

Chapter 2

Process Modelling and Simulation Scenarios

The wastewater research community has extensively applied benchmark models to develop and evaluate control strategies for WWTPs. The large number of journal papers and conferences related to the use of benchmarks in WWTPs, issued up to the present, prove the utility of these tools. This book also makes use of benchmark models to test and compare the proposed control strategies. These benchmarks are briefly described in the first section of this chapter.

The WWTP benchmarks include basic control strategies, which are commonly applied in WWTPs. They are usually used in the literature in order to compare the results achieved with new control strategies or techniques, in terms of control performance and/or plant performance. These default control strategies are described in the second section of this chapter.

2.1 Working Scenarios

In order to simulate the behavior of a wastewater treatment plant and to evaluate different control strategies, two benchmarks have been used in this book, which are called BSM1 [1] and BSM2 [24]. They have been widely applied to test control strategies and to optimize the plant design.

BSM1 and BSM2 are composed by different models developed by the International Association on Water Pollution Research and Control (IAWPRC)

- The Activated Sludge Model No. 1 (ASM1) [30] describes the biological phenomena that takes place in the biological reactors.
- The model developed in [59] describes the physical separation processes that take place inside the secondary settler.
- The Anaerobic Digestion Model No. 1 (ADM1) [5] describes the dynamics of the anaerobic digester.

BSM1 represents an activated sludge system that operates according to ASM1 with a secondary clarifier.

BSM2 integrates BSM1 with wastewater pre-treatment and sludge treatment including ADM1.

2.1.1 Benchmark Simulation Model No. 1

This section provides a description of the BSM1 working scenario. This is a simulation environment defining a plant layout, a simulation model, the procedures for carrying out the tests, the criteria for evaluating the results and a default control strategy.

Plant Layout

The schematic representation of the WWTP layout considered in BSM1 is presented in Fig. 2.1. The plant consists of five biological reactor tanks connected in series, followed by a secondary settler. The first two tanks have a volume of 1000 m^3 each and are anoxic and perfectly mixed. The rest three tanks have a volume of 1333 m^3 each and are aerated. The settler has a total volume of 6000 m^3 and is modeled in ten layers, being the 6th layer, counting from bottom to top, the feed layer. Two recycle flows, the first from the last tank and the second from the underflow of the settler, complete the system. The sludge from the settler that is not recycled is led to be disposed and is called wasteage.

The plant is designed for an average influent dry weather flow rate of $18,446 \text{ m}^3/\text{d}$ and an average biodegradable chemical oxygen demand (COD) in the influent of $300 \text{ g}/\text{m}^3$. Its hydraulic retention time, based on the average dry weather flow rate and the total tank and settler volume ($12,000 \text{ m}^3$), is 14.4 h. Q_w is fixed to $385 \text{ m}^3/\text{d}$ that determines, based on the total amount of biomass present in the system, a biomass sludge age of about 9 days.

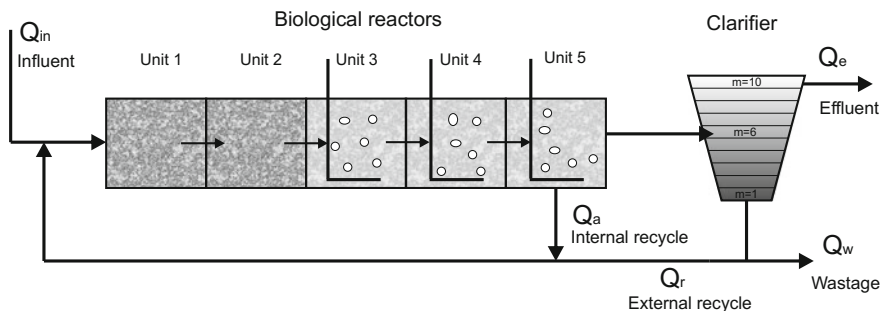


Fig. 2.1 Benchmark simulation model 1

The nitrogen removal is achieved using a denitrification step performed in the anoxic tanks and a nitrification step carried out in the aerated tanks. The internal recycle is used to supply the denitrification step with S_{NO} .

Models

The biological phenomena of the reactors are simulated by using the ASM1 that considers eight different biological processes. The vertical transfers between layers in the settler are simulated by the double-exponential settling velocity model [59]. None biological reaction is considered in the settler. The two models are internationally accepted and include 13 state variables.

The general equations for mass balancing are as follows:

- For reactor 1:

$$\frac{dZ_1}{dt} = \frac{1}{V_1} (Q_a \cdot Z_a + Q_r \cdot Z_r + Q_{in} \cdot Z_{in} + r_{z,1} \cdot V_1 - Q_1 \cdot Z_1) \quad (2.1)$$

- For reactors 2–5:

$$\frac{dZ_k}{dt} = \frac{1}{V_k} (Q_{k-1} \cdot Z_{k-1} + r_{z,k} \cdot V_k - Q_k \cdot Z_k) \quad (2.2)$$

where Z is any concentration of the process, Z_1 is Z in the first reactor, Z_a is Z in the internal recirculation, Z_r is Z in the external recirculation, Z_{in} is Z from the influent, V is the volume, V_1 is V in the first reactor, Q_r is the external recirculation flow rate, Q_{in} is the flow rate of the influent, Q_1 is the flow rate in the first tank and it is equal to the sum of Q_a , Q_r and Q_{in} , k is the number of reactor and Q_k is equal to Q_{k-1} .

The proposed control strategies in this work are based on the conversion rates of S_{NH} (r_{NH}) and S_{NO} (r_{NO}). They are expressed as:

$$r_{NH} = -0.08\rho_1 - 0.08\rho_2 - \left(0.08 + \frac{1}{0.24}\right)\rho_3 + \rho_6 \quad (2.3)$$

$$r_{NO} = -0.1722\rho_2 + 4.1667\rho_3 \quad (2.4)$$

where ρ_1 , ρ_2 , ρ_3 , ρ_6 are four of the eight biological processes defined in ASM1. Specifically, ρ_1 is the aerobic growth of heterotrophs, ρ_2 is the anoxic growth of heterotrophs, ρ_3 is the aerobic growth of autotrophs and ρ_6 is the ammonification of soluble organic nitrogen (S_{ND}). They are defined as

$$\rho_1 = 4 \left(\frac{S_S}{10 + S_S} \right) \left(\frac{S_O}{0.2 + S_O} \right) X_{B,H} \quad (2.5)$$

$$\rho_2 = 4 \left(\frac{S_S}{10 + S_S} \right) \left(\frac{0.2}{0.2 + S_O} \right) \left(\frac{S_{NO}}{0.5 + S_{NO}} \right) 0.8 \cdot X_{B,H} \quad (2.6)$$

$$\rho_3 = 0.5 \left(\frac{NH}{1 + NH} \right) \left(\frac{S_O}{0.4 + S_O} \right) X_{B,A} \quad (2.7)$$

$$\rho_6 = 0.05 \cdot S_{ND} \cdot X_{B,H} \quad (2.8)$$

where S_S is the readily biodegradable substrate, $X_{B,H}$ the active heterotrophic biomass and $X_{B,A}$ the active autotrophic biomass. The biological parameter values used in the BSM1 correspond approximately to a temperature of 15 °C.

Test Procedure

BSM1 [13] defines four different influent data: constant, dry weather, rain weather, and storm weather. Each scenario contains 14 days of influent data with sampling intervals of 15 min. A simulation protocol is established to assure that results are got under the same conditions and can be compared. Thus, first a 150 days period of stabilization in closed-loop using constant influent data has to be completed to drive the system to a steady-state, next a simulation with dry weather is run and finally the desired influent data (dry, rain or storm) is tested. Only the results of the last 7 days are considered for the plant operation evaluation.

Evaluation Criteria

In order to compare the different control strategies, different criteria are defined. The performance assessment is made at two levels. The first level concerns the control. Basically, this serves as a proof that the proposed control strategy has been applied properly. It is assessed by Integral of the Squared Error (ISE), Integral of the Absolute Error (IAE), and average of the absolute error (mean ($|e|$)) criteria.

$$ISE = \int_{t=7days}^{t=14days} e_i^2 \cdot dt \quad (2.9)$$

$$IAE = \int_{t=7days}^{t=14days} |e_i| \cdot dt \quad (2.10)$$

$$mean(|e|) = \frac{1}{T_s} \sum_{i=1}^{i=T_s} |e_i| \quad (2.11)$$

where e_i is the error in each sample between the set-point and the measured value and T_s is the total number of samples.

The second level of evaluation provides measures for the effect of the control strategy on plant performance. It includes effluent violations, Effluent Quality Index (EQI), and Overall Cost Index (OCI).

The evaluation must include the percentage of time that the effluent limits are not met. The effluent concentrations of $S_{N_{tot}}$, Total COD (COD_t), NH, TSS, and Biological Oxygen Demand (BOD_5) should obey the limits given in Table 2.1.

Table 2.1 Effluent quality limits

Variable	Value
$S_{N_{tot}}$	$<18 \text{ g N} \cdot \text{m}^{-3}$
COD_t	$<100 \text{ g COD} \cdot \text{m}^{-3}$
NH	$<4 \text{ g N} \cdot \text{m}^{-3}$
TSS	$<30 \text{ g SS} \cdot \text{m}^{-3}$
BOD_5	$<10 \text{ g BOD} \cdot \text{m}^{-3}$

Table 2.2 B_i values

Factor	B_{TSS}	B_{COD}	B_{NKj}	B_{SNO}	B_{BOD_5}
Value (g pollution unit g^{-1})	2	1	30	10	2

$S_{N_{tot}}$ is calculated as the sum of S_{NO} and Kjeldahl nitrogen (NKj), being this the sum of organic nitrogen and S_{NH} .

EQI is defined to evaluate the quality of the effluent. It is related with the fines to be paid due to the discharge of pollution. EQI is averaged over a 7 days observation period and it is calculated weighting the different compounds of the effluent loads.

$$EQI = \frac{1}{1000 \cdot T} \int_{t=7days}^{t=14days} (B_{TSS} \cdot TSS(t) + B_{COD} \cdot COD(t) + B_{NKj} \cdot NKj(t) + B_{SNO} \cdot S_{NO}(t) + B_{BOD_5} \cdot BOD_5(t)) Q(t) \cdot dt \quad (2.12)$$

where B_i are weighting factors (Table 2.2) and T is the total time.

OCI is defined as

$$OCI = AE + PE + 5 \cdot SP + 3 \cdot EC + ME \quad (2.13)$$

where AE is the aeration energy, PE is the pumping energy, SP is the sludge production to be disposed, EC is the consumption of carbon from external source and ME is the mixing energy.

AE is calculated according to the following relation:

$$AE = \frac{S_o^{sat}}{T \cdot 1.8 \cdot 1000} \int_{t=7days}^{t=14days} \sum_{i=1}^5 V_i \cdot K_L a_i(t) \cdot dt \quad (2.14)$$

where i is the reactor number and S_o^{sat} is the saturation concentration for oxygen that is equal to 8 mg/l.

PE is calculated as:

$$PE = \frac{1}{T} \int_{7days}^{14days} (0.004 \cdot Q_{in}(t) + 0.008 \cdot Q_a(t) + 0.05 \cdot Q_w(t)) dt \quad (2.15)$$

SP is calculated from the TSS in the flow wastage (TSS_w) and the solids accumulated in the system:

$$SP = \frac{1}{T} (TSS_a(14days) - TSS_a(7days) + TSS_s(14days) - TSS_s(7days) + \int_{t=7days}^{t=14days} TSS_w \cdot Q_w \cdot dt) \quad (2.16)$$

where TSS_a is TSS in the reactors and TSS_s is TSS in the settler.

EC refers to the carbon that could be added to improve denitrification.

$$EC = \frac{COD_{EC}}{T \cdot 1000} \int_{t=7days}^{t=14days} \left(\sum_{i=1}^{i=n} q_{EC,i} \right) dt \quad (2.17)$$

where $q_{EC,i}$ is external carbon flow rate (q_{EC}) added to compartment i , $COD_{EC} = 400 \text{ gCOD} \cdot \text{m}^{-3}$ is the concentration of readily biodegradable substrate in the external carbon source.

ME is a function of the compartment volume

$$ME = \frac{24}{T} \int_{t=7days}^{t=14days} \sum_{i=1}^5 [0.005 \cdot V_i \text{ if } K_L a_i(t) < 20 d^{-1} \text{ otherwise } 0] dt \quad (2.18)$$

2.1.2 Benchmark Simulation Model No. 2

In order to include plant-wide operation considerations, BSM1 was extended in a new version, BSM2, in [33] which was updated in [46]. BSM2 also defines a plant layout, a simulation model, a test procedure, evaluation criteria and default control strategies.

Plant Layout

The finalized BSM2 layout (Fig. 2.2) includes BSM1 for the biological treatment of the wastewater and the sludge treatment. A primary clarifier, a thickener for the sludge wasted from the clarifier of biological treatment, a digester for treatment of the solids wasted from the primary clarifier and the thickened secondary sludge, as well as a dewatering unit have been added. The liquids collected in the thickening and dewatering steps are recycled ahead of the primary settler.

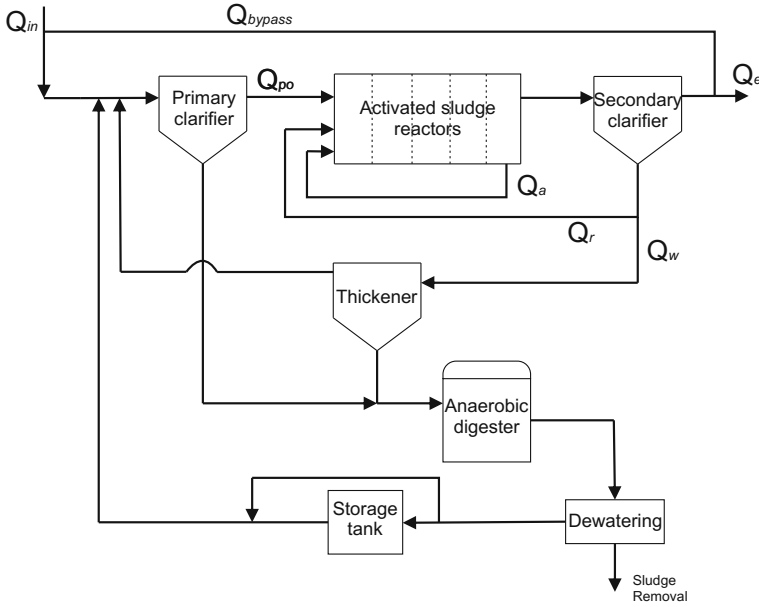


Fig. 2.2 BSM2 plant with notation used for flow rates

Models

This book is based on the implementation of control strategies in the zone of biological treatment of BSM2. For this reason, the explanation of the simulation model is focused on the activated sludge reactors. As in BSM1, the activated sludge reactors consist in five biological reactor tanks connected in series. Q_a from the last tank complete the system. The design of the BSM2 plant is modified with respect to BSM1. It has an average influent dry weather flow rate of 20,648.36 m³/d and an average COD in the influent of 592.53 mg/l. The total volume of the bioreactor is 12,000, 1500 m³ each anoxic tank and 3000 m³ each aerobic tank. Its hydraulic retention time, based on the average dry weather flow rate and the total tank volume, is 14 h. The internal recycle is used to supply the denitrification step with S_{NO} .

ASM1 also describes the biological phenomena that take place in the biological reactors of BSM2. However, unlike BSM1, the temperature is considered in the BSM2.

The general equations for mass balancing are the same as in BSM1, but in this case Q_{in} and Z_{in} are replaced by Q from the primary clarifier (Q_{po}) and Z from the primary clarifier (Z_{po}), respectively

- For reactor 1:

$$\frac{dZ_1}{dt} = \frac{1}{V_1} (Q_a \cdot Z_a + Q_r \cdot Z_r + Q_{po} \cdot Z_{po} + r_{z,1} \cdot V_1 - Q_1 \cdot Z_1) \quad (2.19)$$

- For reactors 2–5:

$$\frac{dZ_k}{dt} = \frac{1}{V_k} (Q_{k-1} \cdot Z_{k-1} + r_{z,k} \cdot V_k - Q_k \cdot Z_k) \quad (2.20)$$

The proposed control strategies in this work are based on r_{NH} and r_{NO} . They are shown in the following equations:

$$r_{NH} = -0.08\rho_1 - 0.08\rho_2 - \left(0.08 + \frac{1}{0.24}\right)\rho_3 + \rho_6 \quad (2.21)$$

$$r_{NO} = -0.1722\rho_2 + 4.1667\rho_3 \quad (2.22)$$

where ρ_1 , ρ_2 , ρ_3 , ρ_6 are four of the eight biological processes defined in ASM1. Specifically, ρ_1 is the aerobic growth of heterotrophs, ρ_2 is the anoxic growth of heterotrophs, ρ_3 is the aerobic growth of autotrophs and ρ_6 is the ammonification of S_{ND} . They are defined as

$$\rho_1 = \mu_{HT} \left(\frac{S_S}{10 + S_S} \right) \left(\frac{S_O}{0.2 + S_O} \right) X_{B,H} \quad (2.23)$$

where μ_{HT} is

$$\mu_{HT} = 4 \cdot \exp \left(\left(\frac{\ln \left(\frac{4}{3} \right)}{5} \right) (T_{as} - 15) \right) \quad (2.24)$$

where T_{as} is the temperature

$$\rho_2 = \mu_{HT} \left(\frac{S_S}{10 + S_S} \right) \left(\frac{0.2}{0.2 + S_O} \right) \left(\frac{S_{NO}}{0.5 + S_{NO}} \right) 0.8 \cdot X_{B,H} \quad (2.25)$$

$$\rho_3 = \mu_{AT} \left(\frac{S_{NH}}{1 + S_{NH}} \right) \left(\frac{S_O}{0.4 + S_O} \right) X_{B,A} \quad (2.26)$$

where μ_{AT} is:

$$\mu_{AT} = 0.5 \cdot \exp \left(\left(\frac{\ln \left(\frac{0.5}{0.3} \right)}{5} \right) (T_{as} - 15) \right) \quad (2.27)$$

$$\rho_6 = k_{aT} \cdot S_{ND} \cdot X_{B,H} \quad (2.28)$$

where k_{aT} is defined as:

$$k_{aT} = 0.05 \cdot \exp \left(\left(\frac{\ln \left(\frac{0.05}{0.04} \right)}{5} \right) (T_{as} - 15) \right) \quad (2.29)$$

Test Procedure

The influent dynamics are defined for 609 days by means of a single file, which takes into account rainfall effect and temperature. Following the simulation protocol, a 200-day period of stabilization in closed-loop using constant inputs with no noise on the measurements has to be completed before using the influent file (609 days). Nevertheless, only the data generated during the final 364 days of the dynamic simulation are used for plant performance evaluation.

Evaluation Criteria

In the same way, as in BSM1, the assessment is made at two levels. The control performance is assessed by the ISE and IAE criteria, whereas the plant performance is evaluated by EQI, OCI, and the percentage that the pollutants concentration is over the limits given in Table 2.1. However, in this case OCI is modified adding the methane production (MET_{prod}) generated in the anaerobic digester and the net heating energy (HE_{net}), which is calculated as:

$$HE^{net} = \max(0, HE - 7 \cdot MET_{prod}) \quad (2.30)$$

where HE is the necessary energy to heat the anaerobic digester to the operating temperature, and it is calculated as:

$$HE = \frac{1000 \cdot 4.186}{86400 \cdot T} \int_{t=245days}^{t=609days} (T_{ad} - T_{ad,i}) Q_{ad}(t) \cdot dt \quad (2.31)$$

where T_{ad} is the temperature of the anaerobic digester, $T_{ad,i}$ is the temperature in the entrance of the anaerobic digester and Q_{ad} is the flow rate of the anaerobic digester.

Finally, the OCI in BSM2 is calculated as

$$OCI = AE + PE + 3 \cdot SP + 3 \cdot EC + ME - 6 \cdot MET_{prod} + HE_{net} \quad (2.32)$$

2.2 Basic Plant Operation

The definition of the BSM1 and BSM2 scenarios include default control strategies, which are commonly used as a reference for comparison.

The default control strategy of BSM1 [1] uses two Proportional-Integral (PI) control loops as shown in Fig. 2.3. The first one involves the control of $S_{O,5}$ by manipulating $K_L a$ in the fifth tank (K_{La5}). The set-point for $S_{O,5}$ is 2 mg/l. The second control loop has to maintain $S_{NO,2}$ at a set-point of 1 mg/l by manipulating Q_a .

In the case of BSM2, [33] proposes a default control strategy (defCL). Its closed-loop control configuration consists of a PI that controls S_O in the fourth tank ($S_{O,4}$) at

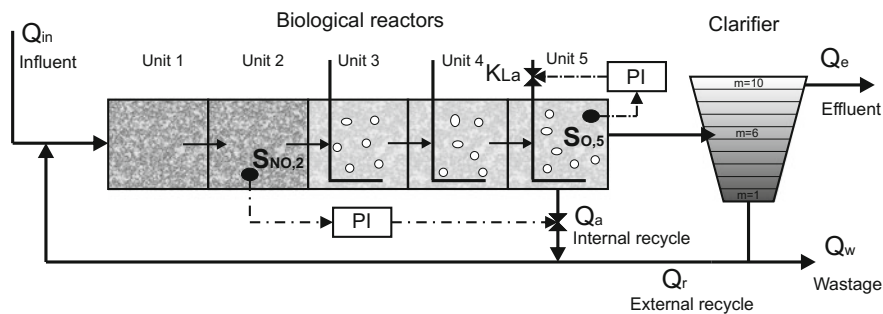


Fig. 2.3 Default control strategy of BSM1

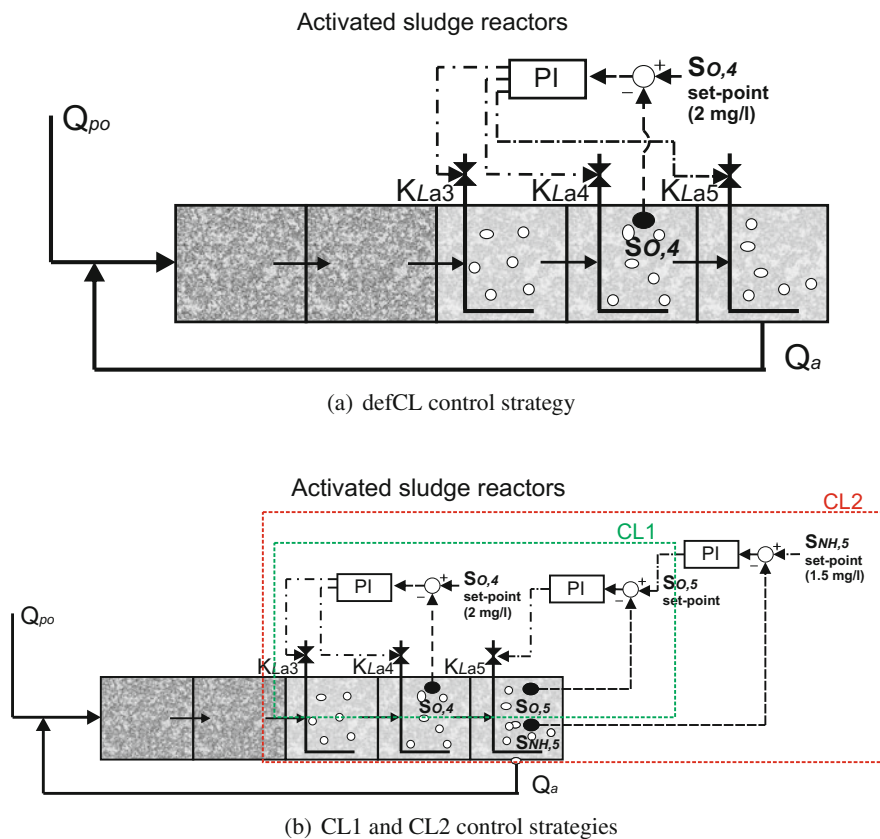


Fig. 2.4 Default control strategies of BSM2

a set-point of 2 mg/l by manipulating $K_L a$ in the third tank (K_{La3}), $K_L a$ in the fourth tank (K_{La4}) and K_{La5} , with K_{La5} set to the half value of K_{La3} and K_{La4} . In addition, q_{EC} in the first reactor ($q_{EC,1}$) is added at a constant flow rate of 2 m³/d. Two different Q_w values are imposed dependent on time of the year: from 0 to 180 days and from 364 to 454 days Q_w is set to 300 m³/d; and for the remaining time periods Q_w is set to 450 m³/d.

The finalisation of BSM2 plant layout is reported in [46], in which two new control strategies are proposed. The first control strategy (CL1) is based on modifying the defCL, controlling the $S_{O,4}$ set-point at 2 mg/l, by manipulating K_{La3} and K_{La4} , and adding another loop to control $S_{O,5}$ by manipulating K_{La5} . PI controllers are applied for both control loops. The second control strategy (CL2) adds a hierarchical control to CL1. Therefore, a PI controller is applied to control S_{NH} in the fifth tank ($S_{NH,5}$) at a set-point of 1.5 mg/l by manipulating $S_{O,5}$ set-point. In the case of CL2, $q_{EC,1}$ is added at a constant value of 1 m³/d.

Figure 2.4 shows the three explained control strategies.

2.3 Summary

This chapter has introduced the scenarios where the evaluation of the control and operation approaches will be tested. These scenarios are based upon the well known benchmarks commonly used within the wastewater research community. A short description of the BSM1 and BSM2 as well as their basic control strategies have been provided. They are used in the literature in order to compare the results achieved with new control strategies or techniques, in terms of control performance and/or plant performance.

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