Model predictive control of purple bacteria in raceway reactors
Handling microbial competition, disturbances, and performance

Moradvandi, Ali; De Schutter, Bart; Abraham, Edo; Lindeboom, Ralph E.F.

DOI
10.1016/j.compchemeng.2024.108981

Publication date
2024

Document Version
Final published version

Published in
Computers and Chemical Engineering

Computers and Chemical Engineering 194 (2025) 108981

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/cace

Model predictive control of purple bacteria in raceway reactors: Handling microbial competition, disturbances, and performance

Ali Moradvandi [a,b,*], Bart De Schutter [b], Edo Abraham [a], Ralph E.F. Lindeboom [a]

[a] Department of Water Management, Delft University of Technology, Mekelweg 5, 2628 CD, Delft, The Netherlands
[b] Delft Center for Systems and Control, Delft University of Technology, Mekelweg 2, 2628 CD, Delft, The Netherlands

ARTICLE INFO

Keywords:
Purple bacteria
Model predictive control
Supervisory control
Hierarchical decision-making control
Override control

ABSTRACT

Purple Phototrophic Bacteria (PPB) are increasingly being applied in resource recovery from wastewater. Open raceway-pond reactors offer a more cost-effective option, but subject to biological and environmental perturbations. This study proposes a hierarchical control system based on Adaptive Generalized Model Predictive Control (AGMPC) for PPB raceway reactors. The AGMPC uses simple linear models updated adaptively to project the complex process dynamics and capture changes. The hierarchical approach uses the AGMPC controller to optimize PPB growth as the core of the system. The developed supervisory layer adjusts set-points for the core controller based on two operational scenarios: maximizing PPB concentration for quality, or increasing yield for quantity through effluent recycling. Lastly, due to competing PPB and non-PPB bacteria during start-up phase, an override strategy for this transition is investigated through simulation studies. The Purple Bacteria Model (PBM) simulates this process, and simulation results demonstrate the control system's effectiveness and robustness.

1. Introduction

Cultivation of Purple Phototrophic Bacteria (PPB) has been gaining importance as a promising alternative for microalgae for nutrient and resource recovery in general. The beneficial aspect of nutrient recovery, coupled with the assimilation of Chemical Oxygen Demand (COD) in wastewater treatment, positions PPB as a viable solution for industrial wastewater resources, consequently contributing to the fertilizer-feed-food-fork chain (Capson-Tojo et al., 2020). It reflects the increasing interests into the application of PPB under various growth conditions over the last decade (Hulsen et al., 2016; Cerruti et al., 2020; Capson-Tojo et al., 2023b).

Owing to PPB's metabolic versatility, they can use a broad range of organic compounds for growth, both in the presence and absence of light (photoheterotrophic and chemoheterotrophic grown) and oxygen (aerobic and anaerobic conditions) (Capson-Tojo et al., 2020). PPB cultivation has proven effective in anaerobic closed photobioreactors. Puyol et al. (2017) have discussed the mechanistic growth metabolisms of PPB in this type of reactor environments and have proposed the Photo-Anaerobic Model (PAnM). While closed controlled systems like membrane and tubular photobioreactors and illuminated stirred reactors offer ideal conditions for maximizing PPB microbial selectivity, open raceway-pond reactors require lower capital and operational expenses (Alloul et al., 2021). The PAnM accurately represents PPB performances for controlled reactors in research labs, however, the extended PAnM (ePAnM) (Capson-Tojo et al., 2023a) and Purple Bacteria Model (PBM) (Alloul et al., 2023) are not limited to photo-anaerobic conditions by taking diverse metabolic capabilities of PPB across various varying environmental conditions into account. More specifically, the PBM mechanistically represents PPB growth in a sequencing batch configuration of raceway reactors, and has been calibrated for alternating aerobic and anaerobic conditions as well as various metabolic growth pathways of PPB (Alloul et al., 2023).

Although raceway reactors are potentially cost-effective industrial options for scale-up, biomass growth productivity can be easily perturbed due to limited control over operating conditions (de Andrade et al., 2016). Therefore, implementing automatic control systems can be a solution for ensuring bioreactor robustness against inevitable operational variations. In recent years, control of microalgae biomass production in tubular and raceway reactors have been studied by proposing various advanced control strategies, like linear active disturbance rejection control (Carreño-Zagarra et al., 2019), hierarchical optimization-based control (Fernández et al., 2016), and learning-based model predictive control (Pataro et al., 2023). These methods have been tailored for microalgae and their dynamics and metabolisms, while PPB responds differently to environmental conditions owing to their different and highly versatile metabolisms, like ability for high

* Corresponding author.
E-mail address: a.moradvandi@tudelft.nl (A. Moradvandi).

https://doi.org/10.1016/j.compchemeng.2024.108981
Received 29 July 2024; Received in revised form 4 December 2024; Accepted 10 December 2024
Available online 17 December 2024

yield on organic carbon sources and utilization of the near infrared light spectrum. Alloul et al. (2019) have shown that efficient PPB production can be achieved utilizing fermented wastewater that is enriched in volatile fatty acids (VFAs). They have also experimentally investigated various operational strategies impacting the PPB growth in raceway reactors (Alloul et al., 2021).

The mechanistical understanding acquired through the aforementioned investigations has been incorporated in the PBM. Basically, the system configuration is made on a fixed daily sequencing batch through a natural 12 h dark and 12 h light regime, fed by VFAs, while taking the stirring effect of the paddle wheel into account. The growth of PPB encompasses three main pathways: photo-, aerobic, and anaerobic chemotrophic metabolisms. Observations have shown that due to the constant transition between dark and light conditions, all these pathways can contribute to PPB growth, even when a specific operational condition seems predominant (Alloul et al., 2021). This metabolic-mechanistic switch (Alloul et al., 2023) has been incorporated into the PBM by introducing an empirical constant for parallel metabolic growth (Alloul et al., 2023). Although this parameter can be fine-tuned through dedicated experiments, it remains a significant source of model mismatch. Furthermore, the open reactor environment of a raceway pond is conducive for microbial competition between PPB and non-PPB, when PPB are not the dominant trophic group. From the work by Alloul et al. (2021), as a consequence of being exposed to air with fluctuating diffusion causing by paddle wheel operation, the low but alternating dissolved oxygen concentration, seems to be particularly important. Light intensity and wavelength are other factors affecting PPB growth in raceway reactors that would affect the growth if not controlled (Cerruti et al., 2022).

Thus, design of a control system to optimize reactor performance under these challenging conditions is desired. As discussed above, such a control system would need to enhance the stability and efficiency of PPB cultivation under complex biological dynamics and meteorological fluctuations. Advanced control strategies like model predictive control (MPC) has shown its applicability and credibility for various biological wastewater treatment systems (Gupta et al., 2022; Han et al., 2021). The adaptive version of Generalized Model Predictive Control (GMPC) (Clarke et al., 1987) presents a control strategy for processes with intricate dynamics, such as the sophisticated microbial dynamics of PPB as described by the PBM. This approach involves simplifying the complex system into input–output dynamics and continuously updating parameters to mimic the evolving behavior of the actual process under varying operational conditions, uncertainties, and perturbations. Furthermore, the continuous changes in operational conditions pose the challenge of adapting the set-point to optimize process performance throughout the operation, which can be effectively tackled through a hierarchical control strategy assigning an appropriate set-point (Sadeghassadi et al., 2018; Ghanavati et al., 2021).

According to the authors' best knowledge, advanced control of PPB-based raceway reactor has not reported in the existing literature. Therefore, this paper introduces a control configuration for a PPB-based raceway reactor. The primary controller is based on Adaptive GMPC (AGMPC), and a supervisory layer is responsible for determining an appropriate set-point given an operational decision strategy and current process status. An operational decision is made based on either a water quality-driven scenario, which reduces effluent VFA as much as possible to increase PPB concentration as well as treatment efficiency, or a quantity-driven scenario, which increases the production rate, and thereafter the yield, by recycling unconverted effluent VFA. Additionally, an override control strategy is integrated into the system to facilitate the transition from the start-up phase to the PPB-dominant phase. The proposed control strategy is operationally advantageous in the following ways:

- Assigning appropriate time varying set-points for PPB concentration, employing a supervisory layer to determine based on two operational scenarios, i.e. quality-driven and quantity-driven under varying operational scenarios.
- Maintaining PPB concentration at the desired set-point under different illumination scenarios and light perturbations.
- Maintaining PPB concentration at the desired set-point even when parallel metabolic growth constant is unknown and the contribution of the different metabolic PPB pathways (photoheterotrophic, anaerobic, and aerobic chemoheterotrophic) to the overall PPB growth cannot be quantified.
- Suppressing the growth of other competing bacterial species, enabling moving towards the desired set-point for PPB concentration under non-steady-state conditions more swiftly (i.e. start up phase) using override phase-based control that regulates the paddlewheel.
- The proposed applied controller, based on an adaptively updated linear input–output model, ensures a low computational burden, and utilizes available measurements to effectively capture process variations and disturbances at each time step.

The paper is organized as follows. Section 2 includes the PPB process description and the corresponding control challenges to be addressed. Section 3 presents the PPB control system by discussing the control configuration for PPB-based raceway reactor integrating adaptive generalized model predictive control, override phased-based control, and decision-making supervisory layer. Finally, the proposed control strategy is assessed via comprehensive simulation studies in Section 4, and in the last section, conclusions are drawn.

2. PPB process description

A first-principle model, describing a biological wastewater treatment process, is a valuable tool to design, optimize, and control a process. Purple Phototrophic Bacteria (PPB) dynamics can be mechanistically represented by the Purple Bacteria Model (PBM) (Alloul et al., 2023). The PBM is the extended model based on the PAnM (Puyol et al., 2017) and the ePAnM (Capson-Tojo et al., 2023a) for growth of PPB in open raceway-pond reactors. A summary of the model dynamics is provided in Appendix. The PBM thus serves as a reliable benchmark to analyze the PPB dynamics, considering the complexity of microbial versatility of PPB as well as competition between PPB and non-PPB. Therefore, in this work, it will be used as a benchmark to simulate the growth of PPB in a raceway-pond reactor and assess the performance of the proposed control system. In this section, a few notable behaviors of the process are described with respect to the PBM, which should be taken into account for designing a control system and assessing its performance.

2.1. Metabolic versatility of PPB

The PBM describes the PPB's microbial versatility among the photoheterotrophic ($X_{PB,ph}$), and both anaerobic ($X_{PB,anc}$) and aerobic chemoheterotrophic ($X_{PB,aec}$) growth of PPB. This mechanistic-metabolic microbial dynamical selection is modeled through an empirical constant called the parallel metabolic growth constant (M_S). This factor is responsible for the contribution of alternative pathways to PPB growth alongside the dominant pathway, resulting in model mismatches. These mismatches stem from its variations during operation, transitions between light and dark conditions, and the challenge of precisely determining the constant empirically through timely experiments (Alloul et al., 2021). Variations of M_S result in different values of PPB concentration during operation, as all these pathways can contribute to PPB growth.

2.2. PPB competitors

In addition to PPB, non-PPB are considered within the microbial biomass of the PBM. Non-PPB are divided into aerobic bacteria (X_{AEB}) and anaerobic bacteria (X_{ANB}). Since the raceway-pond reactor is an open system, aerobic bacteria are the main competitor of PPB. This competition can impact control performance, especially during the start-up phase when PPB concentration is not dominant. Although, the oxygen concentration in raceway reactors is nearly zero, using the paddlewheel to pass oxygen through the bulk, it affects the competition between PPB and non-PPB, particularly when PPB are not the dominant species.

2.3. Light irradiance, attenuation, and distribution

Light is a crucial input factor to support the photoheterotrophic growth of PPB. Light intensity is considered constant during daylight times; this assumption can be reliable if an artificial illumination system is used (Cerruti et al., 2022). Otherwise, the controller should be able to deal with a Gaussian-like illumination intensity that represents the real-world scenario in which the circadian rhythm is perturbed with cloud formation. Therefore, meteorological fluctuations and incoming suspended solids may disturb light distribution and attenuation.

2.4. Maximum yield of PPB

PPB is metabolically capable of using energy and carbon sources to grow (Imhoff, 2006). In other words, light as an energy source and chemical oxygen demand (COD) in wastewater as a carbon source are required to efficiently cultivate PPB. In this sense, fermented wastewater including mostly volatile fatty acids (VFAs) has been considered by Alloul et al. (2019) and Capson-Tojo et al. (2020) as favorable carbon sources for PPB microbial selectivity. Depending on the availability of varying amounts of these two sources, the maximum yield achievable during operation can vary. Therefore, the control system should be designed in such way that it makes best use of available sources, subject to fluctuations, to enhance the process performance.

3. PPB control system

In this section, a step-by-step design of an advanced control system aimed at tackling the mentioned control challenges for PPB utilization in raceway reactors is discussed. The primary control objective is to regulate the concentration of PPB during operation, subject to biological and meteorological fluctuations. Among the advanced control strategies, model predictive control (MPC), which has demonstrated its efficiency and applicability in various biological wastewater treatment processes (Han et al., 2021; Ghanavati et al., 2021), is selected as the core of the control system. To improve efficiency, a supervisory layer is also developed, accounting for an appropriate set-point to be assigned for the MPC controller based on two operational scenarios. An override control strategy is also proposed for the condition when the PPB are not dominant. The developed control system for the raceway reactor is illustrated in Fig. 1. It includes three main components: (i) phased-based controller: it serves as an override control mechanism, facilitating the transition to the MPC controller for PPB concentration during the start-up operation; (ii) main controller: this component is dedicated to regulating PPB concentration and to manage process uncertainties and potential disturbances effectively; and (iii) Decision-making supervisory layer: it acts as a supervisory layer to assign an appropriate PPB set-point concentration based on the preferred operational strategy and the process condition. In the following, the adaptation of the control architecture based on MPC for PPB cultivation in a raceway-pond reactor, and developing the supervisory layer and the override control strategy will be discussed.

3.1. Control of PPB raceway reactors

PPB raceway reactors are modeled as a sequential batch process with daily cycles of filling and extracting the reactor with influent and effluent, respectively. As discussed by Alloul et al. (2021), a favorable operational strategy is 12 h light/12 h dark condition with 24 h stirring, where the reactor is fed by the VFA-based medium before the start of the light condition. To maintain a constant reactor volume, the feeding and extraction rates are kept equal. From an automatic control point of view, practical manipulated variables include the concentration and the flowrate of influent. If the concentration of the incoming medium is assumed to be constant, the feeding flowrate is the feasible control action to regulate PPB concentration.

Given the operational conditions of the raceway reactor, the significance of employing MPC becomes evident. With the reactor being fed once a day and the complex behavior of microorganisms characterized by long response times, making predictions over a horizon and controlling the process accordingly becomes crucial. Therefore, while the simulation (process) time step is an hour, the controller time step is a day (24 h). As depicted in Fig. 2, at time step $24k$, where k is an integer value, measured PPB concentrations (measured X_{PB}) and implemented feeding rates (past u) at past times like $24(k-1)$, $24(k-2)$, $24(k-3)$, etc. are utilized to predict PPB concentrations over a prediction horizon (N_p) and calculate planned control action over a control horizon (N_u) accordingly. This concept is similar to event-based MPC (Pawlowski et al., 2012, 2014), where the event is fixed in this work. This concept also allows for sufficient time to determine PPB concentration daily with an off-line spectroscopic measurement combined with conventional TSS/VSS monitoring if real-time monitoring is not available (Cerruti et al., 2020).

3.2. Adaptive GMPC algorithm: main controller

Model predictive control is a model-based control strategy. Although the mechanistic PBM model provides detailed process dynamics, using it as the base model for MPC controller presents significant challenges. Due to its complex biological characteristics and integrated structure, the PBM model is highly nonlinear. As a result, employing such a large model for MPC controller design leads to a nonlinear non-convex optimization problem that must be solved at each control step, causing computational complexities and a heavy burden (Ahmed and Rodríguez, 2020). Furthermore, designing an MPC controller based on this model requires either measurements or estimations of every state variable at each control step. Measuring all the state variables is economically and practically unfeasible (Dochain, 2013), while developing a state estimator is also challenging, particularly for PPB states that grow through different pathways ($X_{PB,ph}$, $X_{PB,anc}$, and $X_{PB,aec}$). Additionally, the effectiveness of MPC relies on the accuracy of the model, but the PBM model is susceptible to potential mismatches, such as those related to the parallel PPB growth constant (M_S). Therefore, an input–output model is employed in this work to characterize the relationship between the feeding flow rate and the PPB concentration. To capture the variation of the process as those related to the nature of the process like parallel growth pathways as well as external disturbances, an adaptive version of the input–output model is employed. This adaptive approach allows the model parameters to be updated based on a new set of observations, ensuring accurateness of predictions as well as robustness of the controller against biological and meteorological variations. Given the input–output model as the basis of MPC, the generalized model predictive control (GMPC) algorithm can be used as a feedback controller (Clarke et al., 1987). In this method, the GMPC controller calculates the control actions over a control horizon (N_u) that minimizes a cost function based on a prediction horizon (N_p). The cost function, J, is defined as follows:

$$J = \sum_{j=1}^{N_p} \delta\,[\hat{y}(k+j|k) - w(k+j)]^2 + \sum_{j=1}^{N_u} \lambda\,[\Delta u(k+j-1)]^2, \tag{1}$$

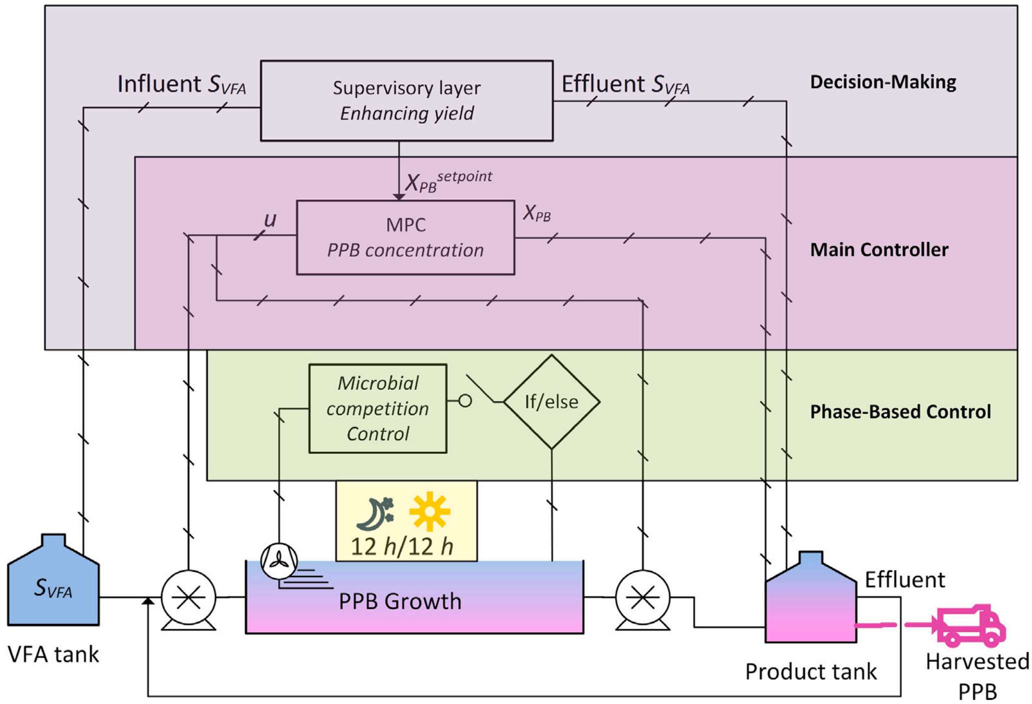

Fig. 1. MPC-based control system architecture for a raceway reactor. The figure illustrates the three main components of the control system: (i) the phased-based controller for transitioning to the MPC controller, (ii) the main controller for regulating the PPB concentration while handling uncertainties and disturbances, and (iii) the decision-making supervisory layer for assigning the PPB set-point concentration based on a preferred operational strategy.

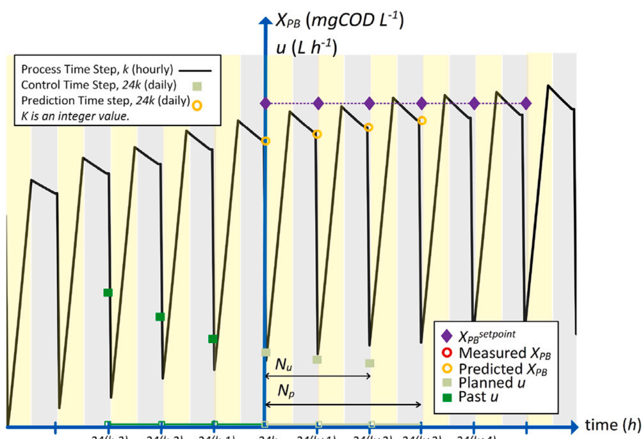

Fig. 2. Schematic representation of the raceway reactor operation and the integration of model predictive control: hourly process time step vs daily control time step.

where $\hat{y}(k+j)$, $w(k+j)$, and $\Delta u(k+j)$ denote the $j-$step ahead prediction on data up to time step k, the future set-point, and the planned control increment, respectively. Moreover, δ and λ are the controller design parameters representing the error and the control weighting factors. The predicted output, $\hat{y}$, of the actual output, y, over the prediction horizon N_p is obtained by a single-input single-output discrete time linear model as follows:

$$A(q^{-1})y(k) = B(q^{-1})u(k) + \epsilon(k)/\Delta, \tag{2}$$

in which

$$\Delta = 1 - q^{-1}, \tag{3}$$

where ϵ denotes zero mean white noise, and $A(q^{-1})$ and $B(q^{-1})$ are the linear models. These linear models are the rational functions of the time shift operator q^{-1} (i.e. $q^{-d}x_k = x_{k-d}$ for $d \in \mathbb{Z}$) that can be written as follows:

$$A(q^{-1}) = 1 + a_1 q^{-1} + \cdots + a_{n_a} q^{-n_a}, \tag{4a}$$

$$B(q^{-1}) = b_0 + b_1 q^{-1} + \cdots + b_{n_b} q^{-n_b}, \tag{4b}$$

in which n_a and n_b express the order of the system with respect to the outputs and inputs, respectively. Since, the adaptive version of the GMPC controller is considered to tackle with improper future predictions, the parameters of model (2) should be updated. If we consider $\theta = [a_1, \dots, a_{n_a}, b_0, \dots, b_{n_b}]^T$ as the vector of the linear model coefficients, the online estimation of this parameter vector at time step k, i.e. $\hat{\theta}(k)$, can be derived using the least-squares method as follows:

$$\hat{\theta}(k) = \hat{\theta}(k-1) + \frac{P(k-1)\phi^T(k)}{1 + \phi^T(k)P(k-1)\phi(k)}(y(k) - \hat{y}(k)), \tag{5}$$

where $\phi(k)$ is the augmented vector of past input and output observations, $P(k)$ is the covariance matrix, and $\hat{y}(k)$ is the prediction output. The identification process can be written as follows:

$$\phi(k) = [y(k-1), \dots, y(k-n_a), u(k), \dots, u(k-n_b)]^T, \tag{6a}$$

$$P(k) = P(k-1) + \frac{P(k-1)\phi^T(k)\phi(k)P(k-1)}{1 + \phi^T(k)P(k-1)\phi(k)}, \tag{6b}$$

$$\hat{y}(k) = \phi^T(k)\hat{\theta}(k-1). \tag{6c}$$

Given this adaptive model, the minimization of the cost function J expressed by (1) can be explicitly derived, assuming no constraints on the control signals (Camacho et al., 2007). Therefore, if $\mathbf{f}$ is defined as the free response of the process, the optimal vector of the planned control actions, i.e. $\mathbf{u}$ can be written as

$$\mathbf{u} = (\mathbf{G}^T\mathbf{G} + \lambda\mathbf{I})^{-1}\mathbf{G}^T(\mathbf{w} - \mathbf{f}), \tag{7}$$

where $\mathbf{G}$, $\mathbf{I}$, and $\mathbf{w}$ express the step response matrix of the system, the identity matrix, and the vector of the future set-points, respectively. However, the actual control action sent to the process, is the first element of the vector $\mathbf{u}$ that can be written as

$$\Delta u = \mathbf{K}(\mathbf{w} - \mathbf{f}), \tag{8}$$

where $\mathbf{K}$ denotes the first row of the matrix $(\mathbf{G}^T\mathbf{G}+\lambda\mathbf{I})^{-1}\mathbf{G}^T$. Now, the first element of Δu is the implemented control action, and the rest of the elements are planned ones that will be re-updated during next control time steps. The adaptation of the system parameters is reflected in the response matrix of the system ($\mathbf{G}$) and the free response ($\mathbf{f}$). In other words, to derive $\mathbf{G}$, we need to find two polynomials E_j and F_j based on the Diophantine equation as follows:

$$1 = E_j(q^{-1})\Delta A(q^{-1}) + q^{-j}F_j(q^{-1}), \tag{9}$$

in which the degrees of polynomials E_j and F_j are n_a and $j-1$ (j as in (1)), respectively, and they can be derived by dividing 1 by $\Delta A(q^{-1})$ until the reminder is a factor of $q^{-j}F_j(q^{-1})$, and then, the quotient is $E_j(q^{-1})$. Therefore, the polynomial $G_j(q^{-1})$ can be written as

$$G_j(q^{-1}) = E_j(q^{-1})B(q^{-1}). \tag{10}$$

The matrix $\mathbf{G}$ is, then, an $N_u \times N_u$ matrix based on coefficients of the polynomial $G_j(q^{-1})$ (Camacho et al., 2007). The elements of the free response vector $\mathbf{f}$ can also be written as follows:

$$\mathbf{f}_{j+1} = q(1-\Delta A(q^{-1}))\mathbf{f}_j + B(q^{-1})\Delta u(k-d+j) \tag{11}$$

in which $\mathbf{f}_1 = y(k)$. Therefore, as can be seen in (9), (10), and (11), these are derived based on the system polynomials of $A(q^{-1})$ and $B(q^{-1})$. Therefore, as these system polynomials are updated at each time step, the response matrix of the system ($\mathbf{G}$) and the free response ($\mathbf{f}$) are also updated accordingly.

It should also be highlighted that the only physical constraint that may be taken into account in the actuator limits as follows:

$$u_{min} \le u \le u_{max}, \tag{12}$$

where u_{min} and u_{max} express the upper and lower bounds of the actuator inputs. Considering the reactor configuration, the lower bound is zero, while the upper bound can be defined based on the volume of the reactor. In case of taking the constraint into account, the optimization problem written by (1) subject to inequality constraint of (12) has to be solved numerically (Camacho et al., 2007).

3.3. Supervisory layer: decision-making operational scenarios

As discussed in Section 2.4, maximum productivity of PPB depends on availability of two sources, i.e. the light intensity and the VFA concentration in influent. From a design perspective, the daily product extraction is scheduled before sunrise. This implies that if there is too much VFA in the influent, such that the illumination of one day was insufficient to cultivate maximum productivity, there will be some unconverted VFA in the effluent. Therefore, determining an appropriate value for the desired PPB set-point concentration of the controller (w in the objective function J expressed by (1)) enables the control system to operate as efficiently as possible. In addition to this point, variations in each of these two sources highlight the importance of selecting the desired PPB set-point concentration.

In thinking of a suitable value for the desired PPB set-point concentration, it is essential to prioritize the operational strategy based on either "*quality*" or "*quantity*". In other words, increasing the feeding rate can enhance quantity but may compromise quality, and vice versa. Quantity and quality can be considered as a higher production rate and a higher PPB concentration, respectively. The production rate at control time step k can be defined as

$$Q(k) = X_{PB}(k)u(k), \tag{13}$$

where Q [mgCOD h^{-1}] denotes the production rate, but since the feeding is configured for only one hour per day, it can be considered as a daily production rate. Hence, increasing u may result in a higher production rate, but reduces the quality, i.e. X_{PB}. The another factor to consider is yield. This comes along as decreasing X_{PB} may lead to unconverted VFA remaining in the effluent. Yield of production, Y, at control time step k can be defined as follows:

$$Y(k) = \frac{Q(k)}{S_{\mathrm{VFA,i}}(k-1)u(k-1)}, \tag{14}$$

where $S_{\mathrm{VFA,i}}$ is the influent VFA concentration. To have some indications towards the factors defined, Table 1 provides the steady-state values of the open-loop process simulation. As can be seen, increasing the feeding flow rate (u) leads to a higher daily production (Q) but with less steady-state PPB concentration (X_{PB}). On the other hand, less PPB concentration results in less yield (Y), but some unconverted VFA in the outlet.

In addition to the discussion above, it is inevitable that fluctuations will occur in both incoming VFA and light intensity. It also highlights the importance of determining an appropriate desired PPB concentration given the process conditions. Therefore, a supervisory layer is developed in this paper to overcome this challenge. The supervisory layer is responsible for decision-making considering the current status of the process. Utilizing such a decision-making supervisory layer within the feedback loop enables the control system to update the desired set-point for the PBB concentration. Therefore, a criterion should be designed for quality-driven and quantity-driven strategies. In this sense, the concentration of VFA in the inlet and outlet plays a crucial role in determining the desired PPB set-point concentration, and thereafter the production rate and the yield. Considering the relations among Q, Y, and X_{PB}, the two following operational scenarios can be discussed:

- *Quality as priority*: In this scenario, the PPB set-point should be set as high as possible. A suitable measurement for tracking this trajectory could be the outlet VFA concentration. As this concentration approaches the minimum assigned value, i.e. S^{min}_{VFA}, it indicates that most portion of carbon sources have been consumed and converted to PPB. This indication provides valuable feedback to the controller subject to possible uncertainties, enabling it to calculate control actions even when no additional information is available for the biological and meteorological conditions. Therefore, a stepwise increase (ΔX_{PB}) is implemented for the set-point until the outlet VFA concentration goes below S^{min}_{VFA}. It should be noted that in practice a buffer range, like $S^{l}_{\mathrm{VFA,o}} \le S_{\mathrm{VFA,o}} < S^{u}_{\mathrm{VFA,o}}$ should be taken into account in order to keep the process operation stable. It should also be highlighted that using this scenario contributes to not only PPB output quality, but also to wastewater treatment by reducing output chemical oxygen demand (COD).
- *Quantity as priority*: In this scenario, by reducing the PPB set-point, the production rate will be increased. However, as can be seen by a few examples provided in Table 1, the yield is also decreased. To tackle this issue, a novel solution is to recycle the soluble effluent, which primarily consists of unconverted VFA. Yield without recycling can be written as (14). Recycling unconverted VFA reduces the amount of VFA required from the VFA tank, thereby increasing the yield to some extent. In other words, it can be written as follows:

$$S_{\mathrm{VFA,i}}(k+1)u(k+1) = S_{\mathrm{VFA,i}}(k+1)u^*(k+1) + S_{\mathrm{VFA,o}}(k)u(k), \tag{15}$$

where u^* is the required flow rate of VFA from the fermented stream, which obviously is less than what should be used without circulation. Given (14), the new yield based on circulation, Y_{rec}, can be written based on u^* as follows:

$$Y_{rec}(k) = \frac{X_{PB}(k)u(k)}{S_{\mathrm{VFA,i}}(k-1)u^*(k-1)}, \tag{16}$$

and by substituting (15), it gives

$$Y_{rec}(k) = \frac{X_{PB}(k)u(k)}{S_{\mathrm{VFA,i}}(k-1)u(k-1) - S_{\mathrm{VFA,o}}(k-2)u(k-2)}, \tag{17}$$

Table 1
Steady-state values of the inlet and outlet VFA, PPB concentration, yield, and daily production rate under three different operational conditions.

Light intensity 12 h dark/12 h light [W m^{-2}]	Paddlewheel 12h dark/12 h light	$S_{\mathrm{VFA,i}}$ [mgCOD L^{-1}]	u [L d^{-1}]	$S_{\mathrm{VFA,o}}$ [mgCOD L^{-1}]	Q [mgCOD d^{-1}]	$Y \times 100$	X_{PB} [mgCOD L^{-1}]
54	On/on	3000	20	≃0	17 792	29.6	889.6
			25	238.6	23 025	30.6	921.0
			30	637.8	25 713	28.6	857.1
60	On/on	3000	20	≃0	19 020	31.7	951.0
			25	127.5	24 332	32.4	973.2
			30	534.1	27 300	30.3	910.0
60	Off/on	2500	20	212.0	14 764	29.5	738.2
			25	594.4	17 187	27.4	687.5
			30	939.3	18 120	24.1	604.0

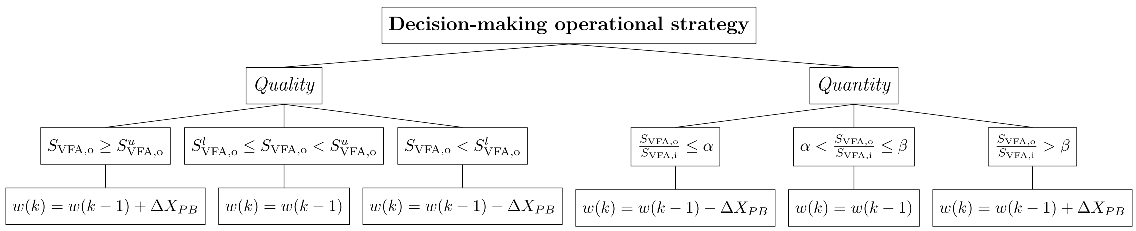

Fig. 3. Decision-making supervisory layer for assigning a suitable PPB concentration set-point based on either quality- or quantity-driven operational strategy.

in which it can be seen that $Y_{rec} > Y$ by comparing (17) and (14). In contrast to the alternative strategy, we should implement a stepwise reduction (ΔX_{PB}). However, we also require an indication for the set-point reduction. To do so, (17) is rewritten as follows:

$$\frac{1}{Y_{rec}(k)} = \frac{S_{\mathrm{VFA,i}}(k-1)u(k-1)}{X_{PB}(k)u(k)} - \frac{S_{\mathrm{VFA,o}}(k-2)u(k-2)}{X_{PB}(k)u(k)}, \tag{18}$$

and

$$\frac{1}{Y_{rec}(k)} = \frac{1}{Y(k)} - \frac{S_{\mathrm{VFA,o}}(k-2)}{S_{\mathrm{VFA,i}}(k-2)} \times \frac{S_{\mathrm{VFA,i}}(k-2)u(k-2)}{X_{PB}(k)u(k)}, \tag{19}$$

Now, it can be seen that a potential measurement indication can be $\frac{S_{\mathrm{VFA,o}}}{S_{\mathrm{VFA,i}}}$. In other words, as the process approaches its steady-state condition considering *recycling effluent*, this factor determines the amount of increase in yield. This strategy not only boosts production rates but also improves yield, which might otherwise decline, but is offset by recirculation. Like the other strategy, a buffer range is also required to be taken into account in practice for operational stability.

Considering these two operational strategies, i.e. *quality-driven* and *quantity-driven*, the decision-making layer can be formulated based on the decision tree given in Fig. 3. The assignment of the design parameters for this mechanistic decision tree, along with the complementary notes on upper and lower bounds ($S^u_{\mathrm{VFA,o}}$, $S^l_{\mathrm{VFA,o}}$, α, and β) will be discussed in a simulation study later.

3.4. Override start-up control: phased-based control

The microbial community considered in the PBM has been divided into three categories: PPB, aerobic bacteria (AEB), and anaerobic bacteria (ANB) (Alloul et al., 2023). Furthermore, three different growth pathways. i.e. photoheterotrophic (ph), aerobic chemoheterotrophic (aec), and anaerobic chemoheterotrophic (anc) have been defined for PPB. Since the operational condition is not favorable for anaerobic growth, concentrations of anaerobic bacteria (X_{ANB}) and anaerobic chemoheterotropic PPB ($X_{PB,anc}$) are very negligible. Therefore, the main competition is between other two types of PPB ($X_{PB,ph}$, $X_{PB,aec}$) with the non-photoheterotrophic aerobic chemoheterotrophic bacteria (X_{AEB}). More specifically, aerobic chemoheterotrophic PPB and aerobic chemoheterotrophic bacteria compete when oxygen levels are high, as both thrive under these conditions. Thus, the reactor environment can be divided into PPB-dominant and competitive phases. The competitive phase predominantly occurs during the start-up phase, when no microbial biomass dominates and the oxygen concentration is high. Once PPB becomes the dominant species, it enhances its growth accordingly. In other words, the reactor is then a PPB-dominated system, because of availability of light, excess in organic carbon, and limited oxygen conditions (Capson-Tojo et al., 2023a).

To facilitate the transition from the competitive phase to the PPB-dominant phase, the high oxygen concentration during start-up should be depleted (Alloul et al., 2021). The paddlewheel in the raceway reactor assists in smooth mixing of the bulk, while also promoting oxygen depletion by accelerating oxygen diffusion for growth, thus reducing the overall oxygen concentration (Alloul et al., 2023). As modeled in the PBM, two modes of operation are considered for the paddlewheel: on and off. The rotation speed is fixed and must not be too fast to avoid disturbing the settling PPB. Therefore, a feasible control action to moderate the transition to the PPB-dominant phase as well as the promotion of the PPB growth is the activation of the paddlewheel. Given that the paddlewheel operates in on/off modes, as explained, on/off control is the only available method. Since the process passes the competitive phase, it can be switched to the main MPC controller like an override control strategy, which brings the process from the start-up phase to the PPB-dominated operation (Chung et al., 2006; Sheik et al., 2022).

As can be seen in Fig. 4, the maximum capacity for PPB cultivation is attained when the paddlewheel operates continuously throughout the day. This outcome is biologically explainable, as lower levels of oxygen enhance the productivity of photoheterotrophic PPB (Capson-Tojo et al., 2021; Alloul et al., 2021). Furthermore, during the start-up phase, the high oxygen levels result in the aerobic bacteria's oxygen affinity being at its maximum level, consequently maximizing their production as depicted in Fig. 4. Therefore, to facilitate a smooth transition from the start-up phase, a heuristic control approach for regulating paddlewheel is implemented in this paper. This controller can effectively suppress the growth of aerobic bacteria. It is worth noting that utilizing this override approach, we can switch from this on/off control to the main MPC controller, when the competition between PPB and non-PPB is minimal. This strategic activation helps preventing any sudden changes that might otherwise destabilize the process. This is chosen because the process stability is crucial, given that the solution

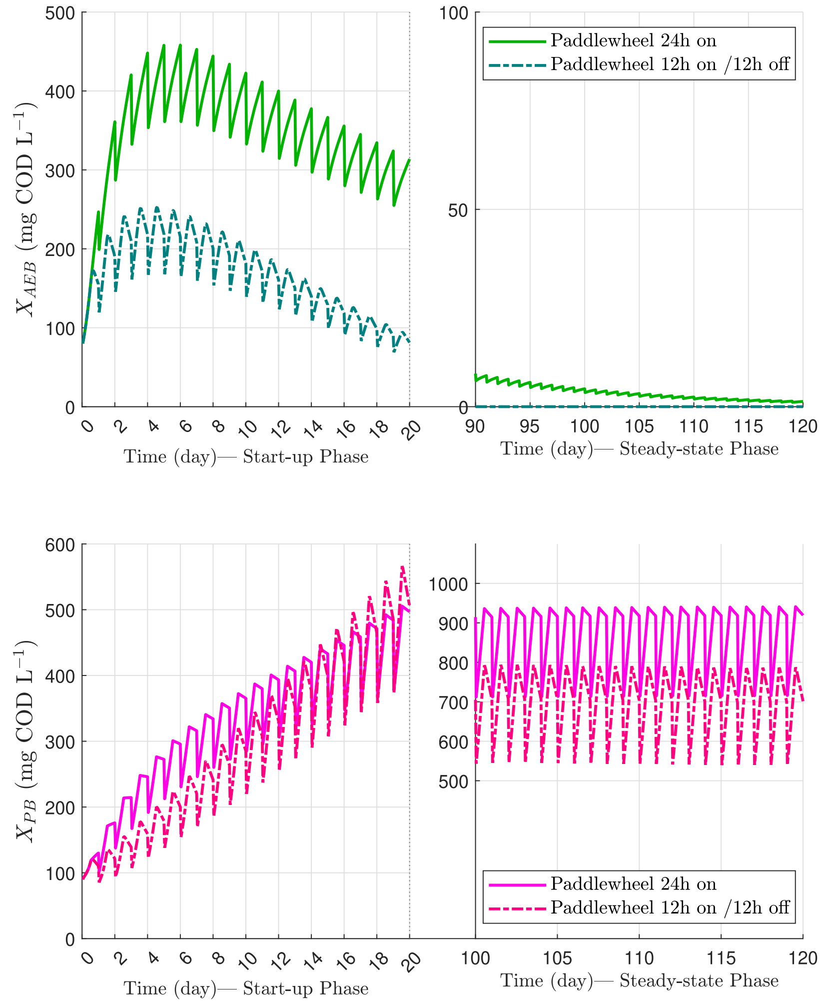

Fig. 4. Open loop outputs for PPB (X_{PB}) and aerobic bacteria (X_{AEB}) for two phases, i.e. start-up and steady-state under two operational conditions w.r.t. the paddlewheel.

of the objective function (1) relies mainly on appropriate initialization. In the next section, the implementation of the developed control system and its results will be discussed.

4. Results and discussions

In this section, the proposed control strategy is assessed via a step-by-step simulation study. First, the main controller is evaluated, including an assessment of its effectiveness and robustness against the most critical model mismatch, namely PPB microbial parallel growth constant, and the most probable disturbances, namely light perturbation and incoming VFA concentration. Secondly, the effectiveness of the phase-based override controller is discussed, and finally, the performance of the main controller coupled with the supervisory layer is assessed.

4.1. MPC for PPB concentration: performance assessment under different perturbations

Given the control structure discussed in Section 3.1, to assess the performance of the proposed controller, the process is considered in the PPB-dominant condition with 24 h paddlewheel in use. Prediction and control horizons are determined based on the process settling time to the open-loop step response. As a role of thumb (Seborg et al., 2016), the control horizon N_c can be chosen between $\frac{t_s}{3\Delta t} < N_c < \frac{t_s}{2\Delta t}$, in which t_s denotes the settling time that is around 8 d in this case for step response w.r.t. the feeding rate, and Δt expresses the sampling time, which is set to 1 d as discussed in Section 3.1. The prediction horizon is also selected close to the control horizon (Seborg et al., 2016). Hence, N_c and N_p are assigned the value of 4 d and 5 d, respectively. The constraint on the control input can be posed based on the reactor volume. Since the total reactor volume is 100 L in the PBM, the upper limit can be physically considered 40 L h^{-1}, while the lower limit can be zero, i.e. $0 \leq u \leq$ 40L/h. In addition, the model expressed by (2) is taken into account as the base model of the MPC controller. The order of model is set to $n_a = 1$ and $n_b = 1$ with respect to the output and the input, respectively. Thus, the parameter vector to be updated at each time step is $\theta = [a_1, b_0, b_1]^T$. As increasing the order did not improve the performance, and the chosen orders provide sufficient control performance, these values are considered fixed for the simulation studies.

Four operating scenarios: (i) set-point tracking without disturbance; (ii) set-point tracking subject to fluctuation in incoming VFA; (iii) set-point tracking under different illumination scenarios; and (iv) set-point tracking with mismatch in the PPB parallel growth constant are considered to assess the controller performance. As depicted in Fig. 5, the AGMPC controller is able to track the assigned set-points by regulating the feeding flow rate as the control action. As mentioned in Table 1, the steady-state equilibrium of the system with initial feeding rate of 25 L h^{-1} is 921 mgCOD L^{-1}, in which by lowering the PPB set-point concentration, the production rate can be increased. Such an observation brought us to design a supervisory layer. Moreover, it has been observed that assigning a set-point either too high may cause process instability, since required amounts of carbon sources may not

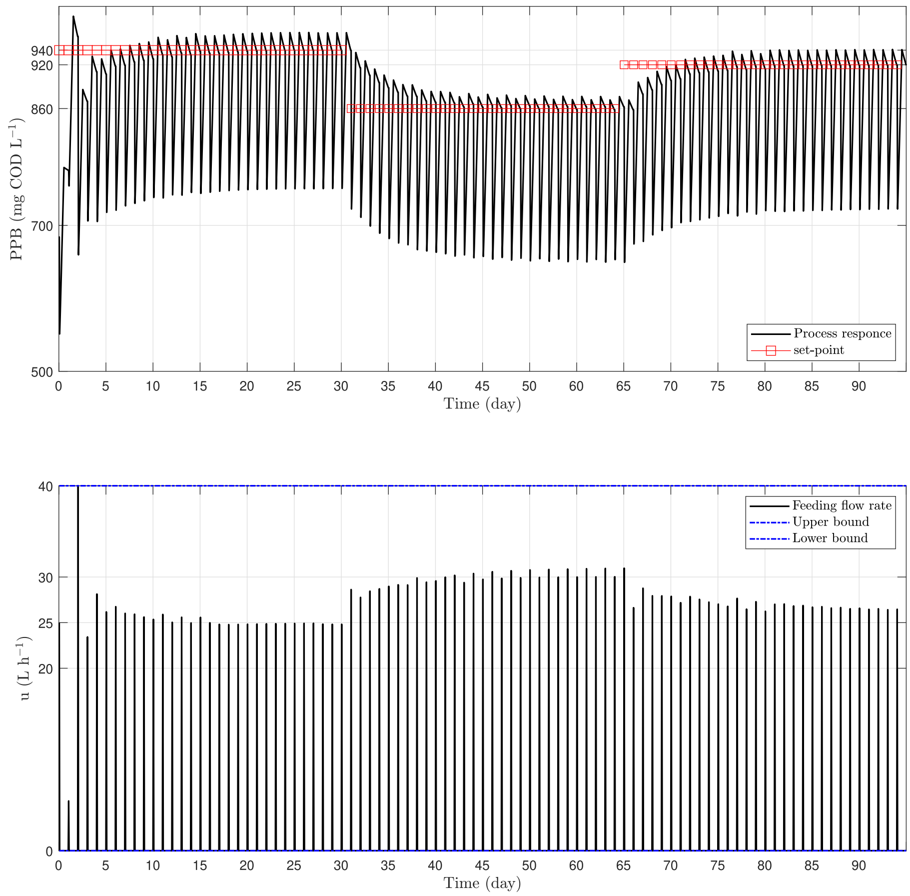

Fig. 5. AGMPC set-point tracking – process response and control action.

be available to convert to PPB, or too low may violate the actuator constraint and drastically decrease the performance and yield. This one also motivates to introduce a supervisory layer to avoid such occurrences.

While having a storage tank for VFA produced from an anaerobic fermentation process helps to stabilize the VFA concentration feeding to the raceway reactor, fluctuations in VFA levels are inevitable. To assess the designed AGMPC controller, a potential $\pm 20\,\%$ disturbances for the nominal incoming VFA concentration is implemented to the process. As shown in Fig. 6, the controller is able to keep the process stable to the assigned set-point, subject to the incoming VFA disturbances. As mentioned previously, light and VFA are the two main sources for PPB growth. In case of a significant decrease in VFA such that there is no sufficient VFA biologically available to convert and reach the designated PPB set-point concentration, especially in the presence of adequate light intensity, the process may become unstable. This instability arises from the absence of an optimal solution for the control action within the considered actuator constraints. For instance, for a $-20\,\%$ decrease in the nominal inlet VFA, the outlet PPB concentration can be deceased by $100\,\mathrm{mgCOD\,L^{-1}}$ without adjusting the feeding rate. Conversely, a significant increase in VFA poses less of a challenge. However, assigning a set-point concentration that is too low can lead to diminished yield and productivity, as significant amounts VFA may remain unconverted. This again highlights the importance of a suitable set-point to be assigned, considering the process status.

To assess the robustness of the proposed control strategy against light intensity, three illumination scenarios are considered, namely (i) controlled (constant) illumination with a constant intensity of $54\,\mathrm{W\,m^{-2}}$, (ii) natural illumination with the total intensity equal to the controlled illumination, and (iii) natural illumination with uncertainty that may happen due to meteorological events, like cloud formation (depicted in Fig. 7 - top figure). As can be seen in Fig. 7, even if the light distribution is varying, the controller keeps the process stable on the assigned PPB set-point. Switching from controlled illumination to natural light, even though the total intensity remains constant, results in a decrease in the feeding flow rate determined by the controller. This indicates that apart from light intensity, the distribution of light also influences growth (in agreement with Capson-Tojo et al., 2023a). These results indicate the automatic controller can handle these perturbations without light distribution information. As the light intensity and distribution may not be the same for every day, in case of meteorological events that perturbs the planned light intensity, the controller still satisfies the control objective as shown in Fig. 7. Once again, if the total intensity becomes too low, in case of too high set-point, there is no potential energy source available to convert to PPB, thereby the process becomes unstable, and the importance of assignment of an appropriate set-point is, then, highlighted.

The robustness of the controller against step changes in incoming VFA concentrations and varying distributions of light intensity has been demonstrated and discussed. Although the design of such a raceway reactor for PPB growth is based on coupling it with high-rate anaerobic digestion for improved performance Alloul et al., 2021; Doki et al., 2024, daily variations in VFA levels are inevitable. Additionally, daily fluctuations in light intensity due to meteorological uncertainties frequently occur in practice. Therefore, two additional scenarios involving daily variations in incoming VFAs and light intensity have also been assessed through simulation studies. As shown in Fig. 8, the controller can keep the track of the set-point despite daily variations in incoming VFAs and light intensity. It can also be observed that the process is more sensitive to daily variations in light intensity than to fluctuations in incoming VFA levels. This is because the available VFA is most effectively converted to PPB when sufficient light energy enables them

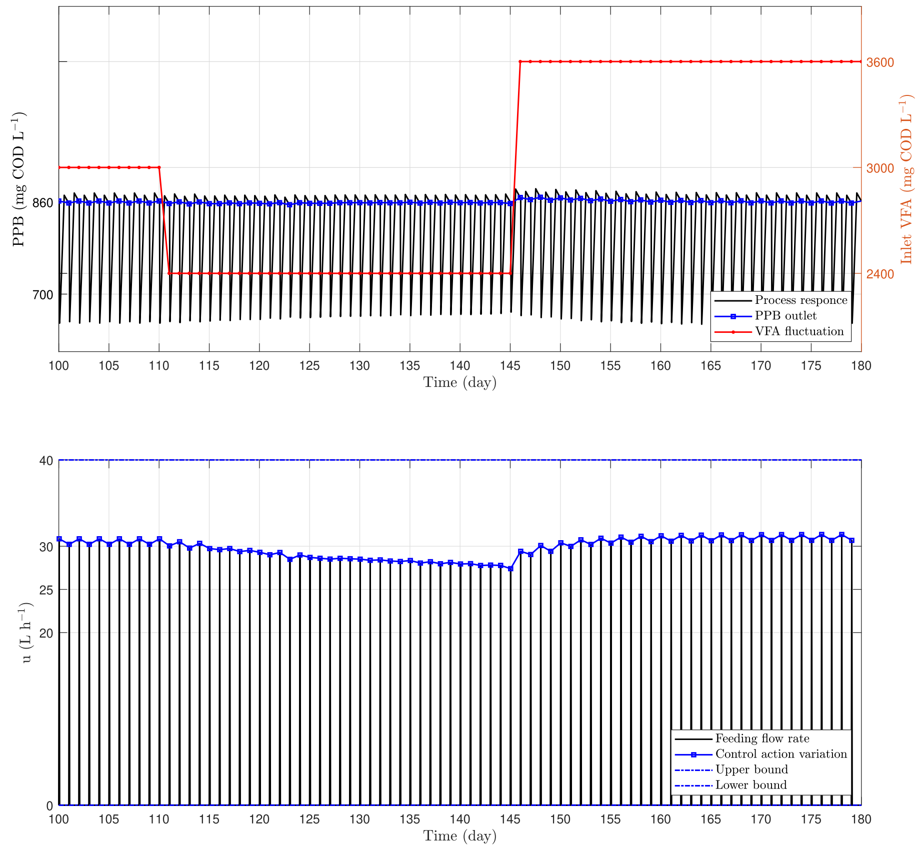

Fig. 6. AGMPC set-point tracking subject to inlet VFA variation – process response and control action.

to outcompete aerobic chemoheterotrophic bacteria. As a result, the impact of daily variations in light intensity is larger than the effect of varying VFA levels. It should also be added that in case of adverse changes in the sources, the set-point should be accordingly adjusted in order to achieve the maximum capacity of PPB growth, considering the process status. To minimize the risk of process failure due to extreme meteorological fluctuations, especially in reactors operating in regions with such conditions, artificial illumination can be a viable solution.

As mentioned in Section 2.1, the most important source of the model mismatch is the parallel metabolic growth constant (M_S). Determination of this parameter is experimentally and mathematically complex, as it may change due to changes in species and continuous daily switching between light/dark conditions (Alloul et al., 2021). The proposed AGMPC controller is robust against uncertainty and model mismatch due to its reliance on an input–output model that is free of mechanistic relationships. Therefore, this model is daily updated based on observed data to accurately capture changes over time. As depicted in Fig. 9, even though the parallel metabolic growth is changed over time, the controller tracks the assigned set-point by regulating the feeding flow rate. To compare the results, the open loop steady-state values of PPB concentration for the different parallel metabolic growth constants on the last five days for the feeding flow rate of $=25\,\mathrm{L\,h^{-1}}$ have been also drawn in Fig. 9. As can be seen, it is an important contributing factor to the PPB concentration, which can drastically change the output concentration without the controller. Thus, the controller keeps the output concentration fixed even when the parallel growth constant changes and no information about these changes is available.

As discussed above, it has been shown that the controller effectively tracks an assigned set-point and can satisfactorily manage two significant potential disturbances: incoming VFA concentration and changes in illumination scenarios, which are the primary resources enabling PPB growth. Moreover, the robustness of the controller against model mismatch of the parallel metabolic growth constant has been demonstrated as well. It has been also investigated, whether in some scenarios with severe fluctuations, one might need to assign an appropriate set-point in order to make the best use of available sources to convert to PPB and to avoid process instability. The simulated examples are for the process conditions wherein PPB are the dominant species. In the following section, the discussion focuses on designing a controller to transition the process from the competition phase (start-up phase) to this PPB dominant phase.

4.2. Override control for microbial competition: phase-based control

According to the discussion in Section 3.4, the paddlewheel is considered as a control regulator for the competition phase during the start-up phase. When the paddlewheel is activated, it boosts the growth of PPB, if it is the dominant bacteria. Alternatively, turning it off suppresses the growth of non-PPB bacteria. Due to inability of the main controller to find a control input within the search domain dictated by the control input constraint, it is suggested to use an override control with a heuristic approach for the first few days during the start-up phase to prevent non-PPB growth by turning the paddlewheel off, and then switch to MPC controller for PPB concentration control and full-time paddlewheel activation to enhance PPB growth to a maximum extent.

As can be seen in Fig. 4, the growth of non-PPB is decreased after 4−7 days. Therefore, by suppressing non-PPB growth during these days, by keeping the paddlewheel deactivated, PPB can be the dominant bacteria in a shorter time, then we can switch to the MPC controller and turn the paddlewheel on 24 h to get the maximum growth of PPB. The switching time for the paddlewheel and the activation of the MPC controller depends on the initial condition (in this case concentration in influent) for non-PPB namely, aerobic heterotrophic bacteria, X_{AHB}.

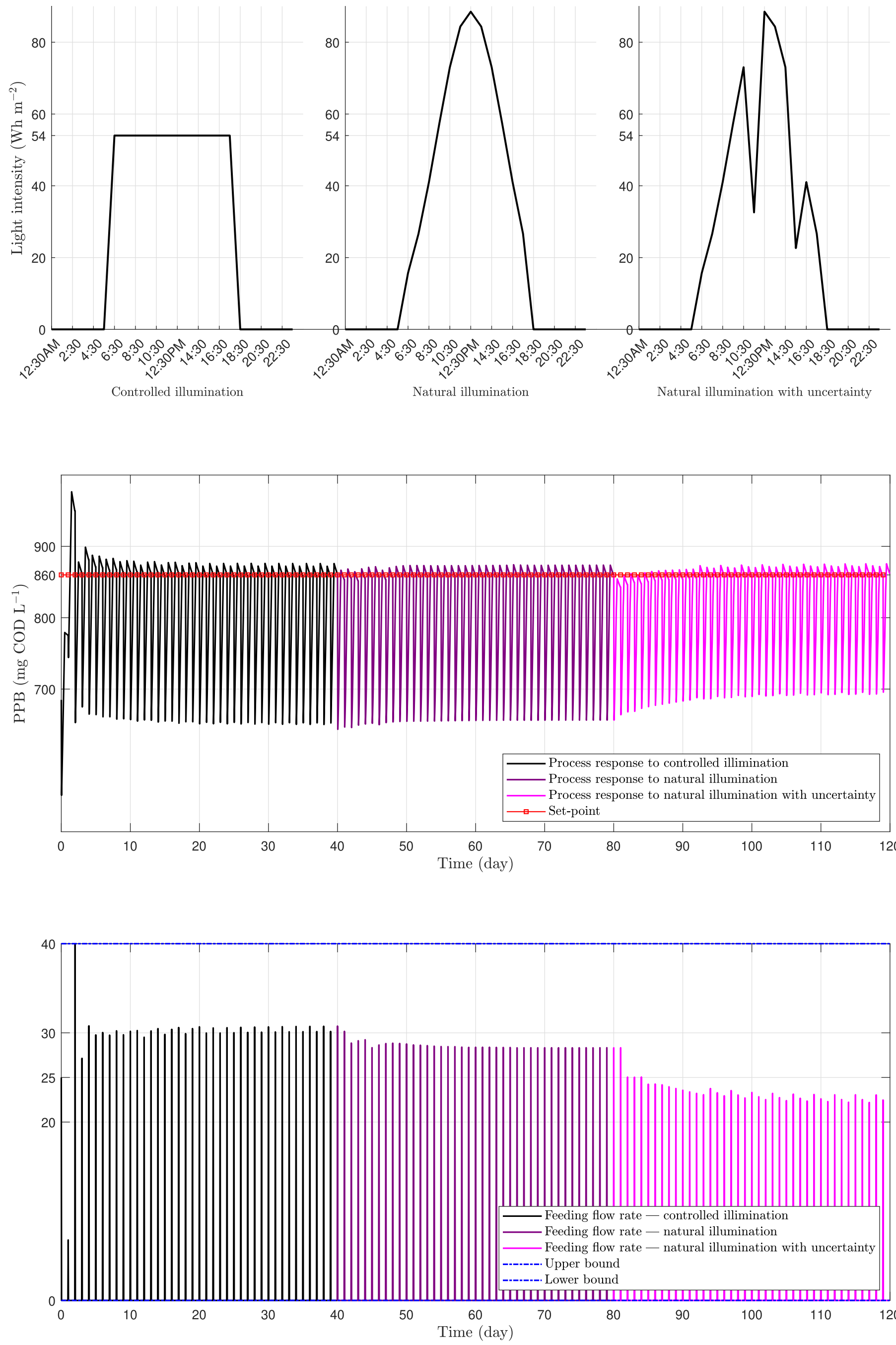

Fig. 7. AGMPC set-point tracking subject to different illumination scenarios – daily illumination intensity, process response, and control action.

As depicted in Fig. 10, when $X_{AHB} = 10$ mgCOD L^{-1}, the transition can occur as early as day 2. For $X_{AHB} = 100$ mgCOD L^{-1}, this transition can take place from day 5 onwards. However, if $X_{AHB} = 200$ mgCOD L^{-1}, switching to the main controller on day 5 may lead to difficulties for AGMPC in stabilizing the PPB concentration at 860 mgCOD L^{-1} as shown. Alternatively, delaying the switch until day 6 can mitigate these control action variations. The process response shown in Fig. 10 also highlights that when the concentration of aerobic heterotrophic bacteria is lower, or when competition decreases due to a delay in switching, the PPB set-point concentration can be reached more rapidly, while maintaining a higher production rate. Therefore, it can be concluded that such an override control benefits the PPB growth.

4.3. *Supervisory layer: discussion on decision-making operational strategies*

As discussed above, the proposed AGMPC control system is able to control the assigned output PPB concentration subject to the model mismatch, influent VFA variations, and different illumination scenarios. According to the discussion in Section 3.3, the main parameter that affects the process performance is the PPB set-point concentration to be assigned. According to an operational decision expressed by the decision tree given in Fig. 3, the design parameters can be assigned as follows:

(i): If the priority is *quality* and reaching water treatment criteria, the PPB set-point concentration should be increased to get the maximum potential of available sources, i.e. incoming VFA concentration

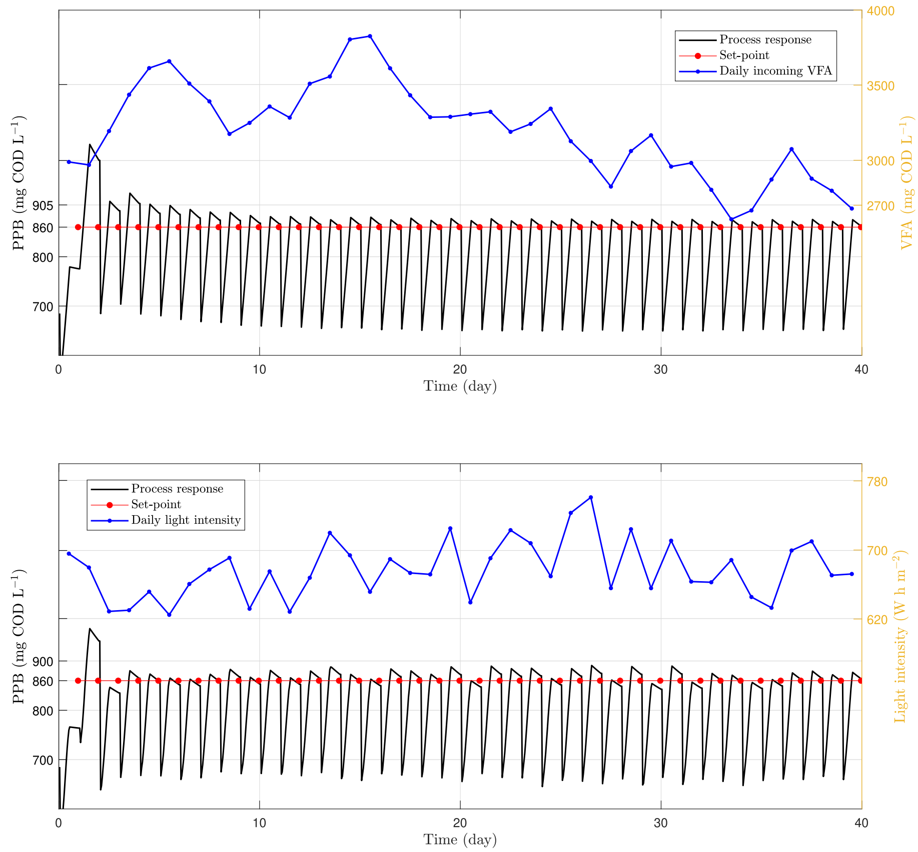

Fig. 8. AGMPC set-point tracking subject to daily variations – process response to daily variation in incoming VFA (top figure), and process response to daily variation in light intensity (bottom figure).

and light intensity for PPB cultivation. As explained, $S_{\mathrm{VFA,o}}$ is a reasonable indication to check how much VFA remains unconverted after one cycle of the process and then to decide for increase/decrease of the PPB set-point. The cross-checking boundaries, i.e $S^1_{\mathrm{VFA,o}}$ and $S^2_{\mathrm{VFA,o}}$ are set to 250 mgCOD L^{-1} and 150 mgCOD L^{-1}, respectively, as can be seen in the decision chart in Fig. 3. Therefore, as long as $S_{\mathrm{VFA,o}} \geq S^1_{\mathrm{VFA,o}}$, the set-point is increased, while if $S_{\mathrm{VFA,o}} < S^2_{\mathrm{VFA,o}}$, the set-point is decreased. Given that the outlet VFA concentration is the only indicator, in instances of significant increases in light intensity resulting from meteorological fluctuations, it may be required to lower the set-point. This adjustment is aimed at preventing process instability, as insufficient VFA may be not available for conversion to PPB, leading to a subsequent drop in outlet PPB concentration. Consequently, the lower bound is considered in such cases to address this concern. The buffer range, i.e $S^l_{\mathrm{VFA,o}} \leq S_{\mathrm{VFA,o}} < S^u_{\mathrm{VFA,o}}$ is also considered keeping the process stable between a specific range of outlet VFA, instead of continuously increasing and decreasing the PPB set-point concentration. Implementing the proposed decision-making layer for *quality* successfully achieves the highest PPB concentration given available sources, as mentioned in Table 2. According to Table 2, for different operational settings in terms of the required sources for PPB utilization, by checking the outlet VFA, the set-point, and consequently the output PPB concentration, are increased. This decision strategy also contributes to COD removal, as the outlet VFA concentration is decreased by regulating the feeding flow rate. The outcomes associated with both PPB concentration and COD removal align with the conclusions drawn by Alloul et al. (2021, 2023), emphasizing the impact of augmenting hydraulic retention time (HRT), achievable through reducing the feeding flow rate as managed by the controller, on both COD removal and PPB concentration.

(ii): For the another operational strategy, *quantity* as a production rate is a priority. It can be achieved by reducing the set-point, which increases the feeding flow rate, and thereafter, the output production rate, according to (13). While the higher production can be achieved, this operational strategy is not appropriate for COD removal. Therefore, it has been suggested to recycle the soluble materials for the subsequent cycle after separation. It helps to reduce the amount of consumption of the VFA tank from the VFA tank, as denoted by u^* in Table 2. As discussed in Section 3.3, $\frac{S_{\mathrm{VFA,o}}}{S_{\mathrm{VFA,i}}}$ can be an appropriate indication to decide for decreasing the PPB set-point concentration. As can be seen in the decision chart in Fig. 3, α and β are the two boundaries to decide for increase/decrease of the PPB set-point.

These parameters are typically regarded as design parameters that should to be determined by a process expert. For instance, they should not be set at levels where control action becomes saturated. Considering the nominal design provided in the original PBM model, α and β are set to $\frac{1}{3}$ and $\frac{2}{5}$. Since in this example, recirculation is taken into account and a portion of feeding rate includes it, the upper actuator limit is also set to 50 L h^{-1}. Investigating data given in Table 2, while increasing the production rate, the required input from the VFA stream, u^* is also decreased due to the recirculation. Therefore, using this operational decision scenario successfully increases the production rate and decreases the amount of VFA that needs to be provided from the VFA tank. This highlights that the VFA feeding rate in this operational strategy is close to the feeding rate computed by the *quality* decision strategy (see the column of u^* in Table 2). Moreover, according to (19) and the factor $\frac{S_{\mathrm{VFA,o}}}{S_{\mathrm{VFA,i}}} \geq \frac{1}{3}$, the yield should exceed $\frac{3}{2}$ of the yield in case of a non-recycling process. In other words, without recirculation, reducing the PPB set-point leads to a corresponding decrease in yield. Conversely, by recycling non-converted VFA, the yield can be increased by almost $\frac{3}{2}$.

The last assessment includes investigating how the supervisory layer reacts to perturbation and uncertainty during operation. In this regard, the following operational conditions are assumed:

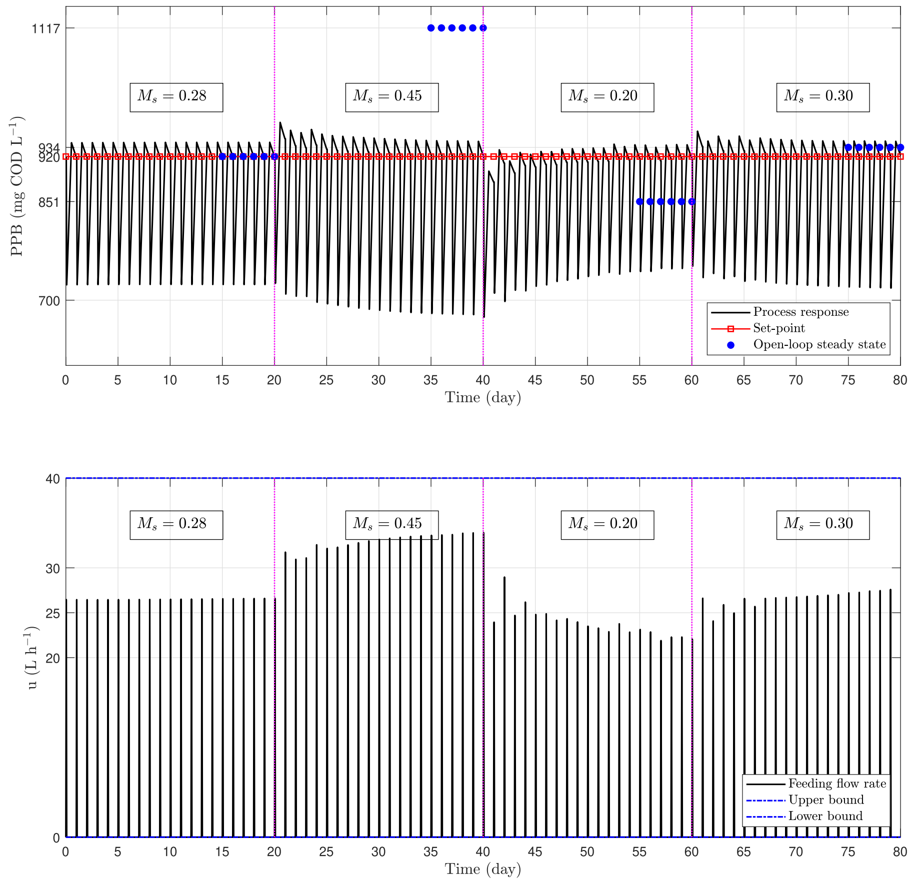

Fig. 9. AGMPC set-point tracking subject to uncertainty of the PPB metabolic growth constant – process response, and control action.

Table 2
Operational conditions (five operational conditions in terms of available sources, i.e. light intensity and incoming VFA, $S_{\mathrm{VFA,i}}$) and performance outcomes: comparative analysis of quality-driven (denoted by #1) and quantity-driven (denoted by #2) approaches in PPB cultivation process.

Operational scenario	Light intensity 12 h dark/12 h light [W m^{-2}]	$S_{\mathrm{VFA,i}}$ [mgCOD L^{-1}]	$S_{\mathrm{VFA,o}}$ [mgCOD L^{-1}]	Q [mgCOD d^{-1}]	$Y \times 100$	X_{PB} [mgCOD L^{-1}]	Output u[L d]	Required input u^*[L d]
#1	54	3000	170.07	22 790.50	31.67	950.00	23.99	23.99
#2			1179.60	28 914.18	39.66	741.96	38.97	24.30
#1	60	3000	191.26	25 244.49	32.99	989.98	25.50	25.50
#2			1117.80	30 631.33	40.96	782.01	39.17	24.93
#1	50	3000	173.61	21 298.37	30.71	989.98	23.12	23.12
#2			1153.2	26.382.78	40.73	782.01	36.26	21.59
#1	54	2500	211.97	25 695.50	34.00	850.00	30.23	30.23
#2			979.48	28 140.02	41.44	629.39	44.71	27.16
#1	54	3500	239.00	21 298.37	28.84	1009.70	20.19	20.19
#2			1355.00	26.382.78	38.69	830.00	32.88	20.15

1. Start: A light intensity of 54 W m^{-2} and incoming VFA concentration of 3000 mgCOD L^{-1} as the nominal condition,
2. Event 1: Perturbation on incoming VFA by 20 % increase on day 100, i.e. a light intensity of 54 W m^{-2} and an incoming VFA concentration of 3600 mgCOD L^{-1},
3. Event 2: Perturbation on light intensity by a 10 % increase on day 200, i.e. a light intensity of 60 W m^{-2} and an incoming VFA concentration of 3600 mgCOD L^{-1},
4. Event 3: Perturbation on light intensity by a 20 % decrease, while considering a mismatch in the parallel growth constant on day 300, i.e. $M_S = 0.32$, a light intensity of 50 W m^{-2} and an incoming VFA concentration of 3600 mgCOD L^{-1}.

As can be seen in Figs. 11 and 12, for the both decision strategies, the PPB concentration should be increased upon Events 1 and 2 by the supervisory layer, as the incoming VFA on Event 1 and the light intensity on Event 2 are increased. The basis of such a decision for the quality-driven scenario is keeping the outlet VFA concentration within the specified range as indicated in Fig. 11 (blue line in top figure), while for the quantity-driven scenario, the criterion is the ratio between the inlet and outlet VFA concentrations, resulting in a higher VFA in the effluent that should be recycled. On Event 3, it is assumed that the parallel growth constant is $M_S = 0.32$ (the nominal constant is $M_S = 0.28$). As discussed in Section 4.1 and more specifically the discussion of Fig. 9, the parallel growth constant is a main source of model mismatch, and therefore, it affects the production, while its value is not known. Therefore, considering this unknown parameter, the supervisory decision layer should determine an appropriate set-point based on the defined criterion. As can be seen in Figs. 11 and 12, however, the light intensity is decreased, but the increase in M_S is the reason of more labor division among different types of PPB (Alloul

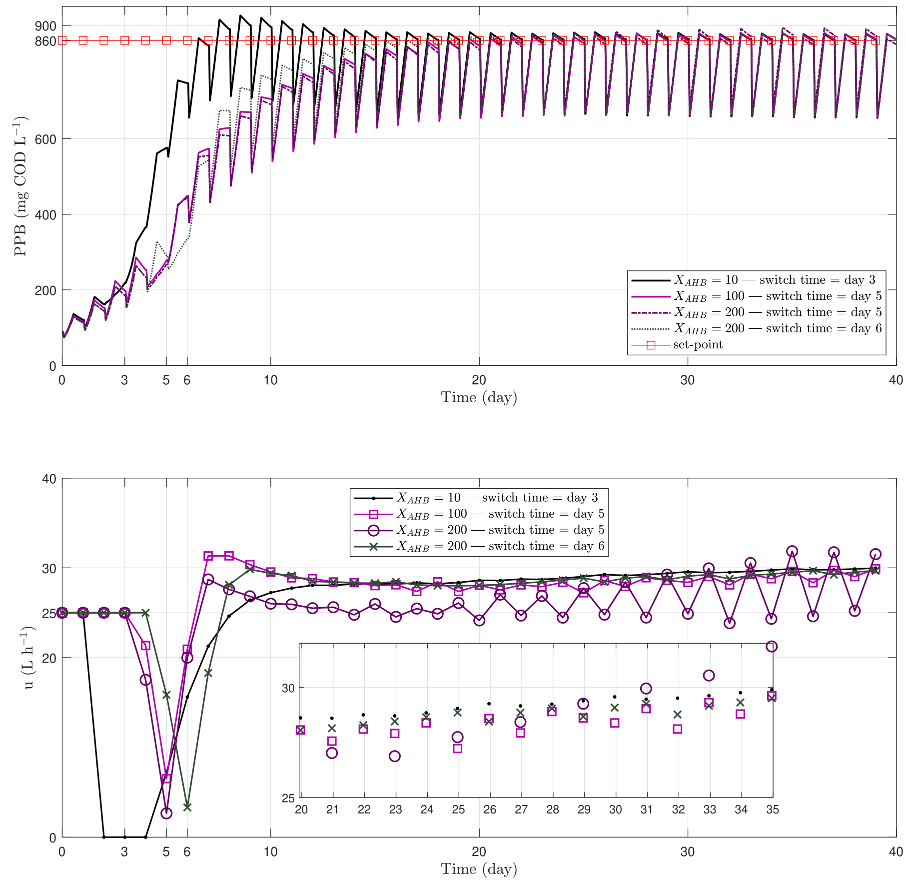

Fig. 10. Override control for microbial competition during the start-up phase. The override control switches to the MPC controller after a specific day.

et al., 2021), and consequently the higher PPB concentration in comparison with Event 1. In terms of the calculated control action for the both scenarios, feeding flow rate is adjusted according to the changes (Figs. 11 and 12, middle ones). On the occurrence of an event, the supervisory layer intervenes to restore stability to the process by addressing the decision criteria that have been violated. Moreover, for the quantity-driven scenario, the flow rate required from the VFA tank (u^* according to Eq. (15)) is also shown in Fig. 12 (red line in middle figure), which is lower than the actual feeding flow rate, as the unconverted VFA is recycled for the next cycle of the process. According to the feeding flow rates depicted in Figs. 11 and 12, the flow rate from the VFA tank is within a similar range ($\simeq$20 L d^{-1}). However, in quantity-driven operational scenarios, the HRT is prolonged due to circulation compared to quality-driven scenarios. This prolonged HRT seems to correspond to an increased yield, aligning with the discussion on PPB aggregation and HRT presented by Blansaer et al. (2022).

Another point to be discussed is the adaptation and switching dynamics. As discussed in Section 3.1 and shown in Fig. 2, the system parameters are theoretically updated every 24 h (daily) based on new observations (measurements). However, as long as the process remains within a stable operating domain, meaning no significant perturbations occur, the observations reach a steady state, and the system parameters remain unchanged. This can be clearly seen in Figs. 11 and 12 (bottom ones), where the parameter vector θ starts switching when an event occurs, such as on days 100, 200, and 300.

4.4. Implications of the proposed control system and further development

The presented control system is the first developed automatic controller for PPB cultivation in a raceway reactor. This reduces the need for skilled labors to supervise the process, not only to ensure process stability against biological perturbations and environmental disturbances, but also to enhance process performance according to the preferred operational strategies mentioned in this work. The best control can be achieved on reliable measurements. Cerruti et al. (2020) have discussed a method to measure PPB concentration. Measurement methods based on flow though cell UV–Vis and NIR spectroscopy (Qi et al., 2023) allow online measurement if only one species, such as PPB are dominant. If some errors occur due to a lack of precise measurements, developing a mathematical prediction method based on reliable available measurements, such as using either a mechanistic model (Piaggio et al., 2024) or an observer (Kemmer et al., 2023), would address data availability for the developed control system. It should be also highlighted the control system is based on input–output model, which allows including delay in measurement by increasing time shift operators. Moreover, if any error occurs for PPB measurement, it can be somehow offset via the supervisory layer by cross-checking outlet VFA consecration, for which more reliable and faster measurement is available, which also highlights another advantage of the developed hierarchical control system.

This paper highlights dealing with the start-up phase for the transition between non-PPB and PPB bacteria communities. This has been addressed by proposing an override control based on mechanistic and heuristic understanding. As mentioned, the capability of the MPC controller to maintain the process on the assigned set-point depends on an appropriate initialization. To include the competition phase into the MPC model, using a simplified mechanistic model instead of such a proposed linear input–output model would address it. Moreover, designing a mechanistic-derived override controller can also be considered as a further development. Finally, a novel supervisory layer based on two proposed operational strategies has been proposed in this work to enhance the process performance. This is based on mechanistic analysis of the process and the simulation model. As a further

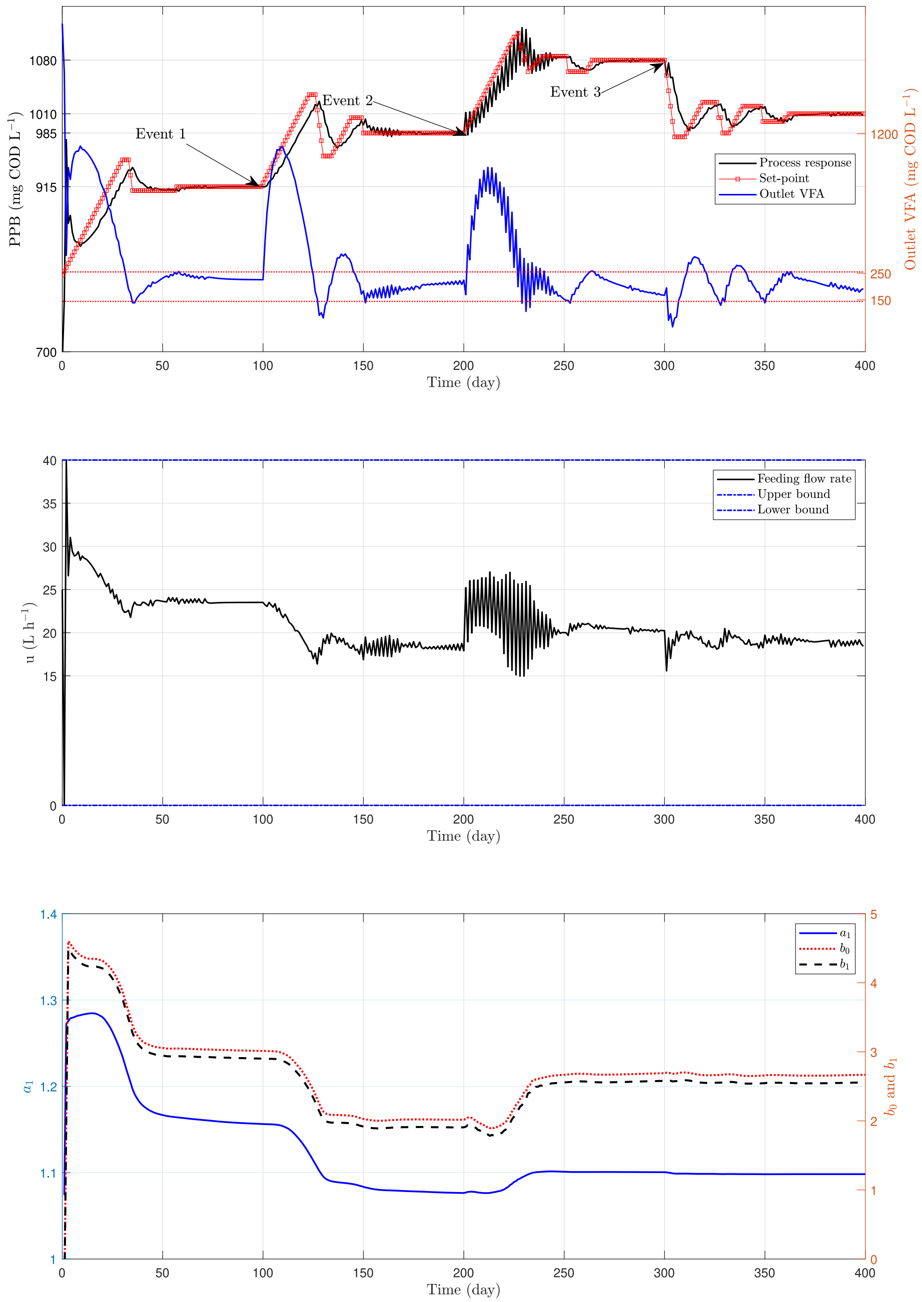

Fig. 11. Quality-driven scenario: AGMPC set-point tracking integrated with the decision-making supervisory layer to assign the appropriate set-point subject to the operational conditions and fluctuations – process response, determined set-point, outlet VFA, feeding flow rate, and adaptations of parameters.

investigation, application of alternative approaches, namely fuzzy logic system (Ghanavati et al., 2021), neural networks (Sadeghassadi et al., 2018), and switched systems (Moradvandi et al., 2024), can be taken into account.

Although the controller can adapt to varying environmental conditions by updating the internal model, the raceway reactor cannot be operated in regions with significantly fluctuating conditions. For example, operating the reactor in areas with limited sunlight (if reliant on natural light) causes practical operational challenges for cultivating PPB. Additionally, as raceway reactors are open systems, temperature is a critical factor. Capson-Tojo et al. (2023a) reported PPB's resilience and a broad survival range to temperature variations, with fixed uptake rate constants between 20 and 40 °C. In case of a wider temperature variation, the proposed control strategy requires further assessment for such regions.

Exploring other types of MPC approaches, such as scenario-based MPC (SMPC) (Calafiore and Fagiano, 2013) and practical nonlinear MPC (PNMPC) (Plucenio et al., 2007), could also be considered as future work. The SMPC controller is well-suited for conditions with high uncertainty, particularly in cases where fluctuations in natural light could significantly disrupt the process. It mitigates these adverse disturbances by accounting for potential scenarios of weather conditions and identifying a solution to handle these variations. Designing an NMPC controller could also be explored; however, it requires a simplified nonlinear model to reduce the computational complexity of the resulting non-convex optimization problem. To address the complexity of the PBM model, it can be simplified using approaches such as principal component analysis by taking into account the availability of real-time measurements as well as controllability and observability of the simplified model (García-Diéguez et al., 2013). Thereafter, some

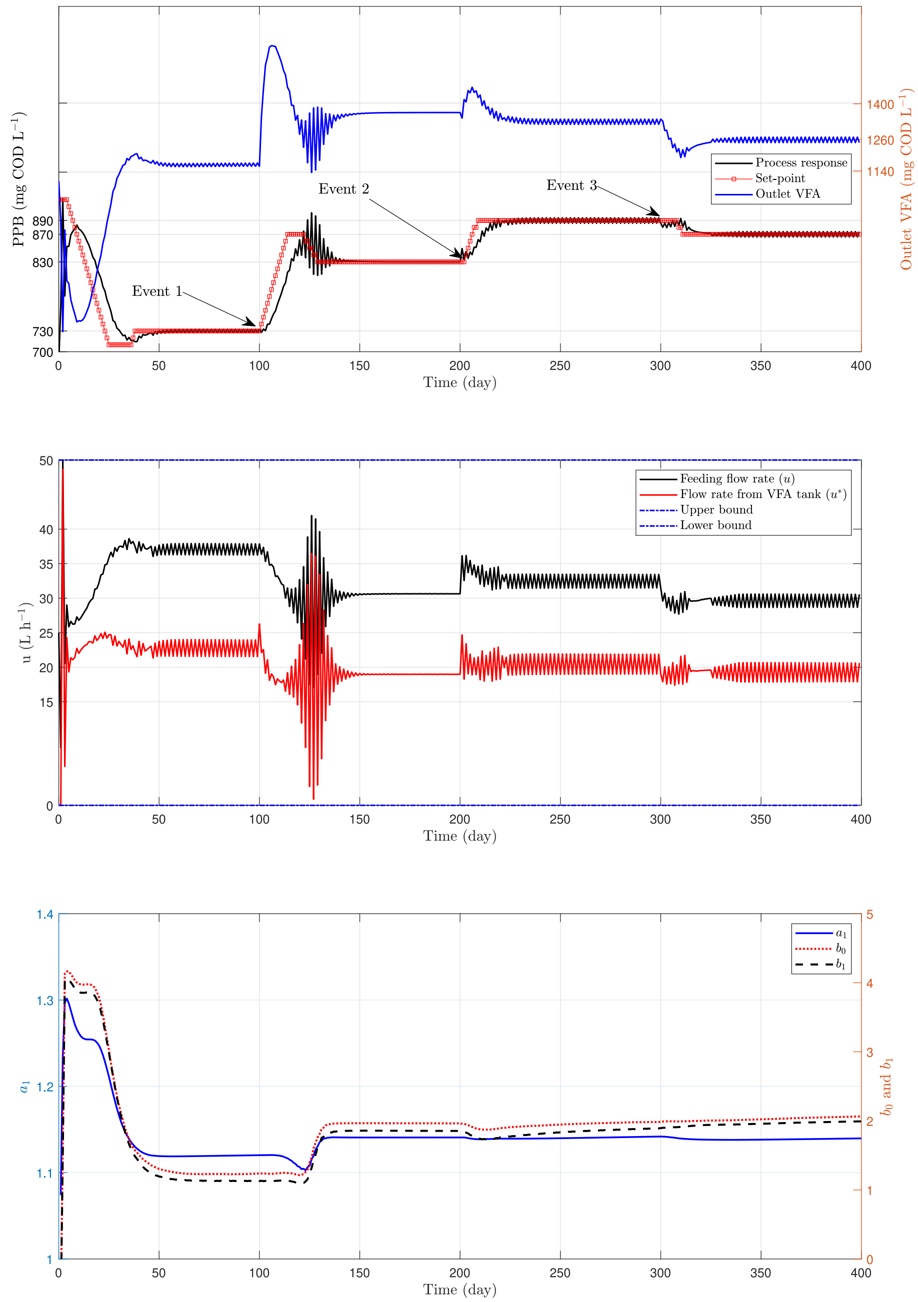

Fig. 12. Quantity-driven scenario: AGMPC set-point tracking integrated with the decision-making supervisory layer to assign the appropriate set-point subject to the operational conditions and fluctuations – process response, determined set-point, outlet VFA, and feeding flow rate, and adaptations of parameters.

computationally effective approaches such as the PNMPC method can be explored for this simplified version of the PBM.

5. Conclusions

In this paper, a control system on the basis of adaptive generalized model predictive control (AGMPC) for PPB raceway reactors is developed. PPB cultivation in raceway reactors is subject to biological and meteorological fluctuations. The proposed control strategy is able to effectively deal with environmental disturbances. However, significant changes in two essential sources for PPB utilization, namely incoming VFA concentration and light intensity, may lead to process and control inefficiency and instability if the set-point is set either too low or too high. Therefore, the AGMPC controller is integrated to a supervisory layer to assign an appropriate set-point given the process condition. Two operational strategies, namely quality-driven and quantity-driven, are developed for assigning a set-point. In both operational strategies, the hierarchical control system is able to fulfill the process objectives under various perturbations. In the quality-driven scenario, maximizing PPB concentration in each cycle can be achieved by monitoring the outlet VFA concentration. This approach also facilitates COD removal, as it ensures minimal outlet VFA concentrations are attained. In the quantity-driven scenario, decreasing the PPB set-point results in an increased production rate. Simultaneously, the system is configured to recycle unconverted outlet VFA, thereby enhancing yield through the extension of HRT. Moreover, an override control strategy is developed in order to transition the process from the microbial competition phase to the PPB-dominant phase. To achieve this, an investigation is conducted to determine the transition, given an initial condition of the process, the paddlewheel should be deactivated for a few days before switching to full-time activation. The effectiveness of the proposed control framework has been assessed via the PBM model as a benchmark. This automatic control framework can also be used for full-scale plants, even they are supervised by unskilled labors.

CRediT authorship contribution statement

Ali Moradvandi: Writing – original draft, Visualization, Software, Methodology, Conceptualization. **Bart De Schutter:** Writing – review & editing, Supervision, Funding acquisition. **Edo Abraham:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization. **Ralph E.F. Lindeboom:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

The authors kindly acknowledge a research grant of the European Horizon 2020 Framework Programme (grant agreement number 821427) under the Project SARASWATI 2.0.

Appendix. The PBM model used for simulation

(i) State variables: The PBM (Alloul et al., 2023) has 15 state variables based on 12 biological and 4 physical processes. Microbial community is divided to three PPB-based bacteria namely photoheterotrophic ($X_{PB,ph}$), anaerobic chemoheterotrophic ($X_{PB,anc}$), and aerobic chemoheterotrophic ($X_{PB,aec}$), and two non-PPB bacteria, namely aerobic bacteria (X_{AEB}) and anaerobic heterotrophic fermenters (X_{ANB}). The other two particulate matters are considered within the incoming feed as slowly biodegradable organic matter (X_S), and inert particulate organic matter (X_I). The other state variables are considered as soluble matters, namely, readily biodegradable organic matter (S_S), volatile fatty acids (S_{VFA}), inert soluble organic matter (S_I), soluble hydrogen (S_{H2}), total inorganic carbon (S_{IC}), total inorganic nitrogen (S_{IN}), total inorganic phosphorus (S_{IP}), and dissolved oxygen (S_{O2}).

(ii) Balances and system dynamics equations: Taking account all the mentioned particulate (X_j; $j = 1, \dots, 7$) and soluble (S_i; $i = 1, \dots, 8$) matters, mass balances of the PBM model can be summarized as follows:

$$\frac{dV}{dt} = Q_{in}(t) - Q_{out}(t), \tag{A.1a}$$

$$\frac{dS_i}{dt} = \frac{S_i^{input} Q_{in}(t) - S_i(Q_{out}(t) + \frac{dV}{dt})}{V_0} + \sum \upsilon_i \rho_i, \tag{A.1b}$$

$$\frac{dX_j}{dt} = \frac{X_j^{input} Q_{in}(t) - X_j(Q_{out}(t) + \frac{dV}{dt} f_{H/S})}{V_0} + \sum \upsilon_j \rho_j. \tag{A.1c}$$

in which V_0, V, Q_{in}, Q_{out} denote the reactor initial and actual volumes, and input and output flow rates, respectively. Besides, $\upsilon_{i \text{ and } j}$ and $\rho_{i \text{ and } j}$ express the stoichiometry factors and the corresponding rate equations, respectively, for consumption and production rates, which details can be found in the Peterson matrix of the model (Alloul et al., 2023). In addition, $f_{H/S}$ is a factor defining the fraction of removed particles.

(iii) PPB metabolic versatility: PPB state variables are the main output of the system. Six biological processes are assigned to them, namely: two photoheterotropic growths on soluble organics and VFAs; two aerobic chemoheterotrophic growths on soluble organics and VFAs; one anaerobic chemoheterotrophic growth on soluble organics; and biomass decay into biodegradable materials and inerts. Therefore, the model is written to account for the ability of PPB to grow on different substrates (carbon sources) or energy sources (light) in parallel. In this regard, a parallel metabolic growth constant (M_S) among the three PPB biomass types is included. Considering the following new variables:

$$f_{ph} = X_{PB,ph} + M_S(X_{PB,aec} + X_{PB,anc}) \tag{A.2a}$$

$$f_{aec} = X_{PB,aec} + M_S(X_{PB,ph} + X_{PB,anc}) \tag{A.2b}$$

$$f_{anc} = X_{PB,anc} + M_S(X_{PB,ph} + X_{PB,aec}) \tag{A.2c}$$

in which f_{ph}, f_{aec}, and f_{anc} represent variables with regard to parallel photoheterotrophic, aerobic chemoheterotrophic, and anaerobic chemoheterotrophic growths, respectively, these variables are used in their corresponding kinetic growth rates. This factor facilities to account the contributions of other parallel growth pathways to the dominant one. Since, the measurement of growth rate of each individual type of PPB is not straightforward and sometime feasible, this factor, i.e. M_S is the main source of uncertainty.

(iv) Inhibition functions: Rate equations ($\rho_{i \text{ and } j}$) are also included the associated inhibition functions, which are based on the Monod type function to describe limitations of organics, ammonium, phosphate, light, and oxygen. As the PBB bacteria is mainly divided to photoheterotrophy and chemoheterotrophy, the light inhibitory factor for PBB photoheterotrophy is the inverse of the light inhibitory factor for PPB chemoheterotrophy. In addition, while the main feed is considered to be VFAs, competitive inhibition function between VFAs and other soluble organics is also included into the PBM.

The details of the PBM dynamics and parameters are provided in https://github.com/Ali-Moradvandi/.

Data availability

No data was used for the research described in the article.

References

Ahmed, W., Rodríguez, J., 2020. A model predictive optimal control system for the practical automatic start-up of anaerobic digesters. Water Res. 174, 115599. http://dx.doi.org/10.1016/j.watres.2020.115599.

Alloul, A., Cerruti, M., Adamczyk, D., Weissbrodt, D.G., Vlaeminck, S.E., 2021. Operational strategies to selectively produce purple bacteria for microbial protein in raceway reactors. Environ. Sci. Technol. 55, 8278–8286. http://dx.doi.org/10.1021/acs.est.0c08204.

Alloul, A., Moradvandi, A., Puyol, D., Molina, R., Gardella, G., Vlaeminck, S.E., De Schutter, B., Abraham, E., Lindeboom, R.E., Weissbrodt, D.G., 2023. A novel mechanistic modelling approach for microbial selection dynamics: Towards improved design and control of raceway reactors for purple bacteria. Bioresour. Technol. 390, 129844. http://dx.doi.org/10.1016/j.biortech.2023.129844.

Alloul, A., Wuyts, S., Lebeer, S., Vlaeminck, S.E., 2019. Volatile fatty acids impacting phototrophic growth kinetics of purple bacteria: Paving the way for protein production on fermented wastewater. Water Res. 152, 138–147. http://dx.doi.org/10.1016/j.watres.2018.12.025.

Blansaer, N., Alloul, A., Verstraete, W., Vlaeminck, S.E., Smets, B.F., 2022. Aggregation of purple bacteria in an upflow photobioreactor to facilitate solid/liquid separation: Impact of organic loading rate, hydraulic retention time and water composition. Bioresour. Technol. 348, 126806. http://dx.doi.org/10.1016/j.biortech.2022.126806.

Calafiore, G.C., Fagiano, L., 2013. Robust model predictive control via scenario optimization. IEEE Trans. Autom. Control 58 (1), 219–224. http://dx.doi.org/10.1109/TAC.2012.2203054.

Camacho, E.F., Bordons, C., Camacho, E.F., Bordons, C., 2007. Constrained Model Predictive Control. Springer.

Capson-Tojo, G., Batstone, D.J., Grassino, M., Vlaeminck, S.E., Puyol, D., Verstraete, W., Kleerebezem, R., Oehmen, A., Ghimire, A., Pikaar, I., Lema, J.M., Hülsen, T., 2020. Purple phototrophic bacteria for resource recovery: Challenges and opportunities. Biotech. Adv. 43, 107567. http://dx.doi.org/10.1016/j.biotechadv.2020.107567.

Capson-Tojo, G., Batstone, D.J., Hülsen, T., 2023a. Expanding mechanistic models to represent purple phototrophic bacteria enriched cultures growing outdoors. Water Res. 229, 119401. http://dx.doi.org/10.1016/j.watres.2022.119401.

Capson-Tojo, G., Lin, S., Batstone, D.J., Hülsen, T., 2021. Purple phototrophic bacteria are outcompeted by aerobic heterotrophs in the presence of oxygen. Water Res. 194, 116941. http://dx.doi.org/10.1016/j.watres.2021.116941.

Capson-Tojo, G., Zuo Meng Gan, A., Ledezma, P., Batstone, D.J., Hülsen, T., 2023b. Resource recovery using enriched purple phototrophic bacteria in an outdoor flat plate photobioreactor: Suspended vs. attached growth. Bioresour. Technol. 373, 128709. http://dx.doi.org/10.1016/j.biortech.2023.128709.

Carreño-Zagarra, J., Guzmán, J., Moreno, J., Villamizar, R., 2019. Linear active disturbance rejection control for a raceway photobioreactor. Control Eng. Pract. 85, 271–279. http://dx.doi.org/10.1016/j.conengprac.2019.02.007.

Cerruti, M., Kim, J.-H., Pabst, M., Van Loosdrecht, M.C.M., Weissbrodt, D.G., 2022. Light intensity defines growth and photopigment content of a mixed culture of purple phototrophic bacteria. Front. Microbiol. 13, http://dx.doi.org/10.3389/fmicb.2022.1014695.

Cerruti, M., Stevens, B., Ebrahimi, S., Alloul, A., Vlaeminck, S.E., Weissbrodt, D.G., 2020. Enrichment and aggregation of purple non-sulfur bacteria in a mixed-culture sequencing-batch photobioreactor for biological nutrient removal from wastewater. Front. Bioeng. Biotechnol. 8, http://dx.doi.org/10.3389/fbioe.2020.557234.

Chung, Y.-C., Chien, I.-L., Chang, D.-M., 2006. Multiple-model control strategy for a fed-batch high cell-density culture processing. J. Process Control 16 (1), 9–26. http://dx.doi.org/10.1016/j.jprocont.2005.05.003.

Clarke, D., Mohtadi, C., Tuffs, P., 1987. Generalized predictive control—Part I. The basic algorithm. Automatica 23 (2), 137–148. http://dx.doi.org/10.1016/0005-1098(87)90087-2.

de Andrade, G., Berenguel, M., Guzmán, J., Pagano, D., Acién, F., 2016. Optimization of biomass production in outdoor tubular photobioreactors. J. Process Control 37, 58–69. http://dx.doi.org/10.1016/j.jprocont.2015.10.001.

Dochain, D., 2013. Automatic Control of Bioprocesses. John Wiley & Sons.

Doki, M.M., Mehta, A.K., Chakraborty, D., Ghangrekar, M.M., Dubey, B.K., Alloul, A., Moradvandi, A., Vlaeminck, S.E., Lindeboom, R.E., 2024. Recovery of purple non-sulfur bacteria-mediated single-cell protein from domestic wastewater in two-stage treatment using high rate digester and raceway pond. Bioresour. Technol. 413, 131467. http://dx.doi.org/10.1016/j.biortech.2024.131467.

Fernández, I., Berenguel, M., Guzmán, J., Acién, F., de Andrade, G., Pagano, D., 2016. Hierarchical control for microalgae biomass production in photobioreactors. Control Eng. Pract. 54, 246–255. http://dx.doi.org/10.1016/j.conengprac.2016.06.007.

García-Diéguez, C., Bernard, O., Roca, E., 2013. Reducing the anaerobic digestion model no. 1 for its application to an industrial wastewater treatment plant treating winery effluent wastewater. Bioresour. Technol. 132, 244–253. http://dx.doi.org/10.1016/j.biortech.2012.12.166.

Ghanavati, M.A., Vafa, E., Shahrokhi, M., 2021. Control of an anaerobic bioreactor using a fuzzy supervisory controller. J. Process Control 103, 87–99. http://dx.doi.org/10.1016/j.jprocont.2021.05.010.

Gupta, N., De, R., Kodamana, H., Bhartiya, S., 2022. Batch to batch adaptive iterative learning control explicit model predictive control two-tier framework for the control of batch transesterification process. ACS Omega 7 (45), 41001–41012. http://dx.doi.org/10.1021/acsomega.2c04255.

Han, H.-G., Fu, S.-J., Sun, H.-Y., Qiao, J.-F., 2021. Hierarchical nonlinear model predictive control with multi-time-scale for wastewater treatment process. J. Process Control 108, 125–135. http://dx.doi.org/10.1016/j.jprocont.2021.11.002.

Hulsen, T., Barry, E.M., Lu, Y., Puyol, D., Keller, J., Batstone, D.J., 2016. Domestic wastewater treatment with purple phototrophic bacteria using a novel continuous photo anaerobic membrane bioreactor. Water Res. 100, 486–495. http://dx.doi.org/10.1016/j.watres.2016.04.061.

Imhoff, J., 2006. The Phototrophic Alpha-Proteobacteria. Springer, New York.

Kemmer, A., Fischer, N., Wilms, T., Cai, L., Groß, S., King, R., Neubauer, P., Cruz Bournazou, M.N., 2023. Nonlinear state estimation as tool for online monitoring and adaptive feed in high throughput cultivations. Biotechnol. Bioeng. 120 (11), 3261–3275. http://dx.doi.org/10.1002/bit.28509.

Moradvandi, A., Abraham, E., Goudjil, A., De Schutter, B., Lindeboom, R.E., 2024. An identification algorithm of switched box-jenkins systems in the presence of bounded disturbances: An approach for approximating complex biological wastewater treatment models. J. Water Process Eng. 60, 105202. http://dx.doi.org/10.1016/j.jwpe.2024.105202.

Pataro, I.M., Gil, J.D., Guzmán, J.L., Berenguel, M., Lemos, J.M., 2023. A learning-based model predictive strategy for pH control in raceway photobioreactors with freshwater and wastewater cultivation media. Control Eng. Pract. 138, 105619. http://dx.doi.org/10.1016/j.conengprac.2023.105619.

Pawlowski, A., Fernández, I., Guzmán, J., Berenguel, M., Acién, F., Normey-Rico, J., 2014. Event-based predictive control of pH in tubular photobioreactors. Comput. Chem. Eng. 65, 28–39. http://dx.doi.org/10.1016/j.compchemeng.2014.03.001.

Pawlowski, A., Guzmán, J., Normey-Rico, J., Berenguel, M., 2012. A practical approach for generalized predictive control within an event-based framework. Comput. Chem. Eng. 41, 52–66. http://dx.doi.org/10.1016/j.compchemeng.2012.03.003.

Piaggio, A.L., Smith, G., de Kreuk, M.K., Lindeboom, R.E., 2024. Application of a simplified model for assessing particle removal in dissolved air flotation (DAF) systems: Experimental verification at laboratory and full-scale level. Sep. Purif. Technol. 340, 126801. http://dx.doi.org/10.1016/j.seppur.2024.126801.

Plucenio, A., Pagano, D., Bruciapaglia, A., Normey-Rico, J., 2007. A practical approach to predictive control for nonlinear processes. IFAC Proc. Vol. 40 (12), 210–215.

Puyol, D., Barry, E., Hülsen, T., Batstone, D., 2017. A mechanistic model for anaerobic phototrophs in domestic wastewater applications: Photo-anaerobic model (PAnM). Water Res. 116, 241–253. http://dx.doi.org/10.1016/j.watres.2017.03.022.

Qi, X., Lian, Y., Xie, L., Wang, Y., Lu, Z., 2023. Water quality detection based on UV-vis and NIR spectroscopy: a review. Appl. Spectrosc. Rev. 1–25. http://dx.doi.org/10.1080/05704928.2023.2294458.

Sadeghassadi, M., Macnab, C.J., Gopaluni, B., Westwick, D., 2018. Application of neural networks for optimal-setpoint design and MPC control in biological wastewater treatment. Comput. Chem. Eng. 115, 150–160. http://dx.doi.org/10.1016/j.compchemeng.2018.04.007.

Seborg, D.E., Edgar, T.F., Mellichamp, D.A., Doyle III, F.J., 2016. Process Dynamics and Control. John Wiley & Sons.

Sheik, A.G., Machavolu, V.R.K., Seepana, M.M., Ambati, S.R., 2022. Integrated supervisory and override control strategies for effective biological phosphorus removal and reduced operational costs in wastewater treatment processes. Chemosphere 132346. http://dx.doi.org/10.1016/j.chemosphere.2021.132346.