Assessment of hydrodynamics based on Computational Fluid Dynamics to optimize the operation of hybrid tubular photobioreactors

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A B S T R A C T

Appropriate hydrodynamic conditions are crucial in photobioreactors (PBR) in order to prevent sedimentation of microalgal biomass and to ensure the uniform exposure of microalgae cells to light and nutrients. Hydrodynamic conditions are also important to guarantee efficient mass transfer and proper shear stress on the transparent walls of the PBR, which can avoid the formation of undesired biofilm. Numerical simulations based on Computational Fluid Dynamics (CFD) can assist to improve the hydrodynamic design and optimization of PBRs. In this study, CFD was used as a tool to investigate the hydrodynamics of a hybrid horizontal tubular PBR designed for microalgae cultivation and wastewater treatment. The flow regime, average circulation time and shear stress distribution in the tubes were evaluated. To establish the reliability of the simulation study, the CFD model was validated using tracer experimental tests and ultrasonic flow meter measurements. Results showed that the hydrodynamic conditions in the tubes resembled plug flow with small axial dispersion. The simulated velocity profile in the tube corresponded to the analytical velocity profile based on experimental data. Simulations also showed that, even increasing flow velocities, low velocity zones were present in some zones of the PBR. The shear stress distribution in the tubes showed values higher enough to reduce or avoid the formation of biofilm, nevertheless the shear stress value is not sufficient to remove the already formed biofilm. Based on the numerical investigation and practical evaluation, this study demonstrated that CFD is a useful tool to optimize PBR design and operation in order to enhance microalgae production and boost the scale-up of this technology.

1. Introduction

Microalgae are part of a large and diverse group of simple aquatic organisms [1]. The characteristic of microalgae is that they are able to convert sunlight, CO₂ and nutrients to biomass through photosynthesis in the same way as other plants. They can grow at a faster rate than other land-based crops and can live in diverse aquatic environments with basic nutrient requirements [2]. Due to these attractive features, microalgae biomass can be cultivated for several purposes. For instance, the use of microalgae for human consumption has beneficial aspects including improved immune response, improved fertility, and better weight control. However, the use of microalgae for food is restricted to very few species due to the strict food safety regulations. On the other hand, microalgae are also the natural feed source for fish and shrimps. In addition, some conversion technologies allow using microalgae in agricultural applications as a biofertilizer [3]. Also, microalgae offer a sustainable alternative to wastewater treatment technologies [4]. It is possible to use them in biological treatment as they are able to remove nutrients and convert them into biomass, while producing oxygen (through photosynthesis) required by heterotrophic and autotrophic bacteria for organic and inorganic pollutants removal from wastewater [5].

Microalgae can be cultivated in open systems (called high rate algal ponds or raceways) or in closed photobioreactors (PBRs). Proper microalgae growth and productivity depend basically on nutrients concentrations, light and temperature. Open systems are less expensive and simpler than closed systems, however productivity is usually lower in open systems with an increased risk of contamination of the desired species. In closed PBRs, the specific conditions required by each microalgae strain can be more carefully controlled. Novel hybrid configurations or semi-closed PBRs, combining open and closed units, arise...
recently proposed and tested at lab scale a PBR configuration combining a closed bubble column reactor with open illuminated tubular structures, with the objective of reducing the required surface area. In a different approach, Uggetti et al. [7] evaluated the performance of a hybrid PBR combining open tanks and closed horizontal transparent tubes, for microalgae-based treatment system within a biorefinery concept. The performance of these systems is significantly influenced by the hydrodynamic conditions. Indeed, the PBR design and operation must ensure proper mixing of the culture medium in order to avoid the formation of biofilm on the walls, especially in hybrid systems. Photobioreactors differ in their design and operating conditions as well. The scale of the photobioreactor also has an important effect on the hydrodynamics. Therefore, scale-up of those systems is limited precisely due to the non-transferability of hydrodynamic conditions from laboratory to pilot or industrial scale.

In the case of tubular PBR, a well-known drawback is that biofilm can develop attached to the inner wall of the transparent tubes, thus reducing the light exposure within the culture medium. Therefore, a proper velocity of the culture medium inside the tubes should be chosen in order to ensure sufficient mixing and shear stress avoiding the formation of biofilm on the walls. On the other hand, excessively high flow velocities should be avoided to prevent cell stress [8,9] and to avoid unnecessary energy consumption. Indeed, the selection of the optimal operating condition of the system can reduce the PBRs costs [10,11]. Determining the distribution of shear stress in a turbulent flow regime is complex and is based on semi-empirical analysis. Therefore, defining a critical value of shear stress that prevents the formation of biofilm is very complicated. Using numerical simulations, it is possible to study in detail the influence of operating conditions on the hydrodynamics of the PBR and to estimate the shear stress. The validated numerical model can help to optimize operating and design conditions in order to intensify the production of microalgae.

Computational Fluid Dynamics (CFD) is a tool based on the fluid dynamics theory, whose application to engineering has experienced a great growth in the last decades. Fluid flows are described by partial differential equations and CFD replaces these equations by algebraic equations, which can be subsequently numerically solved. These equations describe how the single operating parameters are related. CFD models can complement the limitations of laboratory experiments and provide comprehensive hydrodynamic information, such as spatial flow and velocity fields. They can be used either in the initial PBR design or for optimization of the PBR operation. The mixing behavior in different PBRs can be explored without doing expensive experiments and design modification can be further adjusted [12]. Hadiyanto et al. [13] and Gómez-Pérez et al. [10] described several CFD applications to model PBRs in the recent years. Most of these studies are focused on a reduction of energy consumption and operating costs. CFD simulation can be used for optimization of real-scale photobioreactor design and operating conditions as well [14]. Further studies are focused on the effect of flow velocity on biofilm formation in the dead zones of the PBRs. Qin and Wu [15] and Salguero-Rodríguez et al. [16] described the influence of static mixers application in tubular PBR tubes on operating conditions and energy consumption. Bitog et al. [17] review the status of CFD modeling for PBRs and the application of CFD in the design of PBR for microalgae production in different cultivation systems as well. To determine the optimal operating conditions of novel PBR according to the proper mixing of the culture medium and to prevent the formation of biofilm on transparent walls, it is important to specify and describe the hydrodynamics of the culture medium. Using a validated CFD model, it is possible to assess in detail the local values of flow velocities, shear stresses and mixing intensity depending on the operating conditions of a PBR. In turn, CFD model can be used as a powerful tool to adapt PBR operation and/or design in order to improve microalgae production.

The aim of this paper was to analyze and enhance hydrodynamic conditions in a demonstrative scale hybrid tubular PBR by CFD simulations. The specific design of the PBR was aimed at combining advantages of both open and closed systems for microalgae cultivation and wastewater treatment within the biorefinery concept. This is the first study performing a comprehensive hydrodynamic evaluation of this hybrid tubular PBR, addressing three specific objectives: (i) to gain insight about the hydrodynamic behavior of the system, (ii) to optimize the operational conditions of the PBR, and (iii) to evaluate the shear stress to assess the feasibility of preventing or reducing the formation of biofilm. The numerical model was calibrated and validated on the basis of experimental data, confirming its reliability and suitability. Based on the validated numerical model, the influence of PBR design and operating parameters on the hydrodynamics of the culture medium can be investigated without any further complex experiment. This can help increasing microalgae production by changing operating parameters and/or PBR design in accordance with hydrodynamics conditions. Consequently, CFD simulation can be a powerful tool for promoting PBR upscaling.

2. Material and methods

2.1. Description of experiments

2.1.1. Photobioreactor

A demonstrative plant was built in the Agròpolis experimental campus of the Universitat Politècnica de Catalunya-BarcelonaTech within the framework of the H2020 EU project INCOVER “Innovative Eco-technologies for Resource Recovery from Wastewater” (GA 689242). The plant included 3 identical hybrid, semi-closed horizontal tubular PBRs designed and operated to produce microalgal biomass from agricultural and domestic wastewater.

Each hybrid horizontal tubular PBR consists of 2 open tanks connected through 16 low-density polyethylene transparent tubes with 125 mm inner diameter and wall thickness of 0.3 mm, as shown in the

Fig. 1. Hybrid horizontal tubular PBR.
photography in Fig. 1 and the scheme in Fig. 2a. Total volume of culture medium in each PBR is 11.7 m$^3$ (9.2 m$^3$ within the tubes and 2.5 m$^3$ in the 2 open tanks). The scheme of the PBR and section of open tank are shown in Figs. 2a and 2b, respectively. Both tanks are equipped with a paddle wheel, which is driven by a 0.25 kW engine. The system is inspired by the high rate algal ponds or raceway ponds used for wastewater treatment, which use paddle wheels for liquid circulation in the pond. Paddle wheels are simple to operate and have low energy consumption compared to other devices. The paddle wheel speed in the PBR is varied by a frequency converter in the range of 0–12 rpm, which is in the range of the rotational speed of paddle wheels in conventional raceway ponds, usually up to 20 rpm [14]. The energy requirement of the paddle wheels at full capacity reaches 40 W per m$^3$ of culture medium, which is significantly lower than that in conventional tubular PBRs with centrifugal pumps (about 500 W m$^{-3}$) [18].

The flow circulation of the culture medium through the PBR is performed as follows. An overflow plate is located in each tank below the paddle wheel (Fig. 2b). The paddle wheel moves the culture medium from one side of the tank over the overflow to the other side, creating a difference of culture medium level $\Delta h$ (m) between both sides. The higher level in one side of the tank causes the flow of culture medium through 8 of the transparent tubes from one tank to the other. In the second tank, the medium is moved through the overflow again causing the flow from the second tank to the first one through the other 8 tubes, thus, continuous circulation in the PBR is ensured. The culture medium is exposed to the solar radiation during circulation through the transparent tubes. The speed of rotation of the paddle wheels determines the level of the culture medium in the suction and discharge section of the paddle wheel, $h_2$ (m) and $h_1$ (m) respectively. Therefore, the hydrodynamic conditions in the PBR can be adjusted modifying the speed of the paddle wheels. Additionally, the transparent tubes were periodically cleaned with a brush, in order to remove the biofilm growing in the inner wall. The brush was passed through the tubes several times until removing the biofilm. Each tube was cleaned approximately every fortnight.

The PBRs were located outdoors, exposed to the solar radiation and weather conditions in the location of the plant (Viladecans, Barcelona, 41.288 N and 2.043 E UTM). A volume of 2.3 m$^3$ of a mix of agricultural and domestic wastewater was fed daily to each PBR in semi-batch mode.

Nutrients were injected into the PBRs mostly in dissolved form from the agricultural and domestic wastewater. The specific design of the PBRs was initially chosen in order to treat agricultural and domestic wastewater while promoting the selection of cyanobacteria and accumulation of polyhydroxyalkanoates. The design specifications of the PBRs are shown in Table 1. Further description and details about the pilot plant, the PBR design, the characteristics of the influent wastewater and the results during more than one year of operation are reported in Diez-Montero et al. [19], García et al. [20] and Rueda et al. [21].

2.1.2. Experimental tests for hydrodynamic characterization of the PBR

A set of experimental tracer tests was performed in the tubes of the PBR in order to determine the residence time distribution (RTD). The tests were performed in the tubes, instead of the whole PBR, aimed at estimating the mean residence time and main hydrodynamic characteristics in the irradiated area of the PBR. The RTD of a system or reactor can be obtained from tracer tests and is expressed by Eq. (1) assuming a constant flow [22].

$$E(t) = \frac{C(t)}{\int_0^t C(t) dt}$$

where $E(t)$ is the RTD ($s^{-1}$), $C$ (mg L$^{-1}$) is the concentration of tracer in the outlet of the system or reactor at any given time $t$ (s). Subsequently, the mean residence time $t_m$ (s) inside the tube can be calculated from the first moment of the function Eq. (2).

$$t_m = \int_0^\infty t \cdot E(t) dt$$

<table>
<thead>
<tr>
<th>Description</th>
<th>Parameter</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume of culture medium in PBR</td>
<td>11.7</td>
<td>m$^3$</td>
</tr>
<tr>
<td>Water level in open tank, inlet to the tubes ($h_1$)</td>
<td>0.35</td>
<td>m</td>
</tr>
<tr>
<td>Water level in open tank, outlet of the tubes ($h_2$)</td>
<td>0.15</td>
<td>m</td>
</tr>
<tr>
<td>Number of transparent tubes</td>
<td>2 × 8</td>
<td></td>
</tr>
<tr>
<td>Inner diameter of the transparent tube</td>
<td>0.125</td>
<td>m</td>
</tr>
<tr>
<td>Length of the transparent tube</td>
<td>47</td>
<td>m</td>
</tr>
<tr>
<td>Paddle wheel rotational speed</td>
<td>0–12</td>
<td>rpm</td>
</tr>
</tbody>
</table>

Table 1
Horizontal tubular photobioreactor characteristics.

Fig. 2. Scheme of hybrid horizontal tubular PBR, (a) 3D isometric view, (b) section of one open tank.
By substituting Eq. (1) into Eq. (2), and discretizing for given intervals of time, the mean residence time can be determined in discrete form as expressed in Eq. (3).

$$t_m = \frac{\sum_i t_i C_i \Delta t}{\sum_i C_i \Delta t}$$  \hspace{1cm} (3)

where the $t_i$ (s) is the discrete time, $C_i$ (mg L$^{-1}$) is the concentration of tracer in discrete form, $\Delta t$ (s) is the time difference. The variance of the RTD function in discrete form is $\sigma^2_t$ (Eq. (4)).

$$\sigma^2_t = \frac{\sum_i (t_i - t_m)^2 C_i \Delta t}{\sum_i C_i \Delta t}$$  \hspace{1cm} (4)

From Eqs. (3) and (4), the dimensionless variance $\sigma^2_t$ can be obtained (Eq. (5)).

$$\sigma^2 = \frac{\sigma^2_t}{t_m^2}$$  \hspace{1cm} (5)

This dimensionless variance $\sigma^2$ may be used to predict the mixing conditions in the tube. From the dimensionless variance, the dimensionless axial dispersion coefficient $D_{ax}$ can be calculated, and it is assumed to be independent of tracer concentration and of the axial position in the tube (because the concentration is assumed to be radially uniform) [23]. Per definition, $D_{ax}$ depends on the diffusion coefficient $D_{diff}$ (m$^2$ s$^{-1}$), the mean culture medium velocity $u$ (m s$^{-1}$) and the length of the tube $L$ (m) (Eq. (6)).

$$D_{ax} = \frac{D_{diff}}{\pi} \frac{L}{u}$$  \hspace{1cm} (6)

The dispersion coefficient represents a very convenient tool to measure the spread of tracer in the tube and therefore the degree of mixing [23]. For the ideal plug flow $D_{ax}$ approaches to 0, while for perfect mixing $\infty$ [22]. The dispersion coefficient can be estimated from the dimensionless variance obtained in the RTD analysis.

For small extents of dispersion ($D_{ax} < 0.01$), i.e. small deviation from plug flow, Eq. (7) can be used [22].

$$\sigma^2 = 2 \cdot D_{ax}$$  \hspace{1cm} (7)

When the coefficient of dispersion is already estimated, the time normalized (dimensionless) RTD can be calculated from Eq. (8).

$$E_u = \frac{1}{\sqrt{4 \pi D_{ax}}} \exp \left[ -\frac{(1 - \theta)^2}{4 D_{ax}} \right]$$  \hspace{1cm} (8)

where $\theta$ is the normalized time (dimensionless) = $t/t_m$.

The RTD in the horizontal tubes of the PBR was determined experimentally by the pulse-input tracer technique. The experiments were conducted in 8 tubes under the same operational conditions, i.e. the same rotational speed of the paddle wheels. The tests were performed from the inlet of the tubes in one open tank to the outlet in the other open tank. A concentrated solution of sodium chloride (NaCl, 50 g L$^{-1}$) was used as tracer for the RTD tests. A pulse of 100 mL of the tracer solution was injected by means of a syringe at the inlet of each tube at time zero, and the electrical conductivity was continuously measured and recorded at the outlet of the tubes with a HACH CDC40103 probe connected to a HACH HQ40d conductivity meter (Fig. 3a). Subsequently, measured conductivity values were converted to NaCl concentrations (conductivity standards provided by HACH) by assuming that 1 µS cm$^{-1}$ is equivalent to 0.64 mg of NaCl per liter of water. The measurements were performed separately in the 8 tubes. After each measurement, the probe was consecutively moved to the next tube and the syringe was refilled with the same volume of tracer to perform the next test.

Additionally, two more tracer tests were performed in one tube under different operational conditions, modifying the difference in the water level in the open tanks. The rotational speed of the paddle wheels was modified in order to set different water levels in the tanks. These tests were used for validation of the model.

The RTD curves measured experimentally were fitted with the analytical solutions and $D_{ax}$ was calculated from the experimental results. The mean culture medium circulation velocity $u$ (m s$^{-1}$) was determined from the ratio of circulation length $L$ (m) to mean residence time $t_m$ (s).

2.1.3. Onsite velocity measurement

In addition, an ultrasonic flowmeter Flexim Fluxus F601 (accuracy 1.6% of reading 0.01 m s$^{-1}$) was installed as shown in Fig. 3b, in order to measure the actual velocity of the culture medium inside the tubes and to verify the accuracy of the pulse input tracer test. At a distance of 20 m from the exit tank, part of one tube of the PBR was replaced with a rigid PVC tube (about 3 m). Ultrasonic transducers were clamped onto the external wall of the tube (length 2.5 m and diameter 0.11 m) and were never in direct contact with the culture medium flowing inside the tube. Ultrasonic signals were emitted by transducers installed on one side of the pipe. The signals were reflected on the opposite side of the rigid tube and finally received by a second transducer. The signals were emitted alternatively in and against the flow direction. The two ultrasonic transducers were connected to the transmitter of the flowmeter.

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**Fig. 3.** Lateral view of the PBR, including the two open tanks and one tube, representing the: (a) pulse input tracer technique; and (b) ultrasonic flowmeter technique.
2.2. Numerical model setup

Two CFD geometries for PBR simulation were created in ANSYS FLUENT CFD 19.1. The 3D geometry was developed to simulate hydrodynamic conditions in open tanks and the tubes. The 2D mesh was created only for the detail description of hydrodynamics in tubes. In order to reduce cells and have still a good resolution, symmetry was anticipated and only half of the PBR tube was simulated in 2D mesh.

2.2.1. Fluid dynamic model selection

From the analytical calculation of PBR operating conditions, it can be assumed that the flow regime is in the range of low Reynolds number $Re$. Turbulent viscosity is a complex parameter to define, and several semi-empirical theories have been elaborated to determine its approximate value. According to Boussinesq hypothesis, Reynolds stresses are proportional to fluid velocity gradients. This hypothesis is used in the $k$-$\varepsilon$ standard and Re-Normalization Group (RNG) models, and its advantage is the relatively low computational requirement for turbulent viscosity determination. The standard $k$-$\varepsilon$ model is more appropriate for models with high Reynolds number, while RNG model provides an analytically derived differential formula for effective viscosity, which makes the RNG model more accurate and reliable for models with low Reynolds number [24].

Therefore, the RNG $k$-$\varepsilon$ model was used to simulate the fluid dynamics behavior in tubular horizontal PBR. The governing equations of the turbulent kinetic energy $k$ ($m^2 \cdot s^{-2}$) and dissipation rate $\varepsilon$ ($m^2 \cdot s^{-3}$) are given by Eqs. (9) and (10).

\[
\frac{\partial}{\partial x_i}(\rho k) = \frac{\partial}{\partial x_i} \left[ \alpha_i (\mu + \mu_t) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho \varepsilon \quad (9)
\]

\[
\frac{\partial}{\partial x_i}(\rho \varepsilon) = \frac{\partial}{\partial x_i} \left[ \alpha_i (\mu + \mu_t) \frac{\partial \varepsilon}{\partial x_i} \right] + \frac{C_1}{k} G_k - C_2 \rho \varepsilon^2 \quad (10)
\]

where $G_k$ is the generation of turbulence kinetic energy due to the mean velocity gradients, $G_b$ represents the generation of turbulence kinetic energy due to buoyancy. The model constants $C_{1k} = 1.44$, $C_{2k} = 1.68$, are analytically derived by RNG theory, $\alpha_k = \alpha_\varepsilon = 1.393$ represent the inverse effective Prandtl numbers. Effective viscosity is represented by sum of dynamic viscosity $\mu$ and turbulent viscosity $\mu_t$ given by Eq. (11).

\[
\mu_t = \rho C_{\mu t} \frac{k^2}{\varepsilon} \quad (11)
\]

where constant $C_{\mu t} = 0.0845$ is derived using RNG model theory [24]. The calculations obtained using RNG methods should always be verified by experiments or at least by a qualitative comparison with literature results. The hydrodynamic conditions were numerically simulated with ANSYS FLUENT CFD 19.1. software.

2.2.2. Mesh generation

The 3D model consisted of 8 tubes connecting 2 tanks (one with higher water level and the other with lower water level), since the hydrodynamic conditions in the 8 tubes of the second half of the PBR are identical. The grid contains approx. 2,565,305 elements with a 10 mm maximum size. Computations were performed until calculation converged at a residue of $10^{-6}$ between two iterations. The mesh quality was checked using skewness reaching the value of 0.19. Because of the length of each tube, the flow in the PBR can be regarded as a fully developed state, which can be employed for determining steady state flow dynamics of the culture medium.

In order to examine more precisely the hydrodynamic conditions in the transparent tube, a second model with a 2D mesh for one tube was created as well. For a length of 47 m and diameter of 125 mm, the grid contains approx. 1,375,358 elements with a 5 mm maximum size. The inflation function was applied in the area close to the tube wall with the minimum grid size of 0.1 mm. Computations were performed until

2.2.3. Boundary conditions

Properties and physical parameters were set in the model by considering the culture medium as water (excluding microalgal biomass). For the first 3D overall PBR model, the inlet velocities were set according to the range of operating flow rate in outlet cross section of the paddle wheel, and resulted in velocities ranging between 0.385 and 0.606 $m \cdot s^{-1}$. The same conditions were set for outlet flow velocity in the suction cross section of the paddle wheel on the opposite side of the PBR. The outer walls and the internal structures of the tanks were set to no-slip boundary condition to water, and roughness of 0.5 mm in transparent tubes was fixed.

To simulate hydrodynamic conditions in the 2D model representing a transparent tube, the inlet and outlet were located at the beginning and end of the tube, and defined by the hydrostatic pressure derived from the water levels in tanks (Table 3). In order to simulate the effect of microalgae biofilm formation on hydrodynamic conditions, the roughness of 0.5 mm was set. The roughness has been selected according to the biofilm formation on transparent PBR tubes in non-sterile conditions [25]. Roughness selection is described more in detail in paragraph 3.2.

2.3. Hydrodynamic analysis of the hybrid tubular photobioreactor

Once the model was built, simulations were performed in order to comprehensively analyze the hydrodynamics in the tubes and the PBR. First, the model was calibrated according to the velocities obtained by the experimental tracer tests and the velocity profiles inside the tubes. Then, the model was validated with experimental results obtained under different operational conditions of the PBR. Finally, the model was used to analyze the hydrodynamic conditions and estimate the shear stress inside the tubes.

2.3.1. CFD model calibration and validation

The CFD model was calibrated by comparing the simulated velocity profile inside the tubes with the velocity profiles obtained analytically based on the experimental results of the tracer tests. Several empirical velocity profiles exist for turbulent tube flow. Among those, the simplest and the best known is the power-law velocity profile expressed as according to Eq. (12).

\[
u_i = \nu_{max} \left( 1 - \frac{r}{R} \right)^{\frac{1}{n}} \quad (12)
\]

where $R$ (m) is the tube radius, $r$ (m) is the radial coordinate, $\nu_{max}$ ($m \cdot s^{-1}$) is the centerline velocity, and $n$ is the dimensionless constant whose value depends on the Reynolds number $Re$ [26] as described in Eq. (13).

\[n = 1.03 \ln(Re) - 3.6 \quad (13)\]

The centerline velocity can be experimentally determined from the RTD, according to the length of the tube and the time when the concentration of tracer begins to be measured at the outlet of the tube. A

<table>
<thead>
<tr>
<th>Configuration</th>
<th>$h_1$ (m)</th>
<th>$h_2$ (m)</th>
<th>$\Delta h$ (m)</th>
<th>$t_{\text{avg}}$ (s)</th>
<th>$\nu_{\text{max}}$ ($m \cdot s^{-1}$)</th>
<th>$\nu_{\text{bottom}}$ ($m \cdot s^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.35</td>
<td>0.26</td>
<td>0.09</td>
<td>186</td>
<td>0.25</td>
<td>0.249</td>
</tr>
<tr>
<td>B</td>
<td>0.36</td>
<td>0.26</td>
<td>0.10</td>
<td>145</td>
<td>0.32</td>
<td>0.319</td>
</tr>
<tr>
<td>C</td>
<td>0.39</td>
<td>0.26</td>
<td>0.13</td>
<td>128</td>
<td>0.37</td>
<td>0.371</td>
</tr>
</tbody>
</table>
closer examination shows that the power-law profile cannot be valid near the wall, since the velocity gradient is infinite there. In addition, Eq. (12) cannot be precisely valid near the centerline because the first derivative is not smooth in the tube center.

For a further description of the velocity distribution in the tube, it is possible to use the universal velocity profile [27]. The viscous sublayer next to the transparent wall of tube can be specified according to Eq. (14).

\[
    u_i = \frac{r}{\nu} u^* \tag{14}
\]

where \( \nu \) (m\(^2\) s\(^{-1}\)) is the kinematic viscosity and \( u^* \) (m s\(^{-1}\)) is expressed according to Eq. (15).

\[
    u^* = \sqrt{\frac{\tau_{w}}{\rho}} \tag{15}
\]

where \( \tau_w \) (Pa) is the shear stress on the transparent wall of the tube and \( \rho \) (kg m\(^{-3}\)) is the density. The validity of viscous sublayer expression is defined within the range of \( 0 < y^+ < 5 \), where the dimensionless \( y^+ \) is defined by Eq. (16).

\[
    y^+ = \frac{r u^*}{\nu} \tag{16}
\]

In transition area, the velocity profile equation, which is valid within the range of \( 5 < y^+ < 30 \), can be expressed

\[
    u_i = 5 \ln y^+ - 3.05 \tag{17}
\]

For the values \( y^+ > 30 \), turbulent area can be specified

\[
    u_i = 2.5 \ln y^+ + 5.5 \tag{18}
\]

The universal velocity profile describes very well the velocity distribution in smooth tubes except the area close to centerline, where the velocity gradient from Eq. (18) is not zero.

If the height of the tube roughness \( k_s \) (m) exceeds the thickness of the viscous sublayer, the flow of culture medium can be greatly affected. The velocity profile of hydraulically rough tubes can be expressed using Eq. (19) [27].

\[
    u_i = u^* \left( 2.5 \ln \frac{r}{k_s} + 8.5 \right) \tag{19}
\]

In this study, the power-law, the universal smooth tube, and the universal fully rough tube velocity profiles have been assessed and compared to the CFD simulations in order to calibrate the model. Once calibrated, the model has been used to simulate the velocity profile under different operational conditions, and results have been compared to those obtained in experimental tracer tests.

2.3.2. Estimation of the shear stress distribution

The distribution of total shear stress in the tube in turbulent flow consists of a laminar \( \tau_{low} \) (Pa) and a turbulent shear stress \( \tau_{tur} \) (Pa). The total shear stress can be expressed using Eq. (20).

\[
    \tau = \tau_{low} + \tau_{tur} \tag{20}
\]

In turbulent and transition areas, the effect of turbulent shear stress on the total stress distribution is dominant. However, the laminar shear stress is more important in the viscous sublayer near the wall of the tube. The laminar shear stress can be easily defined by the dynamic viscosity \( \mu \) (Pa s) of the flowing medium (Eq. (21)).

\[
    \tau_{low} = \mu \frac{du}{dr} \tag{21}
\]

One of the first attempts of semi-empirical analysis of turbulent flow was the concept developed by Prandtl in 1925 based on mixing length \( l_m \) (m) [27]. Prandtl defined the turbulent viscosity \( \mu_t \) (Pa s) based on the mixing length (Eq. (22)).

\[
    \mu_t = \rho \frac{l_m^3}{\varepsilon} \frac{du}{dr} \tag{22}
\]

where \( \rho \) (kg m\(^{-3}\)) is the density of flowing medium. However, the mixing length parameter is not also easy to determine. Further considerations indicate that \( l_m \) is not a constant throughout the flow field and additional assumptions are needed, according to the mixing length variation throughout the flow. Boussinesq hypothesis (Section 2.2.1.) defines the turbulent shear stress \( \tau_{tur} \) in terms of the turbulent viscosity according to Eq. (23).

\[
    \tau_{tur} = \mu_t \frac{du}{dr} \tag{23}
\]

The use of CFD allows the numerical solution of turbulent viscosity according to Boussinesq hypothesis. The RNG \( k-e \) model provides an analytically-derived differential formula for viscosity, which makes the model more accurate and reliable for a wider class of flows. The RNG model takes into account the effects of swirl or rotation by modifying the turbulent viscosity appropriately. In this study, the turbulent shear stress in the tubes of the PBR was estimated by the Boussinesq hypothesis, according to Eq. (23), using the turbulent viscosity determined by the CFD model (Eq. (11)). Subsequently, the total shear stress distribution was estimated as well.

3. Results and discussion

3.1. Hydrodynamic analysis based on RTD curves

The RTD obtained experimentally in the horizontal tubes of the PBR are shown in Fig. 4. Experimental tests were performed in the eight tubes, however, results corresponding to Tube 4 are not presented since measurements were not reliable due to a high biofilm concentration on the tube walls. It should be highlighted that Tube 4 was not cleaned for a longer time at the time of the experiments, compared to the other tubes. The rotational speed of the paddle wheels of the PBR was set so the water levels \( h_1 \) and \( h_2 \) in the open tanks were 0.28 m and 0.24 m, respectively. The shape of the RTD in all the tubes present a sharp peak, resembling to plug flow with small axial dispersion. All the tubes showed a similar behavior, with the peak occurring close to the normalized time \( \theta = 1 \). Note that the normalized time is obtained based on the measured mean residence time \( t_m \) (s).

The values of mean residence time \( t_m \) and the variance calculated from Eqs. (2) to (5), are presented in Table 2. The \( t_m \) ranged from 250 s in Tube 1–335 s in Tube 7, showing slightly higher values in the tubes located closer to the paddle wheel (6, 7 and 8). This suggests that the flow velocity in the tubes was partly influenced by the distance between each tube and the paddle wheel.

Based on the mean residence time \( t_m \) (s) and the length of the transparent PBR tube (Table 1), it was possible to determine the mean flow velocity \( \bar{v} \) (m s\(^{-1}\)) and Reynolds number \( Re \) in the tubes and the

![Fig. 4. RTD in the horizontal tubes of the PBR. The difference of concentration is \( \Delta C \) and \( \theta \) is the normalized time (dimensionless) = \( t_m / t_{tur} \).](image)
The inner radius of the tube. The flow velocity profiles inside a tube of the PBR, Fig. 5.

The dimensionless dispersion coefficient $D_{ax}$, calculated from Eq. (6). The average flow velocity inside the tubes ranges from 0.14 to 0.19 m s$^{-1}$, in all cases higher than the recommended value of 0.1 m s$^{-1}$ needed to prevent sedimentation of algal biomass [28]. These flow velocities generate a turbulent flow in the tubes, characterized by the Reynolds number ranging from 17,500 to 23,700.

The dispersion coefficient can be used to quantify the extent of the axial dispersion in the tubes. As already mentioned, it is not possible to directly measure the dispersion coefficient $D_{ax}$. However, using the fitting of measured data, it was possible to determine the dispersion coefficient $D_{ax}$ for small extents of dispersion from Eqs. (7) to (8). The results ranged between 0.0022 and 0.0050, in every case clearly below 0.01, thus validating the hypothesis of small dispersion used for the determination of the coefficient and confirming that the hydrodynamic behavior of the tubes was close to ideal plug flow. In addition, the highest extent of dispersion was observed in the tubes located closer to the paddle wheel (6, 7 and 8), which could be attributed to the lower hydrodynamic conditions in the PBR tubes. The dispersion coefficient is needed to precisely determine the fluid field in the hybrid horizontal tubular PBR object of this study.

3.2. CFD model calibration and validation

According to the velocities measured in the tubes, $Re$ reached the value of 23,700, which corresponds to a turbulent flow regime in all the tubes, confirming the appropriateness of the selected fluid dynamic model. Calibration of the CFD 3D model and the subsequent validation of detailed hydrodynamic conditions was performed only for Tube 1, since the variation between the measured average flow velocities in all tubes was low (Table 2). Fig. 5 shows the velocity profile simulated by the CFD model in a cross section of Tube 1, together with the power-law, the universal smooth tube, and the universal fully rough tube velocity profiles based on the experimental data. The maximum centerline velocity $U_{max}$ (m s$^{-1}$) used for the determination of analytical velocity profiles, was determined based on the first response to increasing concentration during the measurement (Table 2). As shown in Fig. 5, the analytical velocity profiles based on experimental data are in good agreement with the CFD simulation. In particular, the universal velocity profile for hydraulically rough tubes ($k_{s}$ was 0.5 mm, the same as in boundary conditions of CFD model) describes the most accurately the distribution of the velocity inside the tube. In the microalgae cultivation process, it is also necessary to consider the effect of biofilm formation on the inner wall of the transparent tubes, due to its influence on the hydrodynamic conditions in the PBR. The thickness of biofilm depends on several factors and ranges from micrometers to millimeters [29,30]. The increase of the biofilm thickness can cause a rise in pressure loss in the tube and consequently lower flow velocity. Decreasing velocity then results in a drop in shear stress that is necessary to prevent further biofilm formation. If the biofilm layer reaches a certain thickness and stiffness, hydrodynamic conditions are not able to remove it or avoid its formation, and it is necessary to stop the operation of the PBR and mechanically remove the biofilm.

Three different operational conditions were selected to validate the CFD simulation. The water levels $h_1$ (m) and $h_2$ (m) in the open tanks were changed by the variation of the paddle wheel rotational speed, resulting in three different setups (A, B, C). Additionally, the flow velocity was verified with an ultrasonic flowmeter. The water levels and main results of the tracer tests and the ultrasonic flowmeter measurements are shown in Table 3.

The velocity profiles inside the tube in the three different conditions were simulated without changing any parameter in the CFD model. The results of the simulations were compared with the universal velocity profiles for rough tubes based on experimental data in Fig. 6. CFD simulations were in good agreement with the analytical profiles. Thus, the numerical predictions were preferably validated by the experimental data, indicating that the established CFD simulation model can simulate precisely the fluid field in the hybrid horizontal tubular PBR object of this study.

3.3. Hydrodynamic analysis based on CFD simulations

This study was focused on the numerical investigation of overall hydrodynamic conditions in horizontal tubular PBR. The hydrodynamics in the open tanks of the PBR was analyzed using the validated 3D model. To this purpose, the hydrodynamic behavior of the PBR was simulated and compared with two different operational conditions. The streamlines in one open tank and at the beginning of the eight tubes with small difference in the water level ($\Delta h = 0.04$ m) and with high

![Fig. 5. Comparison of analytical calculation and numerical simulation of velocity profiles inside a tube of the PBR, r indicates the radial coordinate and R is the inner radius of the tube.](image)

![Fig. 6. Validation of the CFD model: comparison of simulations under the three different conditions considered and the universal velocity profiles for hydraulically rough tubes, r indicates the radial coordinate and R is the inner radius of the tube.](image)
difference in the water level ($\Delta h = 0.2$ m) are shown in Figs. 7a and 7b, respectively. For small differences in water levels (Fig. 7a), low velocities were reached in a significant volume of the tank, in particular in the zone further from the paddle wheel, where the velocity reached values lower than 0.1 m s$^{-1}$. The volume of the open tank consisted of 47% of the medium flowing with velocity lower than 0.1 m s$^{-1}$. This low velocity can cause microalgae sedimentation and accumulation in the open tanks [28].

The increase of the difference in the water level to values closer to the initial design and operational conditions (shown in Table 1) could reduce the formation of low velocities zones in this area. With a difference of 0.2 m (Fig. 7b), the velocity in the zone further from the paddle wheels increased, significantly reducing the volume with low velocity of 23% of total open tank volume. However, flow velocity was still low (lower than 0.1 m s$^{-1}$) in some specific volume of the open tank (Fig. 7b). This suggests that sedimentation and accumulation of microalgae in the tanks cannot be completely avoided by changing the operating conditions. These results also suggest that the shape of the open tanks could be improved in order to further reduce the extent of dead volumes, for instance by substituting the corner located opposite to the paddle wheel and tubes by a chamfer or round shape.

### 3.4. Shear stress analysis based on CFD simulations

Pressure loss in PBR tubes may increase as the biofilm is formed and grows on the inner wall of the tubes. An increasing pressure drop could cause a rising water level in inflow open tank, without increasing the velocity in the tubes and tanks. Therefore, it is always necessary to control biofilm growth inside the tubes, as well as the water levels in the tanks by adjusting the rotational speed of the paddle wheels. Moreover, the shear stress close to the inner wall of the tube is a very important parameter for tubular PBR operation due to its role avoiding biofilm formation and/or excessive growth. In other type of PBRs, such as air lift reactors, the low fluid-induced shear stress can be increased by applying aeration, as reported by Ding et al. in a lab scale experiment [9]. In the PBR analyzed in this study, the shear stress in the tubes can be increased by increasing the water level difference ($\Delta h$) in the open tanks. The estimation of the total shear stress distribution based on CFD simulations for various operational conditions (different $\Delta h$) is shown in Fig. 8. On the one hand, an increase of the shear stress is observed when approaching to the tube wall, as expected, due to the increasing velocity gradient in the radial direction. A sharper increase was observed close to the wall, with a higher slope of the shear stress distribution, due to the no-slip boundary condition. On the other hand, there was an evident increase of wall shear stress when increasing velocity of the culture medium. Shear stress achieved in the wall ranged from 0.3 Pa for the lowest velocity to 1.0 Pa for the largest one. The shear stress values on the wall were higher than the critical value of the shear stress at which microalgae is fixed on the transparent walls in closed systems working in controlled laboratory conditions. At values lower than 0.2 Pa, a biofilm layer is formed in a closed cultivation system. However, in order to disrupt the integrity of the already formed biofilm, it is necessary to reach values of shear stress on the wall higher than 6 Pa [31,32]. It can be assumed that in the PBR processing wastewater in non-sterile conditions, the critical values of wall shear stress will be even higher than in the systems working in laboratory conditions. Therefore, these results suggest that the biofilm could not be removed by the shear stress once it is formed in the PBR. A physical cleaning of the tubes should be periodically performed. However, the shear stress obtained with the highest velocities seems to be able to prevent or reduce the formation of biofilm, thus reducing the need for cleaning or increasing the time interval between consecutive cleanings. It is also important to consider that some of the microalgae strains can be inhibited by high shear stress, while others are not sensitive to values up to 80 Pa [33].

Shear stress in the wall can be increased by increasing the culture medium velocity inside the tubes. In Fig. 9, the velocity and shear stress distribution in the tube are shown for the operating conditions of the initial design (i.e. $\Delta h = 0.2$ m). Due to the increasing velocity of culture medium, there has been a significant increase in the shear stress, reaching a value higher than 1.5 Pa in the wall, which can influence on the biofilm formation. However, even under these conditions, critical values of 6 Pa for disrupting the stability of the formed biofilm cannot be achieved.

Biofilm formation is not only affected by the shear stress, but also by characteristics of the culture medium and by the species of the microalgae present in the PBR [34]. Indeed, in the tubular PBR investigated in this study, during winter season the culture medium was dominated by filamentous microalgae, which are easily trapped within the tube’s walls [20]. On the contrary, in summer season, when the temperature and sunlight irradiation intensity were higher, smaller microalgae were dominating the culture, and the consequent formation of biofilm was significantly slower. Biofilm formation is a very complex issue and the aim of further investigation could be focused on exploration of the shear stress influence directly on biofilm formation. The present study demonstrates that it is possible to simulate the distribution of shear stresses in a PBR tube for various design and operating conditions, and could be

![Fig. 7. Contour plot of the velocity streamlines in the PBR open tank and tubes: (a) $\Delta h = 0.04$ m, (b) $\Delta h = 0.2$ m.](image)

![Fig. 8. Shear stress distribution inside a PBR tube, $r$ indicates the radial coordinate and $R$ is the inner radius of the tube.](image)
further used to investigate the effect on biofilm formation on transparent PBR tubes. All in all, this study demonstrated that CFD simulations can be a useful tool to optimize both design parameters and the operating conditions of PBR for microalgae production, boosting the scale-up of this technology.

4. Conclusion

The aim of this study was to establish and validate a CFD model and to perform a hydrodynamic analysis of a pilot hybrid tubular PBR for microalgae production and wastewater treatment. The reliability of the numerical simulation of culture medium velocity in the horizontal tubes of the PBR was validated by the pulse-input tracer technique and ultrasonic flow meter measurement. Results indicate that the CFD simulation model was accurate for simulating hydrodynamic conditions. The hydrodynamic conditions were reflected by means of CFD, and the hydrodynamic model was compared with analytical velocity profile based on experimental data. The velocity profile inside the tubes of the PBR fitted very well with the universal velocity profiles for rough tubes. The validated CFD model was used to evaluate the hydrodynamic conditions in the open tanks of the PBR. Dead volumes with low velocity, prone to solids settling and therefore unfavorable for microalgae production, were observed in the zone further from the paddle wheels, which can be reduced by increasing the fluid flow velocity. Shear stress inside the tubes was estimated based on the results of the CFD simulations, concluding that shear stress value is high enough to reduce or prevent biofilm formation on transparent walls. However, it is not possible to reach a value of shear stress which could remove the already formed biofilm. The results of hydrodynamic simulations in combination with experimental measurements of the cultivation process can help to intensify the production of microalgae.

CRediT authorship contribution statement

Vojtech Belohlav: Conceptualization, Investigation, Writing - original draft. Enrica Uggetti: Conceptualization, Writing - original draft, Visualization, Writing - review & editing. Joan García: Funding acquisition, Writing, Reviewing and Editing. Tomas Jirout: Conceptualization, Writing - review & editing. Lukas Kratky: Conceptualization, Writing - review & editing. Ruben Díez-Monter: Conceptualization, Investigation, Writing - original draft, Visualization, Writing - review & editing.

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.

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