CFD modeling and experiment of heat transfer in a tubular photo-bioreactor for photo-fermentation bio-hydrogen production

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Abstract: Temperature is one of the most important parameters that need to be controlled in photo-fermentation bio-hydrogen production (PFHP) system. Since the high temperature and big temperature fluctuation have adverse impacts on bio-hydrogen yield, the system numerical simulation based on the operating conditions and environmental factors is desirable. This research focused on the investigation of heat transfer properties of the PFHP system. Enzymatic hydrolysate from agricultural residues was taken as substrate, and up-flow tubular photo-bioreactor was adopted for PFHP. Temperatures inside the photo-bioreactor were monitored. The experimental design and computational modeling for the determination of the heat transfer behavior in tubular photo-bioreactor was presented. Energy balance analysis was conducted to determine the energy efficiency, and optimize the operation parameters in order to obtain higher energy efficiency. The commercial software FLUENT was also adopted in order to predict the transient temperature distribution in the photo-bioreactor. The results showed that mathematical and computational modeling method has a clear potential for improving the performance of photo-bioreactor in the process of PFHP. Up-flow tubular bioreactor has tiny temperature fluctuant, and is suitable for PFHP.

Keywords: photo-fermentation bio-hydrogen production (PFHP), up-flow tubular photo-bioreactor, heat transfer, temperature distribution, numerical simulation

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1 Introduction

Large-scale utilization of fossil fuels in the last few decades with the rapid economic growth has already led to resource exhaustion, climate changes and environmental pollution. The utilization of renewable energy can help addressing these issues, especially the renewable energy derived from biomass[1,2]. Hydrogen is a promising alternative fuel, versatile, clean burning, high energy yield (122 kJ/g), and can be produced biologically from a variety of waste materials such as paper products, sawmill waste, straw and industry waste[3-5]. Biological hydrogen production can be classified into three approaches, bio-photolysis of water, dark fermentation, and photo fermentation. Among of these, photo-fermentation bio-hydrogen production (PFHP) has the highest substrate conversion and can utilize the side products of dark fermentation (such as organic acids, et al.)[6-8]. Nevertheless, the process also suffers from many restrictions, much work is needed to

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develop a large-scale, economically attractive way[9].

Bio-hydrogen production is a complex, multiphase biological, chemical and physical process with many internal interactions between gas, liquid and solid phases. Present researches on bio-hydrogen production have focused on the chemical and biological aspects which affect the efficiency of hydrogen production. While, the physical characteristics such as reactor configuration and hydrodynamics have received very little attention[10]. Light supply, biomass concentration, mixing pattern, cell shear, temperature control and mass transfer rate all influence the photo-bioreactor performance[11]. However, few studies elucidated the heat transfer in the process of bio-hydrogen production[12-15].

In the process of PFHP system, the mixed photosynthetic bacteria (PSB) is sensitive to temperature[16], stable environment is benefit for substrates utilization, light absorption, biomass growth and bio-chemical reaction conduction. PFHP is an enzymatic process, accumulated heat produced by the biochemical reaction and the incident light raise the temperature and possibly deactivate the microbial catalyst[17]. The dinitrogenase in PSB which plays an important role in bio-hydrogen production is active in narrow range of temperature, generally between 30°C and 37℃, so dramatic temperature fluctuation adverse to bio-hydrogen production[18,19]. Knowing that heat is a key feature of life processes and available to govern the microbial dynamics, it is essential to monitor the heat transfer in the bioreactor.

The PFHP system has the co-existence of a quasi-static solid phase (mixed PSB), a mobile fluid phase (fermentation solution) and a mobile gaseous phase (generated through the fermentation, mostly H_2 and CO_2). Few models exist in the literature for numerical simulation and mathematical modeling of tubular photo-bioreactors for the PFHP. Hence, the major objective of this study was to analyze the heat transfer situation inside the bioreactor when using agricultural residue's enzymatic hydrolysates as the carbon source, and to establish the theoretic mathematical heat transfer modeling for PFHP in tubular bioreactor, and then combined with the computational fluid dynamic (CFD) computational method to monitor and control the transient temperature distribution in the tubular photo-bioreactor, in order to achieve a satisfactory hydrogen yield of PSB bio-hydrogen production and help to reduce the number of experiments.

2 Materials and methods

2.1 Microorganisms and inoculum preparation

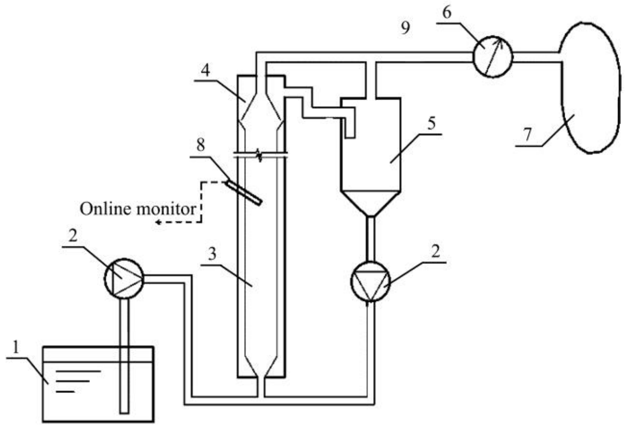
The microorganisms used for photo-fermentation hydrogen production in this study were originally derived from a mixture of sewage sludge, fresh pig manure and cow dung. The mixed strains sequences were analyzed by Basic Local Alignment Search Tool (BALST) comparative analysis method according to National Center for Biotechnology Information (NCBI). Results showed that the mixed strains were *Rhodospirillum rubrum*, *Rhodobacter capsulatus*, and *Rhodopseudomonas palustris*[20].

The growth medium for the mixed strains culture had the following composition: NH_4Cl 1 g/L, $NaHCO_3$ 2 g/L, yeast extract 1 g/L, K_2HPO_4 0.2 g/L, CH_3COONa 4 g/L, $MgSO_4{\cdot}7H_2O$ 0.2 g/L, and NaCl 2 g/L.

The substrate solution utilized for photo-fermentation consisted of reducing sugar contained in the ARPs enzymatic hydrolysates as the carbon source. C, N, P and micro-nutrient of the fermentation medium were supplied in the following dosages: NH_4Cl 0.4 g/L, K_2HPO_4 0.5 g/L, $MgCl_2$ 0.2 g/L, yeast extract 0.1 g/L, NaCl 2 g/L, and sodium glutamate 3.56 g/L. The inoculum load of bacteria during logarithmic phase was 20% (v/v).

2.2 Photo-bioreactor design and set-up

Tubular bioreactor is undoubtedly the most popular choice for PFHP, since it has the biggest surface to capture light energy[21]. Hence, an up-flow tubular photo-bioreactor (UTPB) was employed to investigate the heat transfer in the process of PFHP. The tubular bioreactor is composed of glass tube which is sufficiently transparent to allow good light penetration. Based on the function, the UTPB can be divided into a number of units: gas-liquid separation unit, reaction unit, influent and effluent recycled unit, gas collection unit, and on-line monitoring unit. The effective reaction volume of the bioreactor was 126 mL. The overall structure is shown in Figure 1.



1. Pre-mixed tank 2. Peristaltic pump 3. Tubular photo-bioreactor 4. Gas-liquid separator 5. Effluent liquid collection cylinder 6. Gas meter 7. Air bag 8. Thermometer probe

Figure 1 Schematic diagram of UTPB system

At the beginning of the experiment, fermentation solution was prepared in the pre-mixed tank and then pumped into the tubular bioreactor with a peristaltic pump (HL-2S, HUXI, Shanghai, China) from the bottom inlet diffuser. The volumetric pumping rate was 4.2 mL/min which means the HTR was 0.5 h. A uniform light intensity of 4000 lx was attained at the surface of photo-bioreactors supplied by LED lamps (GF-HO1824YD, 25 W, 120 lx/W). The tubular photo-bioreactor compartment connected to the bottom of gas-liquid separator, which consisted of gas collection cylinder, effluent gas disengage cylinder, effluent liquid collection cylinder, gas outflow pipe, and liquid outflow pipe. The fermentation solution flow upward through tubular photo-bioreactor then flow out from the liquid outflow pipe into effluent liquid collection cylinder which was used to reutilize for bio-hydrogen production. The switch between fresh solution and recycle solution happened when the reaction unit and effluent recycle all filled with fermentation solution. The taper direction of gas collection cylinder also can prevent washout of bacterial granular to some extent. The gas which disengaged from the gas collection cylinder and effluent gas disengaged cylinder flow out through a gas meter then stored in air bags. The temperature was monitored by an online data logger thermometer (YC-747UD, YCT, Tai Wan) which was connected to a computer for realizing on-line record, the accuracy was ±0.1℃. The temperature sensors were placed at the positions mentioned below: feed inlets, discharge holes, center of the bioreactor, and the walls.

The entire experiment process was carried out in a digital biochemical incubator (SPX-250B-III, Shanghai, China) under the ambient temperature of 30°C.

3 Theoretical approach

3.1 Mathematical model

The mathematical and computational model for the tubular photo-bioreactors proposed in this paper accounts for the incident radiation on the tube walls and also in the fluid, the heat generated by biochemical reaction, and the conduction between tube wall and fermentation solution. The entire system was regarded as an adiabatic unit. Fundamental theories combined with the Volume Element Model, which simplifies the partial differential equations into ordinary differential equations, provide a mathematical model which is handled numerically with substantially low computational effort[22]. The model was used to calculate fluid temperature inside the photo-bioreactor. This calculation depends on ambient temperature, velocity of fluid flow, direct light radiation, diffuse radiation, cell concentration and geometry of the photo-bioreactor.

In the bio-hydrogen production system mentioned above, the reaction and heat transfer process are assumed to occur only in the tubular reaction bioreactor. The mathematical domain for bioreactor is divided into two types: the walls (E_w) and the fermentation solution (E_f) that flows inside the bioreactor. Since temperature plays a key role in the bio-hydrogen production, its mathematical modeling is of great value for the governing of the photo-fermentation process and the design of photo-bioreactor.

3.2 Light radiation heat transfer

LED lamp has three heat transfer types of conduction, convection and radiation, Since LED lamps were located in the constant temperature incubator, the effect of heat conduction and convection of the LED on the wall’s temperature can be ignored. The proposed mathematical model used to determine the temperature variation of wall depends on the light radiation and transmissivity of the glass. Beer-Lambert's law is available for quantitative description the monochromatic absorption of material. In order to simplify the model, the transmissivity of 3 mm glass here were calculated according to the Equation (1) mentioned in the reference [23]:

$$\tau = -0.4946i^4 + 0.9654i^3 - 0.725i^2 + 0.1693i + 0.7964 \tag{1}$$

where, i is the incidence angle, (°). In this paper, lights were distributed evenly around the tubular bioreactor, and the diameter of the bioreactor was very thin, so the angle of incidence was regarded as 0°, the transmissivity was 0.7964, the initial intensity of illumination (I_0) was 3000 lx, the intensity of illumination of inside wall (I) was 2389.2 lx, namely 2389.2 W/m^2.

3.3 Convection heat transfer

The PFHP system was conducted in continuous pattern, the fermentation solution flow in the photo-bioreactor with a constant velocity. In order to calculate the temperature of the fluid, the flow regime should be determined. Reynolds number (Re) in the tubular bioreactor was calculated as 3.793, so the flow regime was laminar flow.

The first law of thermodynamics was utilized to depict the heat transfer between the volume elements of wall and fluid. The energy balance of fluid was calculated by Equation (2):

$$Q_{conv}^{i} + mc_f T_f^{i-1} = m_f c_f \Delta T_f^{i} + mc_f T_f^{i} \tag{2}$$

where, Q_{conv}^{i} is convection heat transfer between the wall and fluid, J; m is the mass flow of per time unit, kg; c_f is the specific heat of fluid, J/(kg·℃); T_f^{i-1} is the temperature of i–1 the part fluid, ℃; m_f is the mass of fluid, kg; T_f^{i} is the temperature of the i part fluid, ℃.

3.4 Heat conduction

The fermentation solution flow in the tubular bioreactor, there exist radial temperature difference in each volume element. The temperature of a specified location (T_j) was calculated by basic formula of heat conduction Equation (3):

$$\frac{\lambda(T_w - T_j)}{\Delta L} = q = \frac{h}{T_w - T_f} \tag{3}$$

where, T_w is the temperature of wall, ℃; T_f is the initial temperature of fluid, ℃; λ is the heat conductivity of fluid, W/(m^2·℃); ΔL is the distance between the wall and specified location of T_j, m; h is the surface heat-transfer coefficient, W/(m^2·℃).

3.5 Heat generated by biochemical reaction

Self-heating occurs in bio-hydrogen production process as a result of the biological activity, such as the metabolism of PSB, and glycolysis is the principal metabolic pathway. The metabolic heat production rate is correlated with the stoichiometry of the microbial growth and processes of product formation[17]. Hydrogen is formed through the glycolysis reaction. The reaction equation is shown in Equation (4):

$$C_6H_{12}O_6 + 6H_2O \xrightarrow{light} 12H_2 + 6CO_2 \tag{4}$$

The concentration of exponentially growing mixed strains was measured as 1.2 g dry cell/L. The heat production rate of exponentially growing PSB 0.15 W/g dry cell[26], hence, the heat generate rate is 180 W/m^3.

3.6 Total heat transfer equation

Since the PSB distributes evenly in the fermentation solution, the heat generated by the biochemical reaction was also distributed uniformly. The gas phase in fluid take part contained a very small amount, and the bubbles were tiny which can be negligible, as well as their influence on heat transfer.

The mathematical model that was applied within the volume occupied by fermentation solution for bio-hydrogen production was introduced in Equation (5).

$$mC_f \Delta T_f = Q_{conv}^{i} + mc_f T_f^{i-1} - mc_f T_f^{i} + 180 \tag{5}$$

Heat radiation of light, heat convection between the wall and liquid, heat conductive between the different part of liquid, and heat generated of the micro-organism metabolic inside the fermentation solution are all take into account in the form of a volumetric element heat generation source.

4 Computational fluid dynamics

Based on the theoretical analysis above, the mathematic model of the PFHP system was introduced to calculate temperature distribution in the tubular bioreactor. Advances in CFD approach have also provided an efficient, economical and time saving tool to investigate the heat transfer occurred in bioreactor[27]. FLUENT is one of the most popular commercial CFD softwares, thus it can be utilized to solve various engineering problems involving fluid, heat transfer and chemical reaction[28,29]. In this study, GAMBIT 2.4.6 was employed to mesh photo-bioreactor geometry, and the uncoupled, implicit 2-dimension (2D) solver of FLUENT 6.3.26 was adopted to solve the equations that govern the system for simulating temperature distribution of the fermentation solution within tubular bioreactor. The simulations were carried out on the PC equipped with an Intel Xeon 2.4 GHz processor and 8 GB RAM.

4.1 Simulations of PFHP system

The UTPB system is a multiphase fluid system, and there is the co-existence of a quasi-static solid phase, a mobile bulk liquid phase and a mobile gaseous phase. The solid phase (mixed strain) and gaseous phase (tiny bubble) in the multiphase flow were negligible. The multiphase flow in UTPB was regarded as an incompressible stationary flow.

Computational fluid dynamics simulation includes geometry creation, mesh generation, boundary condition setting and finally iterative solution of governing RTE equation[30]. The governing equations were solved applying finite volume method, using appropriate initial and boundary conditions.

4.2 Mesh generation of the up-flow tubular photo-bioreactor

When developing any CFD model, grid density must be optimized because the quantity and geometry of meshes influence the solution of the exhibition of flow field[31]. In this study, UTPB is axisymmetric, thus the structured grids are uniform, and Quad grid was utilized for the construction of mesh. Two-dimension meshes of the vertical section of UTPB were created by software GAMBIT. Periodicity of translational periodic type was defined for determining the boundary conditions of UTPB.

4.3 Assumption of PFHP system

Following assumptions were made for 2D simulation on the heat distribution in a steady and continuous operation UTPB. (1) Temperature gradient happens in one of the areas of section that can represent others, because tubular is an axial symmetry object, so the model is simplified to 2D. (2) The free surface in the fermenter is set to solid wall, because the normal velocity of free surface can be ignored. (3) The pressure in UTPB is kept in a constant atmospheric pressure because the produced biogases are all discharged through the gas outlet and collected by a constant pressure air bag. The viscosity, thermal conductivity, density and specific heat of the fermentative solutions are assumed to be constant, since the temperature changes a little. (4) The fluid flow inside UTPB is fully developed and no disturbance and back mixing happen. (5) There exists no energy diffusion and viscous dissipation in the heat transfer process, because pressure-based solver is adopted.

4.4 Boundary conditions and convergent condition

Flow characteristics of fermentation solution, radiation of light source and heat conduction in the UTBP were numerically simulated by FLUENT. Viscous model of laminar was adopted to determine the velocity profiles of fermentation solution. Since the UTPB designed in this study for PFHP has a big length/diameter ratio (length is 40 cm, while diameter is 2 cm), thus inlet flow of UTPB can be regarded as fully developed for determining the steady state flow dynamics of fermentation solution.

The fermentation solution inlet was modeled with a velocity-inlet boundary condition, and the outlet was set as pressure-outlet boundary conditions with free slippage for the biogas that produced in UTPB. The remaining boundaries of the model were left as default wall boundary conditions. The thermal condition of the wall was set as radiation heat transfer from exterior, and the external radiation temperature in the model was 34.4℃. Wall thickness was defined for one-dimensional (1D), and there was no need to mesh the wall, heat conduction only calculated in wall-normal direction. There was no slip occurred at the wall, fermentation solution and the photosynthetic bacteria. Inlet fluid velocity and temperature were known as 0.22×10^{-3} m/s, and temperature of 30℃. The outlet of fermentative solutions is set as a static pressure outlet where the atmospheric pressure was specified.

Model parameters applied for the CFD simulation of the 2D fluidized are as below: solution density (ρ) 1125 kg/m^3, viscosity (v) 1.3×10^{-3} kg/(m s), specific heat (c_p) 5.167 kJ/(kg K), thermal conductivity (λ) 0.63 W/(m K).

The simulation was operated in steady state conditions, iterations step was 100 steps. The relative error is specified by using a convergence criterion of 10^{-3} for each scaled residual component.

5 Results and discussion

5.1 Geometrical details

The grid generation or meshing of UTPB is depicted in Figure 2, which is also the 2D computational domain utilized in simulations.

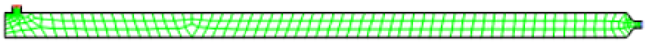


Figure 2 Meshing of UBB fermenter

The computational grid formed consisted of 368 nodes, 288 quadrilateral cells, 655 faces (153 mixed wall faces, two mixed pressure-outlet faces, three mixed velocity-inlet faces and 497 mixed interior faces).

5.2 Numerical solution model validation

The UTPB system was studied at a uniform temperature (30 ℃) and pressure (1 bar). Outlet gas was defined as a pressure outlet, all solid surface were defined as wall. A segregated solution and SIMPLE algorithm were conducted, the solver model was chosen as pressure based solver. An implicit time steps of 0.01 s was utilized with first-order accuracy, the space is 2D, steady-state flow. The gradient option is Green-Gause Cell Based.

Based on the flow regime and assumptions, energy equations including the effects of biochemical reaction, heat conduction and light radiations were considered. *Re* was utilized to determine the flow regime, in this study, the viscous model was determined as laminar flow, whose fluid side heat transfer is approximated as Equation (6):

$$q'' = k\frac{\partial T}{\partial n} \approx k\frac{\Delta T}{\Delta n}\bigg|_n \tag{6}$$

where, n is local coordinate normal to wall.

The energy equation was utilized to activate calculation of heat transfer. In order to include viscous heating terms in energy equation, turn on Viscous Heating in Viscous Model panel. The diffusion energy source option in the Species Model panel was turned off, the volumetric heat sources within solid was a constant value of 180 W/m^3. Since the light radiation is constant, the heat generated in the wall because of light radiation was adopted instead of radiation model, and the temperature was measured as 34.4 ℃. The material properties for heat transfer and thermal boundary conditions are defined, the operation conditions were set as operating pressure of 101 325 Pa, gravitational acceleration of –9.8 m/s^2, the temperature of inlet (velocity-inlet) and outlet (pressure-outlet) were determined by thermometer.

After pre-processing, the model is utilized to simulate temperature distribution of the bio-hydrogen production system in order to investigate the effects of inlet velocity on theat transfer situation and hydrogen production.

5.3 Visualization of temperature field inside up-flow tubular photo-bioreactor

The model in FLUENT was based on discretization of solution controls: standard pressure, first order upwind momentum and energy, residual monitors open. After iterative computations, temperature field was reported by surface monitors, the visualization nephogram of temperature distribution in the UTPB was made to observe the important phenomena, and result is shown in Figure 3.

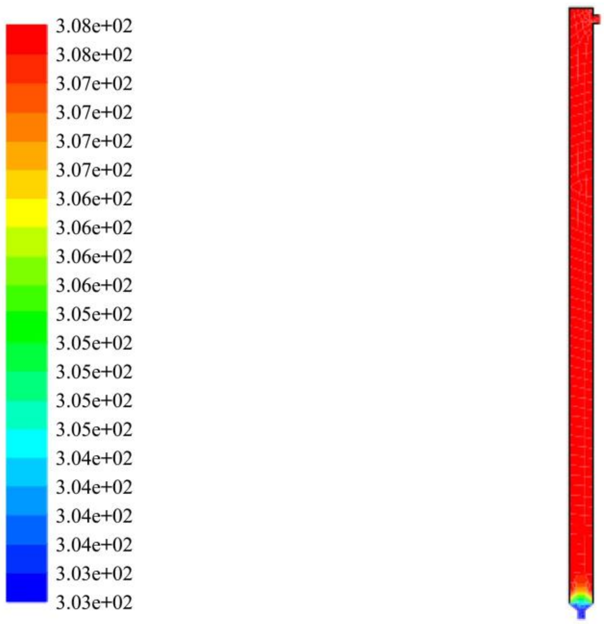


Figure 3 Distribution nephogram of temperature in UTPB

The present FLUENT study focused on describing the detail of the phenomena from experimental results[32]. In this research, the reaction zone of UTPB reactor was analyzed, and the steady state simulation was conducted for describing the temperature distribution and optimizing operation of photo-bioreactor. Changes of color represented the temperature gradients, the higher the color difference was, the bigger the temperature fluctuation was. Higher temperature meant that more heat was accumulated. At the stable running period of UTPB, there is a large temperature gradient distribution within area of inlet. However, in the reaction zone with illumination, there is little temperature fluctuation. The heat uniformly distributed in the bio-reactor at inlet velocity of 0.00022 m/s. Since the diameter of tubular bio-reactor is very thin (2 cm), the heat reached uniformity easily under the action of heat conduction. The minimum temperature was 30℃ in the inlet, and the uniform static temperature was 35.4℃. The entire photo-bioreactor was kept at a stable situation which was beneficial for PSB growth and bio-hydrogen production.

5.4 Comparison of simulated and experimental temperature distribution

Comparisons between simulated values and experimental values of different places of the reactor were conducted, and the results are shown in Figure 4.

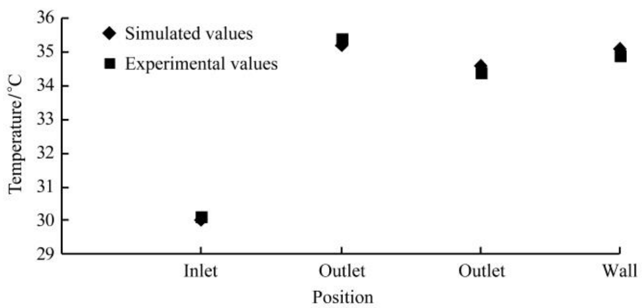


Figure 4 Comparisons between simulated values and experimental values at different positions

Qualitatively, the numerical predictions agree well with the experimental results, which means that the established model is consistent to actual situation. The errors incurred in calculation may be derived from several sources, such as geometry meshing, initial treatment and boundary conditions. It is capable of closely predicting the temperature distribution in PFHP system.

Computational fluid dynamics simulation method can help optimize a bioreactor process by quantifying flow fields and heat transfer characteristics, and the benefits of modeling include monitoring the changes and risks during scale-up and reducing cost with proper design[33].

From calculation using the mathematical and computational methods, the energy balance equation and heat transfer model are suitable for continuous flow system, such as the UTPB mentioned above. While this model cannot be applied to batch systems or to the system which has intensely unsteady hydrodynamic behavior, because of the continuity and steady behavior of model.

Since PFHP needs light throughout the entire process of biochemical reaction, only a minor fraction of light energy absorbed and utilized by the photosynthetic bacteria, while most of it is dissipated as heat[34]. The light radiation was regarded as the most notable factor affecting temperature distribution in the bioreactor. Because of the geometrical shape of bioreactor and the layout of light source, the temperature difference between center and edge regions was tiny, which indicated that this lighting system can provide balanced illumination for the entire model evenly. The LED lamps can provide not only light, but also maintain the fermentative reaction at appropriate temperature range. Therefore, this bioreactor structure is beneficial to the bio-hydrogen production by mixed strain, and this optimized lighting system contributes significantly to reducing the cost of the bioprocess.

6 Conclusions

Photo-bioreactor is the key part in the process of PFHP system, therefore, the determination of heat distribution in the photo-bioreactor is important for high efficiency bio-hydrogen production. Taken the PFHP system from agricultural residues as research object, several conclusions were drawn.

(1) Temperatures inside the photo-bioreactor were monitored, and heat distribution was obtained.

(2) The mathematical models and computational fluid dynamic simulation methods demonstrated an accurate and efficient method for studying the heat transfer behavior in tubular photo-bioreactor for bio-hydrogen production.

(3) Up-flow tubular photo-bioreactor was suitable for PFHP system since there was tiny temperature fluctuation in reaction area.

(4) The numerical simulation confirmed that CFD method could be utilized to optimize the design of the bioreactor and to govern operation parameters.

Acknowledgments

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