5 m$^3$ day$^{-1}$. Figure 3c and Table 2 (column c) show the optimal WWTP configuration and operation conditions obtained. Solution I.C consists of six reaction compartments with volumes of 932, 1096, 13 056, 1241, 1066, and 7766 m$^3$. Around 53% of the influent wastewater flow rate is fed to the first compartment, and the rest to the third one; 57% of the recycle streamflow rate is directed to the first compartment and the remaining 43% to the second compartment. In this configuration, the second, fourth, and fifth compartments are aerated, and according to the prevailing conditions, the sequence of compartments is as follows: *Ana-Ae-(Anox/Ana)-Ae-Ae-Anox*. No external carbon source is dosed, and only the $P_{TOT,ef}$ concentration is at its effluent threshold value. As expected, the NPV is higher than case I.A. The operation costs increase by 28%, the investment costs by 16%, and the NPV by around 24%. Differing from cases I.A and I.B, here the fresh wastewater stream is distributed to the first and third compartments. However, this solution has similarities with solution I.A and I.B. The external sludge recycle is distributed to the first and second compartments. The aerated compartments present the smallest volumes and are placed in the same sequence. The anaerobic compartment is the first one. The anoxic compartment is located at the last place, while a large and hybrid anaerobic/anoxic compartment is placed at the third one.

**7.2. Case Study II.** Here, the WWTP configuration and equipment sizes are supposed given. The goal is optimization of the operation conditions that minimize the annual operation costs, instead of the net present value, using different influent wastewater *compositions*. Specifically, the optimal WWTP configuration obtained for case I.A is selected and supposed given (Figure 3a; Table 2, column a), thus fixing the investment cost. The analysis is focused on the three most relevant influent component concentrations identified from the sensitive analysis performed for solution I.A (Table 4). The concentration of the influent ammonium $S_{NH,fresh}$, slowly biodegradable substrates $X_{S,fresh}$, and inorganic soluble phosphorus $S_{PO,fresh}$ are varied from ±5 to ±25% with respect to the value selected for cases I, keeping the influent flow rate at 18 446 m$^3$ day$^{-1}$ as in case I.A.

The optimal volumes of the six compartments (Figure 3a) determine an investment cost $IC_t$ of 2 382 674 Euros. The investment cost for the three aeration systems required is computed considering an aeration capacity based on a *maximum* $k_La$ value of 360 day$^{-1}$, resulting in 191 042 Euros. It should be noted that this cost is higher than that shown in Table 3 for case I.A ($IC_a$ = 181 764 Euros) since that one was computed based on the *optimal* $k_La$ values (293, 285, and 255 day$^{-1}$). Analogously, the investment cost for the sludge recycle pump $IC_{sr}$ is computed for a *maximum* capacity of $2Q^T_{fresh}$, resulting in 46 884 Euros, which is higher than in solution I.A (35 310 Euros) since that was based on the *optimal* value of the recycle ratio ($0.787Q^T_{fresh}$). As the secondary settler cross area is fixed at 1500 m$^2$, its investment cost $IC_{sett}$ is 442 671 Euros. Finally, the influent wastewater flow rate is fixed at 18 446 m$^3$ day$^{-1}$, resulting in a pumping station investment cost $IC_{ips}$ of 268 985 Euros. Then, the total investment cost $IC^T$ is 3 332 256 Euros.

In the process superstructure model, the units are interconnected through mixers and splitters in such a way to allow flow distribution patterns of the main streams (e.g., fresh wastewater,

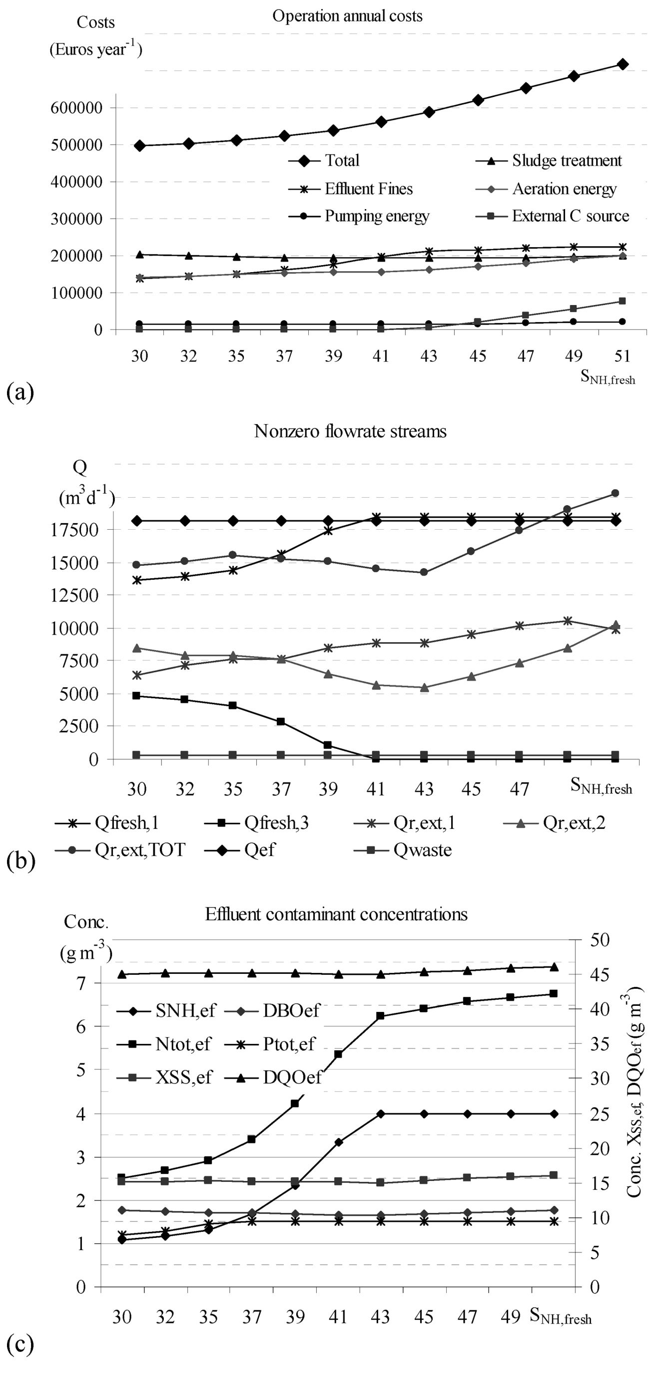

**Figure 4.** Optimization results by varying $S_{NH,fresh}$ concentration for case study II: (a) Annual operating costs, (b) nonzero flow rate streams, and (c) effluent contaminants concentration.

internal recycles and bypasses among compartments, external recycles, and external carbon) but the investment costs related to those accessories are not considered; however, their related operating costs are computed.

Figure 4 shows the optimization results obtained by varying the influent ammonium concentration $S_{NH,fresh}$. The total annual operating cost $OC^{T,Annual}$ increases with the $S_{NH,fresh}$ concentration (Figure 4a). The variation of the fines to be paid due to the effluent quality $OC_{EQ}$ is the most relevant operating cost variation, followed by that related to the external carbon dosed $OC_{ECSD}$ and the energy demand for aeration $OC_a$.

For a 5% increment in $S_{NH,fresh}$ with respect to the reference value (40.60 g of N $m^{-3}$), Figure 4c shows that the effluent $S_{NH}$ reaches its effluent threshold value (4 g of N $m^{-3}$). Figure 4a shows that the fines incurred increase considerably for that variation. However, for higher increments in $S_{NH,fresh}$, the fines $OC_{EQ}$ increase more slightly since the effluent quality deterioration is due to other contaminants present and not to the ammonium, as it has already reached the permitted limit imposed. The cost weighting factors of the other contaminants are comparatively lower than the ammonium's one, leading then to a smoother EQ variation.

The treatment of a fresh stream that is progressively more contaminated with ammonium determines a progressive increase of other cost items involved in the total annual operation cost. Indeed, if $S_{NH,fresh}$ is progressively increased with respect to case I.A, an amount of an external carbon source has to be added to the system and the aeration flow increased to fulfill the effluent permitted limits, increasing their related costs (Figure 4a).

For a 5% increment in $S_{NH,fresh}$ with respect to case I.A, Figure 4b shows a decrement in the external recycle flow rate ($Q^{T}_{r,ext}$), determining an increment in the retention times in the compartments. However, for higher increments in $S_{NH,fresh}$, the tendency changes, resulting in increased external recycle flow rates.

On the other hand, if $S_{NH,fresh}$ is progressively decreased with respect to the referential case I.A, no external carbon is dosed and the aeration requirements decreased, which is reflected by their respective costs in Figure 4a, and as expected, a progressive decrement in the incurred fines is observed since the influent wastewater has a lower content of a main contaminant. In addition, Figure 4b shows that the flow rate fractions of the fresh stream and the recycle sludge both fed to the first compartment ($Q_{fresh,1}$ and $Q_{r,ext,1}$, respectively) decreased, increasing the retention time in the anaerobic compartment, thus improving the P removal process efficiency, as can be seen in Figure 4c. In Figure 4b it can be observed that the flow rate of the external recycle (biomass and nitrate) fed to the second compartment ($Q_{r,ext,2}$) increases, improving the nitrification process, and that the flow rate of the influent wastewater fed to the third compartment ($Q_{fresh,3}$) also increases, thus improving the denitrification process since more carbonaceous matter is available.

Finally, for the smallest reductions in the influent $S_{NH,fresh}$ (5% and 10%), the effluent $S_{NH,ef}$ decreases, while for larger reductions (15% and 20%) the effluent total P ($P_{TOT,ef}$) also decreases. This behavior can be explained by the fact that in the latter cases the N removal processes demand a lower carbon amount, leaving it available for the P removal processes (Figure 4c).

Figure 5 shows the optimization results obtained by varying the influent inorganic soluble phosphorus concentration $S_{PO,fresh}$. The total annual operating cost $OC^{T,Annual}$ increases with the $S_{PO,fresh}$ concentration. However, a variation in the influent $S_{PO,fresh}$ determinates a lower impact in the operating cost than the same variation in the influent $S_{NH,fresh}$. This is in line with the sensitivity analysis results discussed above (Table 4).

The reference value for $S_{PO,fresh}$ concentration, taken from case I.A, is 9.01 g of P $m^{-3}$. If the influent $S_{PO,fresh}$ increases, the external carbon dosed, the waste sludge for disposal produced, and the aeration energy demand also increase, as indicated by their respective costs in Figure 5a ($OC_{ECSD}$, $OC_{SLDGD}$, and $OC_a$, respectively).

For a 5% increment in $S_{PO,fresh}$ with respect to the reference value, the total external recycle flow rate $Q^{T}_{r,ext}$ decreases (Figure 5b) and the fines incurred $OC_{EQ}$ increase significantly (Figure 5a); however, for increments higher than 5%, they remain practically constant.

A reduction in the $S_{PO,fresh}$ with respect to its reference value increases the total external recycle flow rate $Q^{T}_{r,ext}$ (Figure 5b),

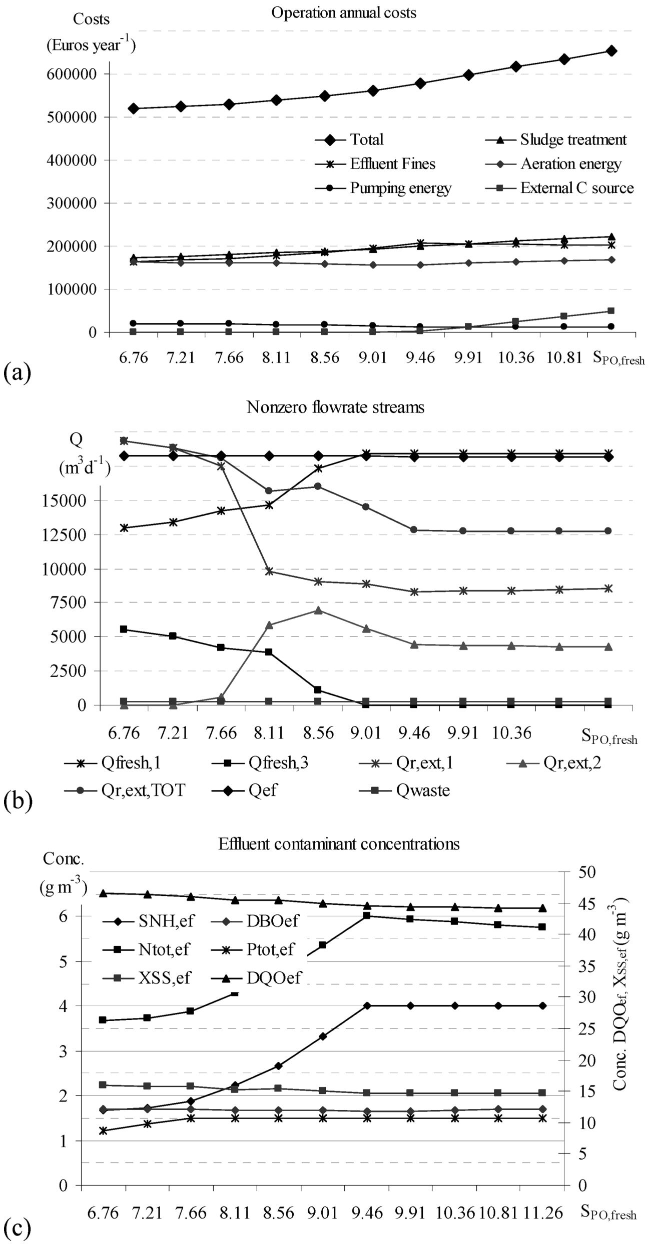

**Figure 5.** Optimization results by varying $S_{PO}$ concentration for case study II: (a) annual operating costs, (b) onzero flow rate streams, and (c) effluent contaminants concentration.

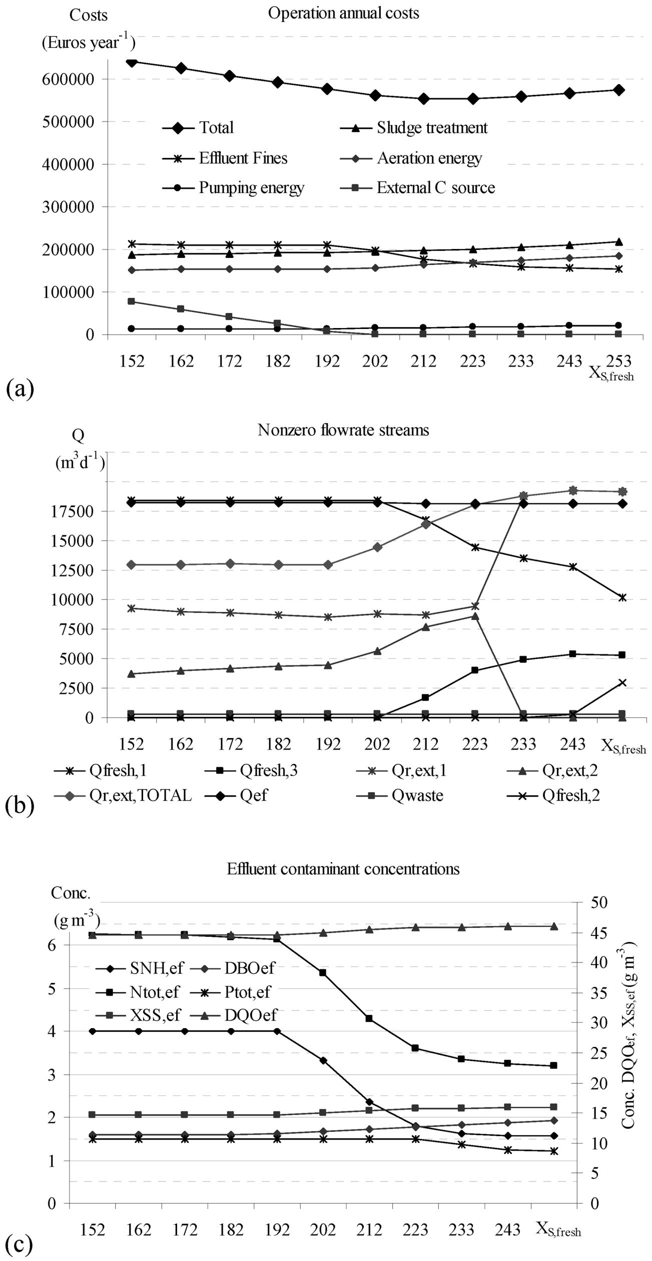

**Figure 6.** Optimization results by varying $X_{S,fresh}$ concentration for case study II: (a) annual operating costs, (b) nonzero flow rate streams, and (c) effluent contaminants concentration.

decreasing the retention times in the compartments and the flow rate of the sludge for disposal as reflected in Figure 5a by its related cost. Now, if $S_{PO,fresh}$ is progressively reduced, the nitrification process is improved by increasing the aeration flow rate and the denitrification process by distributing progressively a greater fraction of the influent flow rate to the third compartment; then, the effluent ammonium concentration $S_{NH,ef}$ and total nitrogen concentration $N_{TOT,ef}$ decreased (Figure 5c) and, consequently, the fines incurred (Figure 5a). The aeration and pumping energy cost increase in a proportion smaller than the reduction in fines and sludge treatment cost, thus improving the total operating cost.

Figure 6 shows the optimization results obtained by varying the influent slowly biodegradable substrates concentration $X_{S,fresh}$. The reference value for $X_{S,fresh}$ concentration, taken from case I.A, is 202.32 g of COD m$^{-3}$. Increments in $X_{S,fresh}$ increase the aeration energy requirements and, consequently, increase the amount of sludge for disposal as more biomass is produced; then, their related costs increase (Figure 6a). However, the effluent quality improves, incurring lower fines. This is explained by the beneficial effect of more carbonaceous organic matter available for the nitrification process, rendering a significantly lower concentration of the total effluent N ($N_{TOT,ef}$), as depicted in Figure 6c. As the total annual operating cost $OC^{T,Annual}$ is concerned, this trade off is favorable for increments in the influent $X_{S,fresh}$ up to 15% (Figure 6a). This tendency changes for larger variations since the increase in the aeration energy and sludge treatment costs exceed the decrease in fines incurred, deteriorating the total operating cost (Figure 6a).

Regarding streamflow distribution patterns, Figure 6b shows that increments of 5% and 10% in $X_{S,fresh}$ decrease progressively the fresh flow rate fraction fed to the first compartment ($Q_{fresh,1}$) and increase proportionally the fraction fed to the third one ($Q_{fresh,3}$) while distributing almost equally the increasing external recycle flow rate ($Q^{T}_{r,ext}$) between the first and second compartments ($Q_{r,ext,1}$ and $Q_{r,ext,2}$, respectively). This stream distribution pattern favors N removal, keeping the effluent P level ($P_{\mathrm{TOT,ef}}$) at its permitted limit (1.5 g of P $\mathrm{m}^{-3}$), as depicted in Figure 6c. Now, for a 15% increment in $X_{\mathrm{S,fresh}}$ a similar flow distribution pattern of the input flow rate is obtained but the external sludge recycle is completely fed to the first compartment, improving the P removal efficiency; the $P_{\mathrm{TOT,ef}}$ concentration computed is lower than its threshold value (Figure 6.c),

On the other hand, if the influent $X_{\mathrm{S,fresh}}$ (i.e., the influent carbon content) decreases from its reference value, an external carbon source has to be added to the system to prevent the effluent N compounds going over the permitted limits. This behavior is shown in Figure 6a by inspecting the operating cost related to it. Moreover, this cost governs the total operation cost since the other ones remain practically constant.

## 8. Conclusions

The optimal synthesis, design, and operation of activated sludge treatment plants for phosphorus and nitrogen removal have been successfully addressed by proposing a superstructure model of the process and formulating and solving a NLP problem. This claim is based on the results obtained from the different case studies considered, which showed the model flexibility and robustness for a wide range of operation conditions and process alternatives.

Although the proposed superstructure model embeds a chain of seven reaction compartments, it can be straightforwardly extended to an arbitrary number of compartments. A distinctive feature of the model is the possibility of flow distribution of the main process streams, which provides flexibility and allows searching for novel or more efficient process configurations.

Besides its applications for optimization tasks and due to mainly its robustness, the proposed model can also be run satisfactorily in "simulation mode" to evaluate and compare the performance of different activated sludge treatment process designs.

The sensitivity analysis performed provides valuable information from a treatment point of view by ranking the main model inputs and parameters according to their relative impacts over the economical objective functions considered. In this sense, it also highlights the capability of the model itself as a useful decision support tool.

Although the *numerical* results reported depend on the model parameter values selected for the scenarios considered, they could be straightforwardly adapted to other regional conditions (local costs) or regulations (effluent permitted limits).

The optimization model helps elucidate the highly interlinked biological, operational, and economical trade offs present, which are not so evident at first glance. For instance, an increment in the influent biological oxygen demand, which determinates a more contaminated liquid, decreases "paradoxically" the computed net present value. This behavior is explained by the fact that more carbonaceous organic matter is available for the nitrogen and phosphorus removal processes, resulting in a more efficient global treatment process. Moreover, in some cases, an external carbon source has to be dosed to the system to meet the nitrogen and phosphorus permitted limits. For case studies I (I.A, I.B, and I.C), optimization of the superstructure model resulted in plant configurations aiming to facilitate suitable environmental conditions for phosphorus removal as it was the most difficult contaminant to remove for the scenarios considered. Finally, as model resolution is concerned, the multiple starting points strategy for model initialization adopted was satisfactory for dealing with locally optimal solutions.

## Nomenclature

$V_i$ = volume of reactor $i$ ($\mathrm{m}^3$)
$k_{\mathrm{L}}a_i$ = oxygen transfer coefficient for reactor $i$ ($\mathrm{d}^{-1}$)

*Volumetric Flow Rates ($m^3$ $d^{-1}$)*

$Q_i$ = volumetric flow rate that leaves/enters reactor $i$
$Q^T_{\mathrm{fresh}}$ = total influent wastewater flow rate
$Q_{\mathrm{fresh},g}$ = influent wastewater flow rate to mixer $g$
$Q_{i,i'}$ = flow rate from reactor $i$ to reactor $i'$
$Q^T_{\mathrm{trans},i}$ = total transversal flow rate of reactor $i$
$Q_{\mathrm{sett,in}}$ = volumetric flow rate fed to the settler
$Q_{\mathrm{trans},i,g}$ = volumetric flow rate from reactor $i$ to mixer $g$
$Q^T_{\mathrm{r,ext}}$ = total external recycle flow rate
$Q_{\mathrm{r,ext},g}$ = external recycle flow rate to mixer $g$
$Q_{\mathrm{ef}}$ = flow rate leaving the clarification settler zone
$Q_{\mathrm{bottom}}$ = flow rate leaving the sedimentation settler zone
$Q_{\mathrm{waste}}$ = sludge flow rate to be wasted

*Mass Flow Rates (g $d^{-1}$)*

$u^{\mathrm{T}}_{\mathrm{ECSD}}$ = total external carbon source rate
$u_{\mathrm{ECSD},g}$ = external carbon source rate dosed to mixer $g$
$u_{x,g}$ = mass of component $x$ dosed to mixer $g$

*Streams Concentrations ($C_x$ = $S_x$ or $X_x$, g of x $m^{-3}$)*

$C_{x,i}$ = concentration of component $x$ in reactor $i$
$C_{x,\mathrm{fresh}}$ = concentration of component $x$ in the influent (fresh) wastewater stream
$C_{x,\mathrm{sett,in}}$ = concentration of component $x$ in the stream fed to the settler
$C_{x,\mathrm{r,ext}}$ = concentration of component $x$ in the external recycle stream
$C_{x,\mathrm{bottom}}$ = concentration of component $x$ in the stream leaving the sedimentation settler zone
$C_{x,\mathrm{ef}}$ = concentration of component $x$ in the stream leaving the clarification settler zone
$C_{x,m}$ = concentration of component $x$ in the settler layer $m$
$C_{x,g}$ = concentration of component $x$ in the stream leaving mixer $g$

*Cost Variables*

NPV = net present value (Euro)
$\mathrm{IC}^{\mathrm{T}}$ = total investment cost (Euro)
$\mathrm{OC}^{\mathrm{T}}$ = total operation cost (Euro)
$\mathrm{OC}^{\mathrm{T,Annual}}$ = total annual operation cost (Euro $\mathrm{year}^{-1}$)
$\Gamma$ = cost updating factor ($\mathrm{year}^{-1}$)
$\mathrm{IC}_t$ = reaction compartments investment cost (Euro)
$\mathrm{IC}_{\mathrm{a}}$ = aeration systems investment cost (Euro)
$\mathrm{IC}_{\mathrm{sett}}$ = secondary settler investment cost (Euro)
$\mathrm{IC}_{\mathrm{ips}}$ = influent pumping station investment cost (Euro)
$\mathrm{IC}_{\mathrm{sr}}$ = sludge recycle pump investment cost (Euro)
$\mathrm{OC}_{\mathrm{a}}$ = aeration energy annual operation cost (Euro $\mathrm{year}^{-1}$)
$\mathrm{OC}_{\mathrm{pump}}$ = pumping energy annual operation cost (Euro $\mathrm{year}^{-1}$)
$\mathrm{OC}_{\mathrm{EQ}}$ = effluent annual fines (Euro $\mathrm{year}^{-1}$)
$\mathrm{OC}_{\mathrm{SLDGD}}$ = sludge treatment annual operation cost (Euro $\mathrm{year}^{-1}$)
$\mathrm{OC}_{\mathrm{ECSD}}$ = external carbon source annual operation cost (Euro $\mathrm{year}^{-1}$)

## Appendix: Model Equations

### A.1. Process Units and Equipment Model Equations.

### A.1.1. Reactor Model Equations.

$$\frac{Q_i}{V_i}(C_{x,g} - C_{x,i}) + r_{x,i} = 0, \forall i, g = i, x \neq O_2 \qquad \text{(A-1)}$$

The reaction term $r_{x,i}$ for each compound $x$ and reactor $i$ is computed as follows

$$r_{x,i} = \sum_{K} \upsilon_{k,x} \cdot \rho_{k,i}, \forall i, x \qquad \text{(A-2)}$$

where $\rho_{k,i}$ is the $k$th process rate in reactor $i$ and $\upsilon_{k,x}$ are the stoichiometric coefficients.

For dissolved oxygen, eq A-1 is modified to account for gas−liquid mass transfer

$$\frac{Q_i}{V_i}(S_{\mathrm{O},g} - S_{\mathrm{O},i}) + k_{\mathrm{L}}a_i(S_{\mathrm{O,sat}} - S_{\mathrm{O},i}) + r_{S_{\mathrm{O}},i} = 0, \forall i, g = i \qquad \text{(A-3)}$$

where $S_{\mathrm{o,sat}}$ is the oxygen saturation concentration at 15 °C ($S_{\mathrm{o,sat}} = 8$ g of $\mathrm{O_2}$ $\mathrm{m^{-3}}$).

Finally, for each compartment $I$, the following constraints are considered for volumes and for the mass transfer coefficient $k_{\mathrm{L}}a_i$

$$V_i \leq V_{\max}, \forall i \qquad \text{(A-4)}$$

$$k_{\mathrm{L}}a_i \leq k_{\mathrm{L}}a_{i,\max}, \forall i \qquad \text{(A-5)}$$

where $V_{\max}$ is a sufficiently large upper bound for reactor volumes and $k_{\mathrm{L}}a_{i,\max}$ is a maximum operating limit ($k_{\mathrm{L}}a_{i,\max} = 360$ $\mathrm{day^{-1}}$).

**A.1.2. Splitter Mass Balances Equations.** The expressions listed below represent the stream splitters needed to model the process superstructure

$$Q_{\mathrm{fresh}}^{T} = \sum_{G} Q_{\mathrm{fresh},g} \qquad \text{(A-6)}$$

$$Q_i = Q_{i,(i+1)} + Q_{\mathrm{trans},i}^{\mathrm{T}}, \forall i \neq I \qquad \text{(A-7)}$$

$$Q_i = Q_{\mathrm{sett,in}} + Q_{\mathrm{trans},i}^{\mathrm{T}}, i = I \qquad \text{(A-8)}$$

$$Q_{\mathrm{trans},i}^{\mathrm{T}} = \sum_{G} Q_{\mathrm{trans},i,g} \forall i \qquad \text{(A-9)}$$

$$Q_{\mathrm{trans},i,g} = 0 \forall i \neq I, g = (i+1) \qquad \text{(A-10)}$$

$$Q_{r,\mathrm{ext}}^{\mathrm{T}} = \sum_{G} Q_{r,\mathrm{ext},g} \qquad \text{(A-11)}$$

$$Q_{\mathrm{bottom}} = Q_{\mathrm{waste}} + Q_{r,\mathrm{ext}}^{\mathrm{T}} \qquad \text{(A-12)}$$

$$u_{\mathrm{ECSD}}^{\mathrm{T}} = \sum_{G} u_{\mathrm{ECSD},g} \qquad \text{(A-13)}$$

Mass components balances

$$C_{x,\mathrm{sett,in}} = C_{x,i}, \forall x, i = I \qquad \text{(A-14)}$$

$$C_{x,r,\mathrm{ext}} = C_{x,\mathrm{bottom}}, \forall x \qquad \text{(A-15)}$$

$$C_{x,\mathrm{bottom}} = C_{x,m}, \forall x, m = 1 \qquad \text{(A-16)}$$

$$C_{x,ef} = C_{x,m}, \forall x, m = 10 \qquad \text{(A-17)}$$

**A.1.3. Mixer Mass Balances Equations.** Analogously, the following expressions are the total and components mass balances for the stream mixers needed to model the superstructure

$$Q_i = Q_{\mathrm{fresh},g} + Q_{r,\mathrm{ext},g} + \sum_{I'} Q_{\mathrm{trans},i',g}, \forall i', i = 1, g = i \qquad \text{(A-18)}$$

$$Q_i = Q_{\mathrm{fresh},g} + Q_{r,\mathrm{ext},g} + \sum_{I'} Q_{\mathrm{trans},i',g} + Q_{(i-1),i}, \quad \forall i \neq 1, g = i, \forall i' \qquad \text{(A-19)}$$

Mass components balances

$$Q_i C_{x,g} = Q_{\mathrm{fresh},g} C_{x,\mathrm{fresh}} + Q_{r,\mathrm{ext},g} C_{x,r,\mathrm{ext}} + \sum_{I'} Q_{\mathrm{trans},i',g} C_{x,i'} + u_{x,g}, \forall i', i = 1, g = i, x \qquad \text{(A-20)}$$

$$Q_i C_{x,g} = Q_{\mathrm{fresh},g} C_{x,\mathrm{fresh}} + Q_{(i-1),i} C_{x,(i-1)} + Q_{r,\mathrm{ext},g} C_{x,r,\mathrm{ext}} + \sum_{I'} Q_{\mathrm{trans},i',g} C_{x,i'} + u_{x,g}, \forall i \neq 1, g = i, x, i' \qquad \text{(A-21)}$$

### A.2. Cost and Performance Models.

$$\mathrm{NPV} = \mathrm{IC}^{\mathrm{T}} + \mathrm{OC}^{\mathrm{T}} \qquad \text{(A-22)}$$

$$\mathrm{IC}^{\mathrm{T}} = \sum_{P} \mathrm{IC}_p \qquad \text{(A-23)}$$

$$\mathrm{OC}^{\mathrm{T}} = \Gamma \mathrm{OC}^{\mathrm{T,Annual}} = \Gamma \sum_{P} \mathrm{OC}_p^{\mathrm{Annual}} \qquad \text{(A-24)}$$

$$\Gamma = \sum_{j=1}^{n} \frac{1}{(1 + id)^j} = \frac{1 - (1 + id)^{-n}}{id} \qquad \text{(A-25)}$$

$$\mathrm{IC}^{\mathrm{T}} = \mathrm{IC}_t + \mathrm{IC}_a + \mathrm{IC}_{\mathrm{sett}} + \mathrm{IC}_{\mathrm{ips}} + \mathrm{IC}_{\mathrm{sr}} \qquad \text{(A-26)}$$

$$\mathrm{i}IC_t = \left( \sum_{i=1}^{7} b_t V_i^{\delta_t} \right) \qquad \text{(A-27)}$$

$$\mathrm{IC_a} = \left( \sum_{i=1}^{7} b_a OxCa_i^{\delta_a} \right) \qquad \text{(A-28)}$$

where $OxCa_i = 3000^{-1}$ kg of $\mathrm{O_2}$ day $(\mathrm{h\ m^3})^{-1}$ $k_{\mathrm{L}}a_i$ $V_i$.

$$\mathrm{IC_{sett}} = b_{\mathrm{sett},1} A_{\mathrm{sett}}^{\delta_{\mathrm{sett},1}} + b_{\mathrm{sett},2} A_{\mathrm{sett}}^{\delta_{\mathrm{sett},2}} \qquad \text{(A-29)}$$

$$\mathrm{IC_{ips}} = b_{\mathrm{ip}s,1} Q_{\mathrm{fresh}}^{\mathrm{T}\delta_{\mathrm{ips},1}} + b_{\mathrm{ips},2} Q_{\mathrm{fresh}}^{\mathrm{T}\delta_{\mathrm{ips},2}} + b_{\mathrm{ips},3} Q_{\mathrm{fresh}}^{\mathrm{T}\delta_{\mathrm{ips},3}} \qquad \text{(A-30)}$$

$$\mathrm{IC_{sr}} = b_{\mathrm{sr}} Q_{r,\mathrm{ext}}^{\mathrm{T}\delta_{\mathrm{sr}}} \qquad \text{(A-31)}$$

$$\mathrm{OC}^{\mathrm{T,Annual}} = \mathrm{OC} = \mathrm{OC_a} + \mathrm{OC_{pump}} + \mathrm{OC_{EQ}} + \mathrm{OC_{SLDGD}} + \mathrm{OC_{ECSD}} \qquad \text{(A-32)}$$

$$\mathrm{OC_a} = (\alpha_{\mathrm{E}} E_{\mathrm{a}}) \qquad \text{(A-33)}$$

$$\mathrm{OC_{pump}} = (\alpha_{\mathrm{E}} E_{\mathrm{pump}}) \qquad \text{(A-34)}$$

$$\mathrm{OC_{EQ}} = (\alpha_{\mathrm{EQ}} EQ) \qquad \text{(A-35)}$$

$$\mathrm{OC_{SLDGD}} = (\alpha_{\mathrm{SLDGD}} u_{\mathrm{SLDGD}} (\mathrm{kg\ 1000^{-1}\ g^{-1}})) \qquad \text{(A-36)}$$

$$\mathrm{OC_{ECSD}} = (\alpha_{\mathrm{ECSD}} u_{\mathrm{ECSD}} (\mathrm{kg\ 1000^{-1}\ g^{-1}})) \qquad \text{(A-37)}$$

$$E_{\mathrm{pump}} = \gamma \left( \sum Q_{\mathrm{trans},i}^{\mathrm{T}} + Q_{r,\mathrm{ext}}^{\mathrm{T}} + Q_{\mathrm{waste}} \right) \quad \text{with } \gamma = 0.04 (\mathrm{kWh\ m^{-3}}) \qquad \text{(A-38)}$$

$$E_a = 24\sum_I\left(2,267.10^{-7}\left(\frac{k_La_iV_i}{24}\right)^2 + 5.612\times10^{-3}\left(\frac{k_La_iV_i}{24}\right)\right) \tag{A-39}$$

$$\begin{aligned}\mathrm{EQ} = \left(\frac{1}{1000}\right)(\beta_{\mathrm{SS}}X_{\mathrm{SS,ef}} + \beta_{\mathrm{COD}}\mathrm{COD}_{\mathrm{ef}} + \beta_{\mathrm{BOD}}\mathrm{BOD}_{\mathrm{ef}} +\\ \beta_{\mathrm{TKN}}\mathrm{TKN}_{\mathrm{ef}} + \beta_{\mathrm{NO}}S_{\mathrm{NO,ef}} + \beta_{\mathrm{Ptot}}P_{\mathrm{tot,ef}})Q_{\mathrm{ef}}\end{aligned} \tag{A-40}$$

$$\begin{aligned}\mathrm{COD}_{\mathrm{ef}} = S_{S,\mathrm{ef}} + S_{I,\mathrm{ef}} + X_{S,\mathrm{ef}} + X_{I,\mathrm{ef}} + X_{H,\mathrm{ef}} + X_{A,\mathrm{ef}} +\\ X_{\mathrm{STO,ef}}X_{\mathrm{PHA,ef}} + X_{\mathrm{PAO,ef}}\end{aligned} \tag{A-41}$$

$$\begin{aligned}\mathrm{BOD}_{\mathrm{ef}} = 0.25(S_{S,\mathrm{ef}} + (1 - f_{S_I})X_{S,\mathrm{ef}} + (1 - f_{X_I})(X_{H,\mathrm{ef}} +\\ X_{A,\mathrm{ef}} + X_{\mathrm{STO,ef}} + X_{\mathrm{PAO,ef}} + X_{\mathrm{PHA,ef}}))\end{aligned} \tag{A-42}$$

$$\begin{aligned}\mathrm{TKN}_{\mathrm{ef}} = (i_{N,SI}S_{I,\mathrm{ef}} + i_{N,SS}S_{S,\mathrm{ef}} + S_{NH,\mathrm{ef}} + i_{N,XS}X_{S,\mathrm{ef}} +\\ i_{N,XI}X_{I,\mathrm{ef}} + i_{N,BM}(X_{H,\mathrm{ef}} + X_{A,\mathrm{ef}} + X_{\mathrm{PAO,ef}}))\end{aligned} \tag{A-43}$$

$$\begin{aligned}P_{\mathrm{TOT'ef}} = (i_{P,SI}S_{I,\mathrm{ef}} + i_{P,SS}S_{S,\mathrm{ef}} + S_{\mathrm{PO4,ef}} + i_{P,XS}X_{S,\mathrm{ef}} +\\ i_{P,XI}X_{I,\mathrm{ef}} + X_{\mathrm{PP,ef}} + i_{P,BM}(X_{H,\mathrm{ef}} + X_{A,\mathrm{ef}} + X_{\mathrm{PAO,ef}}))\end{aligned} \tag{A-44}$$

$$u_{\mathrm{SLDGD}} = (X_{SS,\mathrm{waste}}Q_{\mathrm{waste}}) \tag{A-45}$$

The performance model parameters used are as follows.[1,3] A discount rate *id* of 0.05 and a life span *n* of 20 years are used. Parameters $b$ and $\delta$ for the investment cost functions (eqs A-27−A-31) used are considered valid in the whole search space defined. The parameters $b$ and $\delta$ for the investment cost functions are $b_t = 10\,304$, $b_a = 8590$, $b_{\mathrm{sett},1} = 2630$, $b_{\mathrm{sett},2} = 6338$, $b_{\mathrm{ips},1} = 2334$, $b_{\mathrm{ips},2} = 2123$, $b_{\mathrm{ips},3} = 3090$, $b_{\mathrm{sr}} = 5038$, $\delta_t = 0.477$, $\delta_a = 0.433$, $\delta_{\mathrm{sett},1} = 0.678$, $\delta_{\mathrm{sett},2} = 0.325$, $\delta_{\mathrm{ips},1} = 0.637$, $\delta_{\mathrm{ips},2} = 0.540$, $\delta_{\mathrm{ips},3} = 0.349$, and $\delta_{\mathrm{sr}} = 0.304$. Annual unitary operation costs used in (eqs A-33−A-37) (coefficients α) are $\alpha_{\mathrm{EQ}} = 50$ Euro day (kg of PU year)$^{-1}$, $\alpha_{\mathrm{E}} = 25$ Euro day (kWh year)$^{-1}$, $\alpha_{\mathrm{SLDGD}} = 75$ Euro day (kg of SS year)$^{-1}$, and $\alpha_{\mathrm{ECSD}} = 109.5$ Euro day (kg of COD year)$^{-1}$. Weighting factors $\beta_y$ for the contaminating components used in eq A-40 are (in g of contaminating unit g$^{-1}$): $\beta_{\mathrm{SS}} = 2$, $\beta_{\mathrm{COD}} = 1$, $\beta_{\mathrm{TKN}} = 20$, $\beta_{\mathrm{Ptot}} = 20$, $\beta_{\mathrm{NO}} = 20$, and $\beta_{\mathrm{BOD}} = 2$.

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