

1 **Dynamic Modelling of Microalgae Cultivation Process in High Rate Algal** 2 **Wastewater Pond**

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8 9 **ABSTRACT**

10 In this work, a comprehensive dynamic mathematical modelling to simulate the production of
11 microalgae in a High Rate Algal Pond (HRAP) is attempted. A synergetic algal–bacterial
12 system comprising various interrelated biological and chemical system processes is
13 presented. The dynamic behaviour of HRAP system is studied by solving mass balance
14 equations of different components which account light intensity and gas–liquid mass transfer.
15 The model predictions are compared with the previously reported studies in the literature.
16 The influence of kinetic and operating parameters, including the supply of CO₂, the
17 maximum growth rate, pond depth and dilution rates, on the pond performance are evaluated.
18 The sensitivity analysis of important process parameters is also discussed in this study. The
19 developed model, as a tool, can be used to assess the factors that affect the pond performance
20 criteria, including algal productivity and the dynamics of nutrient requirements.

21 **Keywords:** HRAP; Microalgae; Mathematical modelling; Wastewater treatment.

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24 **1. Introduction**

25 High Rate Algal Ponds (HRAPs) for the treatment of wastewater obtained from municipal,
26 industrial and agricultural sources are a potential technology to be used in cultivating algal
27 biomass, because there is a growing interest in the development of effective and efficient
28 wastewater treatment methods for domestic and industrial wastes with the concurrent need
29 for alternative sources of energy and water. HRAPs are preferred among stabilization ponds
30 because of its simplicity and economy [1]. HRAPs can serve as a potential nutrient provider
31 for cultivating algae, in addition to wastewater treatment, with the possibility of reducing the
32 cost of sustainable commercial production of biofuels from microalgae. The key
33 characteristic feature of HRAPs is the symbiotic relationship between the photoautotrophic
34 algae and the heterotrophic bacteria. Microalgal growth generates oxygen in the pond
35 systems and thus facilitates dissolved oxygen concentration which in turn is required by
36 aerobic bacteria for both oxidation and nitrification processes. Microalgae also consumes
37 CO₂ produced by the bacteria during the mineralization of pollutants. Integrating wastewater
38 treatment with algal biomass production has the potential to reduce oxygen cost, mitigates
39 CO₂, and enhances nutrient assimilation and stripping processes. These processes stabilize
40 wastes, facilitate the sedimentation process, and promote constructively algal growth coupled
41 with driving the aerobic wastewater treatment synergistically [2]. Thus, the use of algal–
42 bacterium consortia has the potential to increase the economic feasibility and effectiveness of
43 microalgae biomass production. Despite numerous benefits, the lack of knowledge on the
44 design and operational parameters coupled with the management of microalgae–based
45 processes has limited their widespread implementation. This is because of various complex
46 physicochemical and biological processes that determine the efficiency of the pond
47 characterization and the performance in HRAPs. These processes are: nutrient requirements
48 for algae growth, dissolved oxygen that induces bacterial growth and biochemical oxidation

49 of organic matters; pH that controls the rate of distinctive biochemical process; a temperature
50 that controls the rate of biochemical reactions and transformations; light input for
51 photosynthesis and hydraulic behaviour that govern the process of mixing in the pond [3]. To
52 understand the process holistically and improve the efficiency of HRAPs from the standpoint
53 of hydrodynamics through chemical and biological interactions, several studies using
54 modelling approach have been attempted in the literature.

55 Buhr and Miller [4] have described a process modelling of biochemical interaction and
56 symbiotic relationship of photosynthetic microalgae, and heterotrophic bacteria, and
57 validated the HRAP process experimentally. The hydrodynamics of the system was
58 considered as a series of continuous stirred tank reactors (CSTR) units with recirculation. The
59 growth of both algae and microorganism was described by Monod kinetics. However, the
60 effects of algal respiration and gaseous transformations in the pond are not being considered.
61 Fallowfield et al. [5] have studied the validation of algal pond models to estimate net
62 productivity, oxygen evolution and wastewater treatment capacity. Jupsin et al. [6] have
63 presented a mathematical model of HRAP based on River Water Quality Model (RWQM)
64 that was capable of simulating HRAP's operating cycles considering sediment oxygen
65 demand. Grobbelaar et al. [7] have developed algal productivity models in terms of
66 temperature and incident light. Recently, Yang [8] has extended the mathematical models
67 developed by Buhr and Miller [4] to estimate the effect of pH, dissolved oxygen and substrate
68 concentrations on CO₂ supply and utilization. He has considered the growth kinetics,
69 thermodynamics and gas mass transfer, and the absorption of gases such as oxygen and
70 ammonium.

71 The objective of the present study is to develop a dynamic model for microalgae production
72 in HRAP under different operational conditions. The present model involves the prediction of
73 biomass concentration, dissolved oxygen, total inorganic carbon and total inorganic nitrogen

74 concentrations. The model also considers the effects of sparging CO₂ with congruent
75 sensitivity analysis of some other important parameters. The modelling methods used in this
76 study are mostly drawn from the previous work of Buhr and Miller [4] and Yang [8].
77 However, there are some differences between this work and the previous literature work [4,
78 8] to build the present model in a simple way. These differences are following. pH limitation
79 in the presented model is considered as the method described by James et al. [9]. This
80 method involves the functional form of the relation between pH and dissolved CO₂ derived
81 from chemical equilibrium theory. CO₂ mass transfer coefficient, k_{lg,CO_2} is calculated as
82 based on the oxygen mass coefficient, k_{lg,O_2} which is considered as a constant value in this
83 work; Yang [8] used gPROMS as process modelling software to solve model equations,
84 whereas, in this work model equations are solved using Matlab tool. The developed model as
85 a tool can be employed to determine the pond performance criteria, including maximum algal
86 productivity and nutrient requirements. Using prediction model, the effect of kinetic and
87 operating parameters, such as supply of CO₂, the maximum growth rate, pond depth and
88 dilution rate, on the pond performance is presented. The sensitivity analysis of some
89 important process parameters is also discussed in this study.

90

91 **2. HRAP model development**

92 The schematic algal pond is represented as shown in Figure 1 to depict the synergetic algal–
93 bacterial system comprising various interrelated biological and chemical processes.
94 Wastewater can be described as a mixture of dissolved oxygen, dissolved inorganic nutrient
95 concentrations and biological oxygen demand (BOD). pH of wastewater is an influential
96 parameter that governs the biochemical transformation and substance balance in the reactor.
97 The HRAP model also considers gaseous CO₂ as a carbonaceous source. The assumptions
98 considered in developing the models in this study are: (i) the pond is modelled as completely

99 stirred tank reactors (CSTR); (ii) algal specific growth rate is a function of light intensity,
 100 total dissolved CO₂ and total inorganic nitrogen; (iii) exchange of O₂ and CO₂ between the
 101 pond and the atmosphere is not included; (iv) evaporative losses are not considered due to
 102 lower water loss. It is noted in the literature that other nutrients such as phosphorus and
 103 micronutrient are not considered to be the limiting factor because these compounds are
 104 usually highly available in wastewater [8, 10]. Thus, in the present study, this effect has not
 105 been explicitly considered with the assumption that the metabolism of the of the microbial
 106 consortium are not limited or inhibited by these compounds. Also, the ammonia volatilization
 107 and the removal of phosphorus by chemical precipitation occurring due to high pH (9-10) and
 108 temperature are not considered in the present study.

109 The model that describes the growth of photosynthetic microalgae in HRAP is a set of
 110 nonlinear differential equations derived from mass balance equations for both liquid and
 111 gaseous species transformations.

112 The average light intensity in the pond can be expressed in terms of concentration and depth
 113 of the pond (z) at a particular time using the Beer–Lambert’s law as [8]

$$114 \quad I_a = \frac{1}{z} \int_0^z I_0 \exp(-K_e z) dz \quad (1)$$

115 where z is the depth of the pond, K_e is the extinction coefficient related to the algal
 116 concentration, X_A expressed as a simple linear relationship

$$117 \quad K_e = K_{e1} + K_{e2} X_A \quad (2)$$

118 Here K_{e1} and K_{e2} are constants and I_0 is the maximum surface light intensity during the
 119 photoperiod (5.00–19.00 hrs).

120 Combining Eqns. (1) and (2), the following relationship between the light intensity and the
 121 distance from the surface is obtained as

$$122 \quad I_a = \frac{I_0}{z} \exp\left(\frac{1 - e^{-(K_{e1} + K_{e2} X_A)z}}{(K_{e1} + K_{e2} X_A)}\right) \quad (3)$$

123 The diurnal variation of the surface light intensity can be estimated as [11]

124 $I_0(t) = \max\left(0, I_0\pi\left(\sin\left(\frac{(t-5)2\pi}{24}\right)\right)\right)$ (4)

125 The light intensity factor for algae growth is thus modelled using Steele's function as [8]

126 $f_I = \frac{I_a}{I_s} \exp\left(1 - \frac{I_a}{I_s}\right)$ (5)

127 where I_s is the saturation or optimum light intensity.

128 The mass balance of algae concentration in the effluent is expressed as [8]

129 $\frac{dX_A}{dt} = \frac{F}{V}(X_{Ain} - X_A) + A_{gr} - r_{dA}$ (6)

130 where X_A , F , V , A_{gr} and r_{dA} are the biomass concentrations per unit culture volume, the total
131 flow rate, the culture volume, the growth rate and the decay rate of algae, respectively.

132 Subscripts *in* is used to indicate the inlet concentration.

133 The growth rate of microalgae, A_{gr} can be expressed as

134 $A_{gr} = \mu_A X_A$ (7)

135 where μ_A and X_A are the respective specific growth rate and mass concentration of algae.

136 The specific growth rate can be expressed in terms of light intensity (f_I), maximum growth
137 (μ_M) and nutrients (dissolved CO_2 , CO_{2D} and total inorganic nitrogen, N_T) in the form of
138 Monod-type function as [8]

139 $\mu_A = \mu_M \left(\frac{CO_{2D}}{K_c + CO_{2D}}\right) \left(\frac{N_T}{KN_A + N_T}\right) f_I$ (8)

140 where μ_M , K_c and KN_A are constants. CO_{2D} can be obtained using pH dependence equation by
141 an iteration method which is described at the end of this section.

142 The mass balance of total inorganic carbon can be written as

143 $\frac{dTIC}{dt} = \frac{F}{V}(TIC_{in} - TIC) + \mu_B X_B Y_{BCO_2} - \mu_A X_A Y_{ACO_2} + f_{CO_2} - k_{lg,CO_2} a(CO_2^* - CO_{2D})$ (9)

144 where TIC_{in} is the influent concentration of total inorganic carbon, Y_{ACO_2} and Y_{BCO_2} are the
145 respective components mass yield, f_{CO_2} is the mass flux of CO_2 , k_{lg,CO_2} is the mass transfer

146 coefficient and CO_2^* is the liquid phase CO_2 concentration which is in equilibrium with the
 147 gaseous CO_2 .

148 The total inorganic carbon concentration, C_{TIC} includes not only the dissolved carbon dioxide
 149 concentration (CO_{2D}), but also takes into account the carbonate concentration ($C_{CO_3^{2-}}$) and
 150 bicarbonate concentration ($C_{HCO_3^-}$) species generated in the system in order to balance total
 151 inorganic carbon.

$$152 \quad C_{TIC} = CO_{2D} + C_{HCO_3^-} + C_{CO_3^{2-}} \quad (10)$$

153 The concentration of carbonate ions entering into the TIC balance equation [10] is computed
 154 by pH dependence and they can be calculated as

$$155 \quad C_{HCO_3^-} = \frac{C_{TIC}}{1 + \frac{[H^+]}{k_1} + \frac{k_2}{[H^+]}} \quad (11)$$

$$156 \quad C_{CO_3^{2-}} = \frac{C_{TIC}}{1 + \frac{[H^+]}{k_2} + \frac{[H^+]^2}{k_1 k_2}} \quad (12)$$

157 where k_1 and k_2 are the dissociations constant for HCO_3^- and CO_3^{2-} respectively. Above
 158 equations (11-12) are derived using Eqn. (10) and the dissociation equations of HCO_3^- and
 159 CO_3^{2-} which are discussed at the end of this section.

160 The equilibrium liquid phase concentration of CO_2 can be written as

$$161 \quad CO_2^* = H_{CO_2} P_{CO_2} \quad (13)$$

162 where P_{CO_2} is the partial pressure of saturated CO_2 and H is the Henry's constant for CO_2 .

163 The mass transfer coefficient of CO_2 in water is used as [12]

$$164 \quad k_{lg,CO_2} = k_{lg,O_2} * \frac{D_{CO_2}}{D_{O_2}} \quad (14)$$

165 where k_{lg,O_2} is the mass transfer coefficient of O_2 in water and D_{CO_2} and D_{O_2} are the
 166 diffusion coefficient of CO_2 and O_2 , respectively.

167 The mass balance of N_T can be written as

$$168 \quad \frac{dN_T}{dt} = \frac{F}{V} (N_{T_{in}} - N_T) - \mu_B X_B Y_{BN_T} - \mu_A X_A Y_{AN_T} \quad (15)$$

169 where N_{Tin} is the influent concentration of total inorganic nitrogen and Y_{ANT} and Y_{BNT} are
170 the respective components mass yield.

171 The decay rate of algae (r_{dA}) can be modelled in terms of dependent variable of algal
172 concentration (X_B) as

$$173 \quad r_{dA} = k_{dA}X_A \quad (16)$$

174 where k_{dA} is constant.

175 Similar to algal mass balance, bacterial concentration can be modelled as

$$176 \quad \frac{dX_B}{dt} = \frac{F}{V}(X_{B0} - X_B) + r_{gB} - r_{dB} \quad (17)$$

177 where X_{B0} is the influent concentration of bacteria.

178 The growth rate of bacteria, r_{gB} can be calculated in the same manner as biomass
179 concentration

$$180 \quad r_{gB} = \mu_B X_B \quad (18)$$

181 where μ_B and X_B are the specific growth rate and mass concentration of bacteria. The
182 nutrients, such as an organic substrate, oxygen and total inorganic nitrogen, are considered in
183 this work. The specific growth rate of bacteria is described in the Monod-type equation can
184 be written as

$$185 \quad \mu_B = \mu_{BM} \left(\frac{S}{K_S + S} \right) \left(\frac{O_2}{K_{O_2} + O_2} \right) \left(\frac{N_T}{K_{NB} + N_T} \right) \quad (19)$$

186 where μ_{BM} , K_S , K_{O_2} and K_{NB} are the half velocity constants and S is the concentration of the
187 substrate (BOD), respectively.

188 The substrate, S balance can be attributed to the stoichiometric reaction of algal and bacterial
189 growth. The balance equation for substrate component can thus be written as

$$190 \quad \frac{dS}{dt} = \frac{F}{V}(S_0 - S) - \mu_B X_B Y_B \quad (20)$$

191 where S_0 and Y_B are the influent concentration of substrate and mass yield of substrate (BOD)
192 consumed per unit mass of bacteria produced.

193 The mass balance of O₂ can be written as

$$194 \frac{dO_2}{dt} = \frac{F}{V} (O_{2in} - O_{2out}) - \mu_B X_B Y_{BO_2} + \mu_A X_A Y_{AO_2} + f_{O_2} - k_{lg,O_2} a (O_2^* - O_2) \quad (21)$$

195 where O_{2in} and O_{2out} are the respective influent and effluent concentrations of O₂,

196 Y_{AO_2} and Y_{BO_2} are the respective components mass yield, f_{O_2} is the mass flux of O₂, and

197 k_{lg,O_2} and O_2^* are the mass transfer coefficient and liquid phase O₂ concentration that is in

198 equilibrium with the gas phase O₂.

199 The equilibrium liquid phase concentration of O₂ can be written as

$$200 O_2^* = H_{O_2} P_{O_2} \quad (22)$$

201 where P is the partial pressure of O₂ and H is the Henry's constant for O₂.

202 The decay rate (r_{dB}) depends on bacterial concentration (X_B) and is modelled as

$$203 r_{dB} = k_{dB} X_B \quad (23)$$

204 where k_{dB} is constant.

205 Now, $f_{g=CO_2,O_2}$ in Eqns. (9) and (21) can be estimated using the following relationship:

$$206 f_g = \frac{1}{Z} \varepsilon \int k_{lg} a (M_g^* - M_g) dz \quad (24)$$

207 Assuming the variation of dissolved CO₂ and O₂ along the height is negligible, f_g can be

208 calculated as

$$f_g = \varepsilon k_{lg} a (M_g^* - M_g) \quad (25)$$

209 where M_g and M_g^* are the liquid phase concentration and equilibrium liquid phase

210 concentration of gas species ($g=CO_2$ and O₂), Z is the depth of the pond, a is the interfacial

211 area ($a=6/d_b$) and ε is the volume fraction of the gas hold up and can be determined as

$$\varepsilon = \frac{n\pi d_b^3 f}{6U_{gb}} \quad (26)$$

212 Here d_b is the bubble diameter. The frequency of bubble formation, f can be estimated from

213 the number of each orifice as

$$f = \frac{6Q_0}{\pi d_0^3} \quad (27)$$

214 The gas volumetric flow rate, Q_0 is related to the number of orifices per unit area (n), total
 215 surface area required for gas flow (A_g) and total gas flow rate (Q) as

$$Q_0 = \frac{Q}{nA_g} \quad (28)$$

216 Furthermore, considering liquid velocity to be very small, bubble liquid slip velocity
 217 (U_{gb}) was approximated with the values of ascending velocity ($U_{gb} = u_{rel}$) and thus,
 218 U_{gb} can be determined as

$$U_{gb} = \sqrt{\frac{4d_b}{3C_D}} \quad (29)$$

219 The drag force coefficient (C_D) can be deduced using the following correlation [8]

$$C_D = \begin{cases} \frac{18.5}{Re^{0.6}} & \text{for } 1 < Re < 1000 \\ 0.44 & \text{for } Re \geq 1000 \end{cases} \quad (30)$$

220 Since the culturing mechanism of microalgae depends on the concentration of substrates,
 221 such as carbon dioxide and nitrogen, pH influences the adsorption and desorption of nutrient
 222 to enhance the bioavailability of organic matter. In this work, pH limitation in this model is
 223 considered as the method described by James et al. [9]. The method involves the functional
 224 form of the relation between pH and dissolved CO_2 derived from chemical equilibrium
 225 theory. Gaseous CO_2 contacts with H_2O to become dissolved CO_2 , which in turn reacts with
 226 H_2O to form carbonic acid:



228 The hydration constant of above equation is [9]

$$229 \quad k_h = \frac{[H_2CO_3]}{CO_{2D}} = 1.7 \times 10^{-3} \quad (32)$$

230 where CO_{2D} is the concentration of dissolved CO_2 and H_2CO_3 is a diprotic acid that can
 231 dissociate into two protons in a two-stage process:





234 The dissociation constants for the above two stages [9] are given by :

235 $k_1 = \frac{[\text{H}^+][\text{HCO}_3^-]}{[\text{H}_2\text{CO}_3]} = 4.45 \times 10^{-7}$ (35)

236 $k_2 = \frac{[\text{H}^+][\text{CO}_3^{2-}]}{[\text{HCO}_3^-]} = 4.69 \times 10^{-11}$ (36)

237 with the assumption that carbonic acid is a weak monoprotic acid, $[\text{CO}_3^{2-}]$ formed during the
 238 second dissociation of $[\text{HCO}_3^-]$ is neglected, the following equation can be obtained
 239 according to James et al. [9] as

240 $k_1 = \frac{[\text{H}^+]([\text{H}^+] - [\text{OH}^-])}{k_h \text{CO}_{2D} - [\text{H}^+] + [\text{OH}^-]}$ (37)

241 Using the hydration constant for water, $k_w = [\text{H}^+][\text{OH}^-] = 1.008 \times 10^{-14}$, and using $[\text{OH}^-] =$
 242 $k_w/[\text{H}^+]$, the simplified expression of k_1 in terms of $[\text{H}^+]$ is

243 $[\text{H}^+]^3 + k_1[\text{H}^+]^2 - (k_1 k_h \text{CO}_{2D} + k_w)[\text{H}^+] - k_1 k_w = 0$ (38)

244 In Eqn.(38), $k_1 k_w$ is negligible due to smaller value ($\sim O(10^{-21})$); so it can be reduced to a
 245 quadratic equation

246 $[\text{H}^+]^2 + k_1[\text{H}^+] - k_1 k_h \text{CO}_{2D} + k_1 = 0$ (39)

247 The above quadratic equation can be solved numerically and approximated into a simple
 248 expression for H^+ as a function of $[\text{CO}_2]$ and is given as

249 $[\text{H}^+] = (k_w + k_1 k_h \text{CO}_{2D})^{0.5}$ (40)

250 In this work, the iterative method is used to calculate CO_{2D} which is further used to find pH
 251 using Eq.(40). At the first iteration, using the initial pH (assumed 7.2) and initial total
 252 inorganic carbon concentration (C_{TIC}), the carbonate ions are computed from Eqns. (11) and
 253 (12). The carbonate ions are further used to calculate CO_{2D} concentration from Eqn. (10).
 254 Using CO_{2D} concentration, the concentration of H ion is calculated from Eq. (40) for the next
 255 iteration. The iterations are running until the difference between the previous iteration and the
 256 current iteration for CO_{2D} is negligible. The iteration method used in this work can be

257 improved by a solving system of algebraic equations of all ionic species which describe
258 chemical equilibrium of CO₂-NH₃-H₂O system. Since this thermodynamic model involves a
259 multi-solute system of CO₂-NH₃-H₂O which requires a substantial work to couple with
260 biological models, the improvement in the present model for pH calculation will be addressed
261 in future.

262

263 **3. Results and Discussion**

264 3.1 Model validation

265 Simulations were conducted using Matlab with ODE23s function. Since the detailed
266 experimental results of co-culture of bacteria and algae for high-rate wastewater treatment
267 ponds are hard to find in the literature, the validation of the present model was performed to
268 simulate microalgae cultivation in wastewater using two different literature studies. First one
269 is the model development for algal-bacteria interaction in the open system and the second one
270 is an algae cultivation in a synthetic medium simulating treated urban wastewater (secondary
271 effluent) in raceways ponds. The experimental and simulation data of Bai [13] was
272 considered for the algae-bacteria interaction in the open system. Bai studied the contribution
273 of bacteria on the microalgae cultivation in open algal systems by accounting carbon cycling
274 and further, developed an expanded algae-bacteria conceptual model which considers the
275 comprehensive carbon and nutrient fluxes in open algal systems, considering the activity of
276 heterotrophic bacteria. A simulation was performed for this specific operating condition
277 described by him to validate the present model. Figure 2a shows the comparison plot of algae
278 concentration between the present model and experimental findings of Bai [13] along with
279 the simulation result reported by him. It is seen that the predicted algae concentration profile
280 of the present model shows the similar trend with a small deviation shown by the
281 experimental observation. However, the trend closely matches with the author's modelling

282 work. Also, it can be seen from the figure that the simulated profile shows a wavelike trend
283 which indicates that the model can be able to reproduce both algae growth and inactivation
284 cycles occurring during daytime and at night, respectively. In another validation study, the
285 experimental and simulation data of Solimeno et al. [10] was considered for algae cultivation
286 using urban wastewater in open raceway ponds. They carried out batch cultivation of algae in
287 an open pond with the volume of 500L. The authors used a synthetic medium which is
288 similar to the mineral composition of wastewater. They had also developed a mechanistic
289 model to simulate microalgae growth, considering carbon-limited growth, transfer of gases,
290 photorespiration and photosynthesis kinetics. Figure 2b shows the comparison plot of algae
291 concentration between the present model and experimental findings of Solimeno et al. [10]
292 along with their simulation result. It is found that the predicted algae concentration profile of
293 the present model matches with the experimental observation reported by Solimeno et al.
294 [10]. It is also worth to mention that the present model shows a better prediction compared to
295 the author's modelling work.

296

297 3.2 Base case simulation

298 Base case simulation of algae-bacteria co-culture for high-rate waste water treatments ponds
299 was conducted to present the dynamics and the performance of the HRAP system. The model
300 parameters used in a base case simulation are presented in Table 1. The design and operating
301 parameters adopted for the simulation are presented in Table 2. Main operating conditions
302 used for the simulation scenarios were constant feed flow rate of $50 \text{ m}^3/\text{day}$ with the dilution
303 rates varies between 0 and 1 day^{-1} , considering the typical HRAPs pond depth of 0.1–0.4 m
304 based on the literature [1, 8, 14, 15]. Figure 3 presents the results of the modelling of the
305 algae biomass growth rate and pH variation during 24hrs period along with the previously
306 reported results by Yang [8] for testing of the present models. The process conditions used in

307 this case are: the pond depth of 0.4m, the dilution rate of 0.35 day^{-1} , the maximum specific
308 growth rate of 0.693 day^{-1} and the CO_2 flow rate of $10\text{m}^3/\text{hr}$. It can be seen from the figure
309 that the model predicted profiles of algae concentration and pH have a similar trend with the
310 previous work of Yang [8]. However, there was a deviation in pH profile between the
311 prediction of the present model prediction and that of Yang [8]. This may be due to the
312 different methods for pH calculation. Also, it is found from Figure 3a that during the
313 photoperiod (5.00–19.00hrs) the growth of algae biomass increases whereas it decreases
314 during the absence of photo light period. It is noteworthy to mention that algal biomass
315 concentration profile follows the pH profile. This implies that the production of algal biomass
316 in HRAPs is based on the influence of pH stemming from the utilisation of CO_2 as a major
317 carbonaceous source. There is a shift in carbonate chemical equilibrium if CO_2 consumed by
318 algae in the pond, which will automatically increase pH as well as the algal biomass
319 production. Therefore, the growth of algae implies the pH control by means of CO_2 addition
320 in the pond [16]. However, the change in CO_2 concentration in the pond induces the change
321 in pH, which is substantially affected by its solubility [17]. Thus, the addition of CO_2 will
322 increase the availability of carbon for algal growth with congruent improvement in the
323 removal efficiency of nutrient [18].

324 Figures 4 (a–c) exhibit the diurnal behaviour of dissolved oxygen, total inorganic carbon and
325 total inorganic nitrogen concentrations in the pond. It is found that the cyclic trend of
326 dissolved oxygen matches with the report of Yang [8]. During the day, when the external
327 irradiance increases, it is shown that the dissolved oxygen increases and reaches to $6.5\text{g}/\text{m}^3$ at
328 19:00hr and then sharply decreases. Similarly, it is shown that the concentration of total
329 inorganic carbon decreases at the same period when the concentration of oxygen increases in
330 the pond which is a clear indication of photosynthetic growth. The dissolved oxygen
331 concentration depends on the organic loads and the type of biomass presents in the HRAP. In

332 fact, pH and DO values were higher in the pond during the day due to photosynthetic activity
333 present in the pond. Figure 4c shows a substantial decreasing trend of total inorganic nitrogen
334 concentration in the pond during the dark period, whereas, in the photoperiod, the total
335 inorganic nitrogen concentration still decreases towards to constant and then increases
336 towards to a constant value in the dark period. The increase in total inorganic nitrogen
337 concentration in the dark period that cannot be seen in the main Figure 4c because of scale is
338 clearly shown in the inset of Figure 4c. Nitrogen is being consumed and reduced in the pond
339 during the day as both the pH and algal biomass productivity increase. Also, the consortium
340 of bacteria present in the system coupled with the loss of nitrogen to the atmosphere at the
341 same time may induce the additional total inorganic nitrogen reduction. Besides bicarbonate
342 equilibrium due to CO₂ gas sparging, the pH is also influenced by the dynamic equilibrium
343 exists between NH₄⁺ ions and NH₃.

344

345 3.3 Influence of CO₂ sparging on algae concentration

346 Figure 5 shows the predicted concentration profiles of algal biomass, pH, dissolved oxygen,
347 and dissolved carbon dioxide versus the time for the cases of both with and without CO₂ inlet
348 flow rate. The process conditions are: the pond depth of 0.4m, the dilution rate of 0.35day⁻¹,
349 and the maximum specific growth rate of 0.693 day⁻¹. It is obvious from Figure 5a that the
350 amount of algae produced in the pond is low when CO₂ is not sparging to the system. This
351 behaviour agrees with the literature [10]. There is the concomitant production of oxygen and
352 consumption of carbon dioxide and increasing pH concentration during the day.

353 3.4 Parameter studies

354 Simulations were conducted to evaluate the effect of some important parameters on the pond
355 performance. The effects of pond depth, dilution rate, and biochemical oxygen demand on the
356 pond performance were thus evaluated. These parameters are paramount to the maximization

357 of algal biomass production and nutrient consumptions efficiency. Moreover, these
358 parameters are interconnected to the biochemical system on the light penetration in the pond,
359 gaseous mass transfer, microalgal growth rate and the extent of organic matter degradation in
360 the pond [8, 10]. Thus, understanding the trend of variation of algae biomass concentration
361 with respect to the pond depth being a design variable and dilution rate being an operating
362 variable is important for algal biomass production and optimization.

363 Figures 6 (a–c) show the effect of algal productivity as the pond depth varies from 0.1 to
364 0.4m, dilution rate varies from 0.1 to 0.4 day⁻¹ and BOD varies from 50 to 300 g/m³. As
365 shown in Figure 6a, the algal areal productivity decreases with the pond depth due to the
366 reduction in the surface area and thus lowers the acquisition of atmospheric CO₂. Similar
367 trends are also reported in the literature [8, 10]. The results reveal that the longer residence
368 time and the lower concentration of microalgae in the pond may lead to the decline of algal
369 productivity. However, Sutherland et al. [19] reported that the increasing pond depth
370 increases the areal productivity, the nutrient removal efficiency as well as increased
371 photosynthetic activity. Nevertheless, increasing pond depth may promote CO₂ fixation and
372 removal efficiency, but it may not promote high algal yield necessarily. Figure 6b represents
373 the plot of dilution rates versus algal areal productivity. Selecting the ranges of dilution rate
374 with unique growth rate helps in achieving a steady state that can be used to optimize
375 biomass productivity. Based on this point, the continuous outdoor culture is composed of
376 cyclic variations in culture conditions that determine day and night biomass productivities.
377 Simulations were performed considering an optical pond depth of 0.1m, maximum growth
378 rate of 0.693day⁻¹, initial biomass concentrations in the pond as 383g/m³ coupled with
379 dilution rates of 0.1, 0.2, 0.25 and 0.35day⁻¹ [11,15]. It is obtained that the areal productivity
380 increases with dilution rates and the maximum dilution rate obtainable under the condition of
381 0.3day⁻¹ which corresponds to the areal productivity of 3.98 kgcm⁻²day⁻¹. A slight variation

382 in algal productivity is found when BOD increases from 50g/m^3 to 400g/m^3 , which is shown
383 in Figure 6c. This is an indication of the consumption of CO_2 by algae that has been produced
384 by bacteria in the pond. But algal productivity decreases after 400g/m^3 due to the nitrogen
385 starvation caused by the simultaneous growth of bacteria and CO_2 consumption by the
386 growth of algae [8].

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389 3.5 Sensitivity analysis

390 Sensitivity analysis was conducted on the few parameters of the present model. For each
391 parameter, three cases were performed to obtain distinctive profiles of microalgae
392 concentration with keeping the rest of the parameters at same as base case condition. A
393 variation of the parameters within the range of $\pm 10\%$ was used for microalgae biomass
394 concentration predictions.

395 Figure 7 presents the results of sensitivity analysis on algae concentration by varying the
396 parameters of algal decay rates (k_{da}), the maximum specific growth rates (μ_M) and the
397 saturation light intensity (I_s) and the half saturations constant (K_C) which are considered as
398 most important predetermined constants of the model. It is found that the model seems to be
399 insensitive to the nutrient determined half saturations constant for cell growth (K_C). A
400 similar finding has been revealed by Park and Li [17]. However, the model has a slightly
401 higher influence on algae concentration by varying of algal decay rates (k_{da}), the maximum
402 specific growth rates (μ_M) and the saturation light intensity factor (I_s).

403

404 4. Conclusion

405 Dynamic characteristics of microalgae culture in HRAP were investigated through the
406 development of a comprehensive mathematical modelling. A combined effect of light

407 intensity, biological model, and gas–liquid mass transfer on the prediction of process
408 parameters was studied in this study. Predictions of various components such as biomass
409 productivity, pH, dissolved oxygen, total inorganic carbon, and total inorganic nitrogen
410 concentrations were reported. The effects of design and operating parameters on the biomass
411 productivity were also investigated. The various conclusions that can be drawn from this
412 study are as follows:

- 413 • The pH and biomass productivity obtained in this study are in accordance with the
414 literature.
- 415 • The addition of CO₂ regulates pH, enhances the biomass productivity and thus, its
416 concentration in the pond is critical, which must be available at a sufficient
417 concentration to maintain a dynamic balance for algal–bacterial consortium.
- 418 • Oxygen production in the pond is mainly from photosynthesis process that is
419 dependent on algal growth rate, light intensity, temperature and pH. Its concentration
420 is inversely related to the concentration of CO₂.
- 421 • The effect of an increase in biomass productivity depends not only on light intensity
422 but also on the imposed dilution rate and pond depth.

423 The present model can be used effectively for simulating various conditions and in further
424 refinement of design and operating procedures for the HRAPs. This model will be useful
425 for scale–up and optimization of microalgal biomass production process.

426 **5. Acknowledgment**

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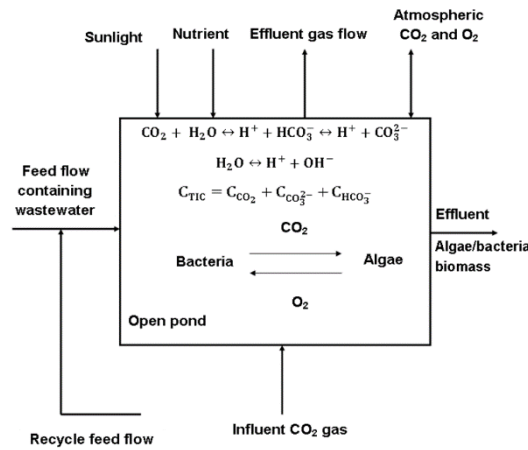
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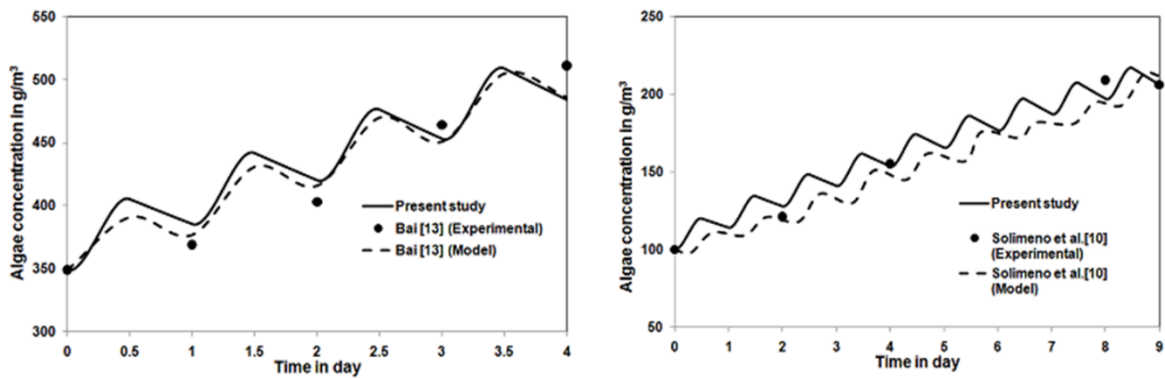
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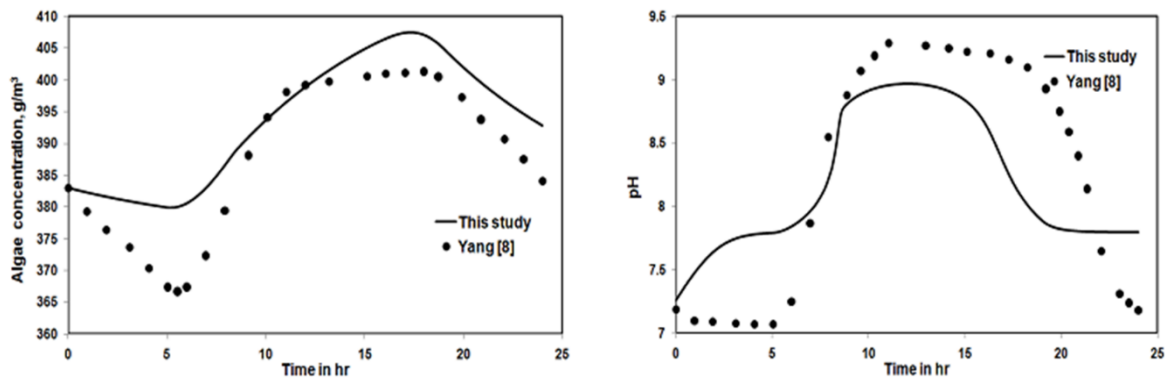
501 **Figure 1:** Schematic diagram of the algal pond system with recirculation [8]



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503 **Figure 2:** A comparison plot of algae concentration between this work and the literature [10,
504 13]

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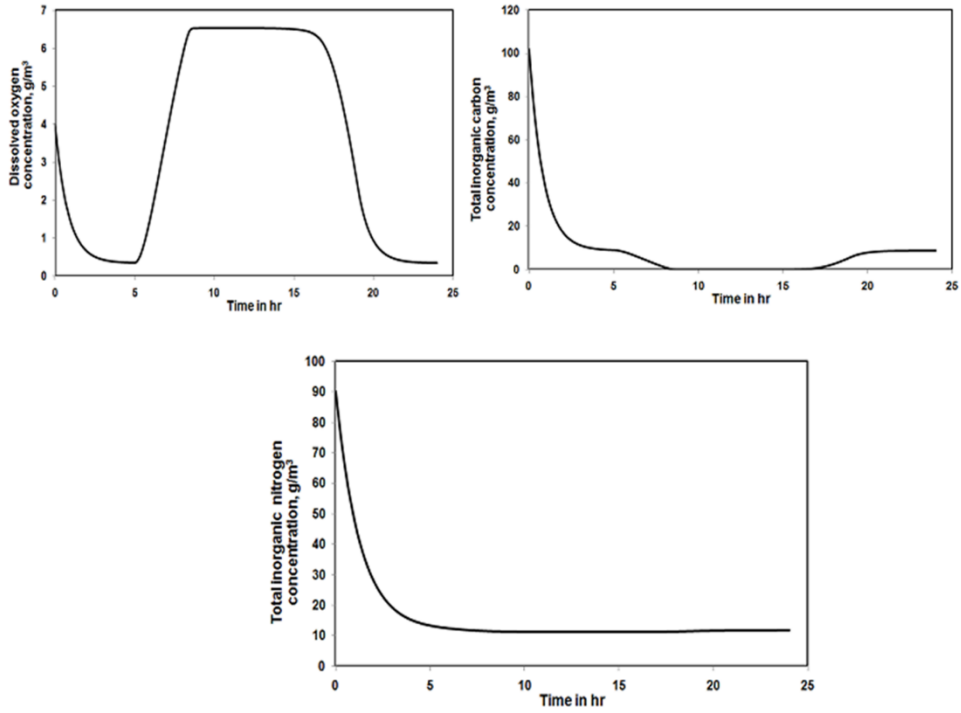


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507 **Figure 3:** (a) Algal concentration and (b) pH validations in HRAP along with 24hrs period

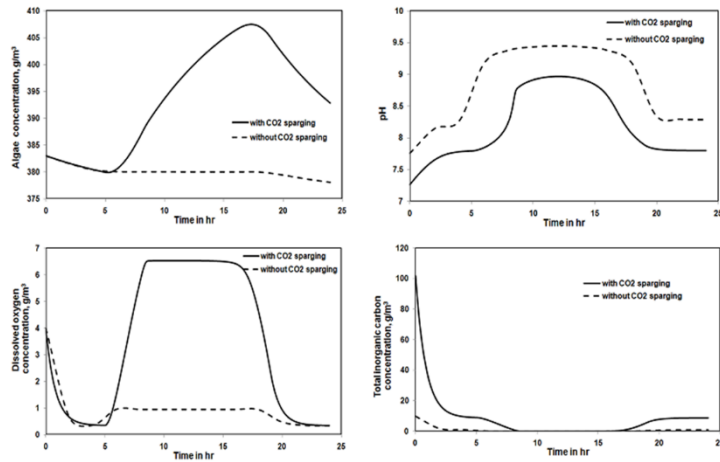
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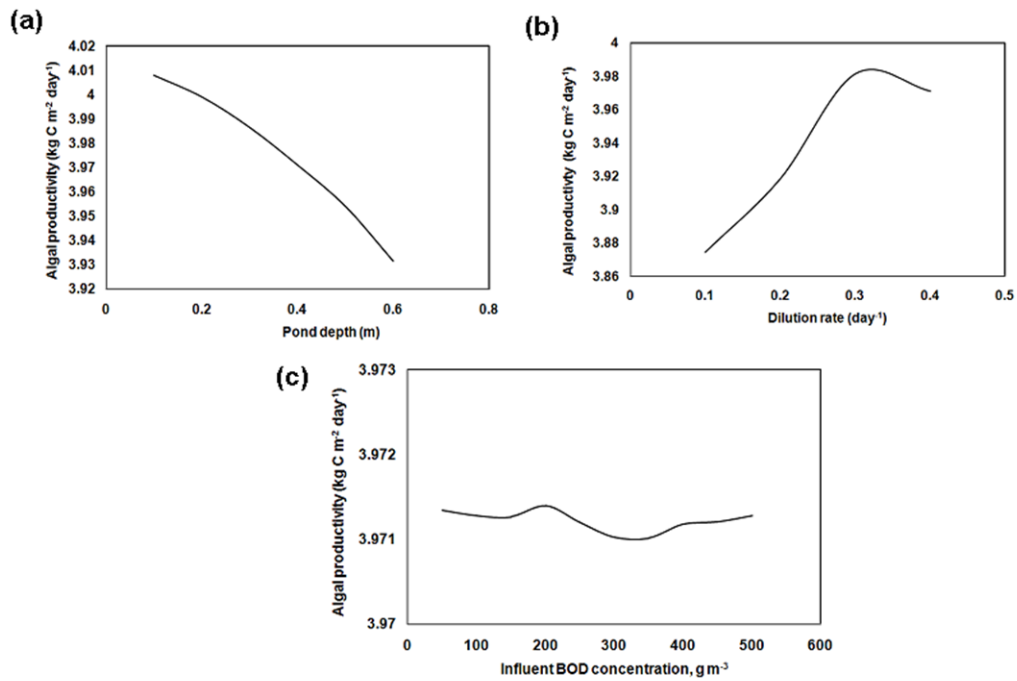
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511 **Figure 4:** (a) Dissolved oxygen (b) Total inorganic carbon and (c) Total inorganic nitrogen
 512 profiles in HRAP along the 24hrs period



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514 **Figure 5:** (a) Algal biomass concentration, (b) pH, (c) Dissolved oxygen (DO) and (d) total
 515 inorganic carbon profiles along the 24hrs period for the case of without CO₂ sparging.



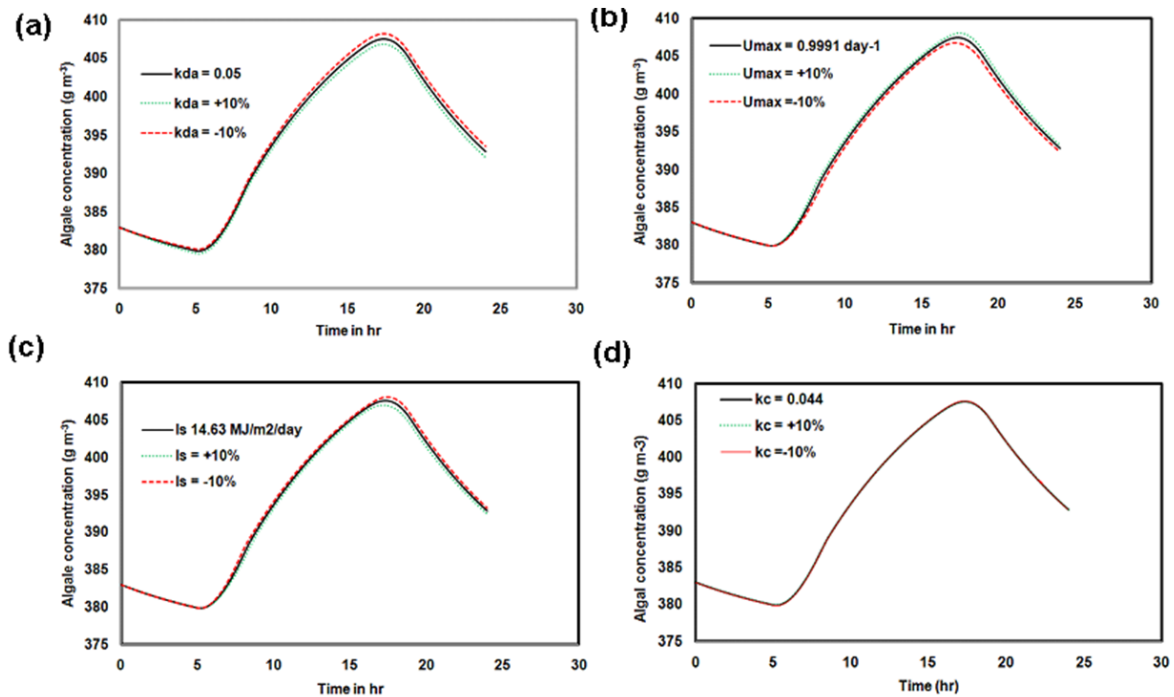
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517 **Figure 6:** Plots of (a) pond depth, (b) dilution rate and (c) BOD versus areal productivity of
 518 algae biomass

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523 **Figure 7:** Sensitivity analysis of (a) decay rate (b) maximum specific growth rate (c)
 524 saturation light intensity (d) nutrient half saturation constant on algal biomass concentration

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List of Tables

Table 1: Values of model parameters employed in simulation

Table 2: Design and Operating Parameters employed in the mathematical model

552

553

Table 1

554

Parameter description	Symbol	Value	Unit	Reference
Maximum specific rate of algae	μ_M	0.9991	$days^{-1}$	Yang [8]
Maximum specific rate of bacteria	μ_{BM}	5.0432	$days^{-1}$	Yang [8]
Henry's constant (Carbon dioxide)	$K_{H(CO_2)}$	0.90315	$g/(m^3 atm)$	Yang [12]
Henry's constant (Oxygen)	$K_{H(O_2)}$	0.04416	$g/(m^3 atm)$	Yang [12]
Dissociation constants for carbonic acids system	K_A	1.76e-05		Ifrim et al. [15]
Dissociation constants for carbonic acids system	K_{1C}	4.38e-07		Ifrim et al. [15]
Dissociation constants for carbonic acids system	K_{2C}	4.65e-11		Ifrim et al. [15]
Yield conversion coefficient (BOD) consumed	Y_B	2.5	$\frac{g \text{ BOD consumed}}{(g \text{ bacteria mass produced})}$	Yang [8]
Yield conversion coefficient of CO ₂ consumed per unit mass of algae produced	Y_{A,CO_2}	2.812	$g \text{ CO}_2 / g \text{ algal mass produced}$	Park and Li [16]
Yield coefficient of oxygen produced per unit mass of algae produced	Y_{A,O_2}	1.587	$g \text{ O}_2 / g \text{ algal mass produced}$	Park and Li [16]
Yield conversion coefficient of Nitrogen consumed per unit mass of algae produced	$Y_{A,N}$	0.091	$g \text{ N} / g \text{ algal mass produced}$	Park and Li [16]
Yield conversion coefficient of CO ₂	Y_{B,CO_2}	3.432	$g \text{ CO}_2 / g \text{ bacteria mass produced}$	Park and Li [16]

Parameter description	Symbol	Value	Unit	Reference
produced per unit mass of bacteria produced				
Yield coefficient of O ₂ consumed per unit mass of bacteria produced	Y_{B,O_2}	2.496	g O ₂ / g bacteria mass produced	Park and Li [16]
Yield coefficient of Nitrogen consumed per unit mass of bacteria produced	$Y_{B,N}$	0.1239	g N/ g bacteria mass produced	
Algae decay coefficient	k_{da}	0.05	days ⁻¹	Yang [8]
Bacteria decay coefficient	K_{db}	0.10	days ⁻¹	Yang [8]
Half velocity constant for carbon dioxide	K_C	0.044	gCO _{2D} m ⁻³	Yang [8]
Half velocity constant for substrate	K_S	150	BOD m ⁻³	Yang [8]
Half velocity constant for ammonia	$K_{NA};$	0.014	g N m ⁻³	Yang [8]
Half velocity constant for oxygen	K_{O_2}	0.256	gCO _{2D} m ⁻³	Yang [8]
Partial pressure of oxygen	P_{O_2}	0.21	atm	Yang [8]
Partial pressure of carbon dioxide	P_{CO_2}	0.00032	atm	Yang [8]
Extinction coefficient	K_{e1}	0.32	m ⁻¹	Yang [8]
Extinction coefficient	K_{e2}	0.03	m ⁻¹ (g/m ³) ⁻¹	Yang [8]
Saturation light intensity	I_S	14.63	M/m ² /day	Yang [8]
Density of liquid	ρ_L	1e3	kg/m ³	Yang [8]
Liquid viscosity of pure water	μ_L	9.07e-4	pa s	
Mass transfer coefficient of O ₂	k_{lg,O_2}	24	day ⁻¹	Bai et al. [11]

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Table 2

Item	Parameter description	Symbol	Nominal value	Unit
pond	Pond depth	z	0.1-0.4	
	Hydraulic retention time	τ		day
	Temperature	T	20	$^{\circ}\text{C}$
	Maximum light intensity	I_0	77.8	MJ/(m ² day)
	Saturation light intensity	I_s	14.63	MJ/(m ² day)

	Number of CSTR	-	20	-
	Photo-period (in a 24-h day)	-	(5.00: 19.00)	hrs
	Dilution rate	R_T	0.1-0.4	day ⁻¹
Influent waste water	Influent waste water flow rate	F	50	m ³ /day
	Biological Oxygen Demand	BOD	0 - 50	g/m ³
	Total Inorganic Carbon	C_T	102	g /m ³
	Total ammonium Nitrogen	N_T	90	g /m ³
	Influent oxygen concentration	M_{OXG}	4	g /m ³
	Total substrate concentration	S	300	g /m ³
	Temperature	T	20	°C
	Total algae concentration	X_a	383	g/m ³
	Total bacteria concentration	X_b	0.005	g/m ³
Supplied gas	Volumetric flow rate	Q_o	240	m ³ / day
	Pressure		0.11e06	pa
	Temperature	T	20	°C
	CO ₂ molar fraction		11	mass fraction (%)

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