Gaining insight in biological hydrogen production by computational approaches

Hydrogen is one of the most important raw materials for the chemical industry and has an undisputed future importance as an environmentally friendly fuel. At present, 96% of the 500 billion m^3 of hydrogen gas that is produced each year are originated from depleting fossil raw materials. To meet the growing demand of hydrogen, it is essential to develop sustainable processes for its bioproduction. The use of solar energy by photosynthesis reveals a promising technique for an ecological hydrogen production.

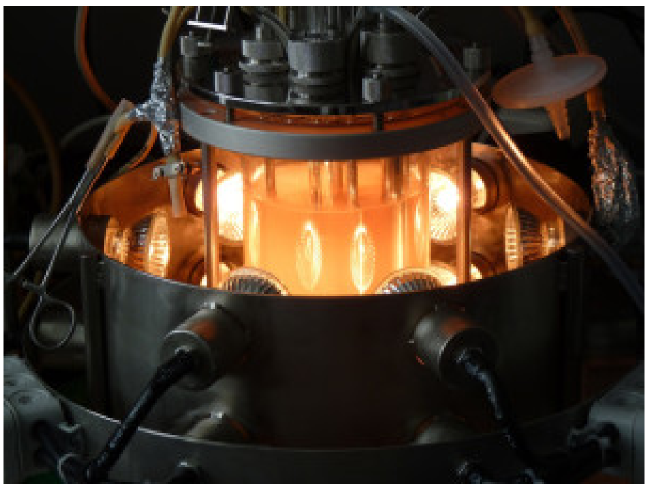

Fig.1. Continuous operated Halogen-photobioreactor using Rhodobacter sphaeroides DSM 158 for the photofermentative hydrogen production.

The purple non-sulfur bacterium Rhodobacter sphaeroides DSM 158 is able to capture light energy via phototsynthetic pigments. At specific process conditions the absorbed light energy promotes the direct conversion of organic substrates into hydrogen gas.

The optimization of photobiological processes is challenging because the supply of phototroph organisms with light energy is a very dynamic process, which depends on the provided light intensity. The cells move between the well-illuminated bioreactor periphery and low-illuminated parts in the center of the bioreactor. In this study, the authors found that the rate of hydrogen production in a continuous-operated and externally illuminated stirred tank photobioreactor (Fig. 1) is dependent on the adjusted stirrer speed. This directly influences the fluid flow and consequently the cellular movement through the high- and low-illuminated parts of the bioreactor.

In order to characterize the time cycles in which the cells have access to light energy at the bioreactor surface a number of simulation tools were used to characterize the light process conditions of the photobioreactor.

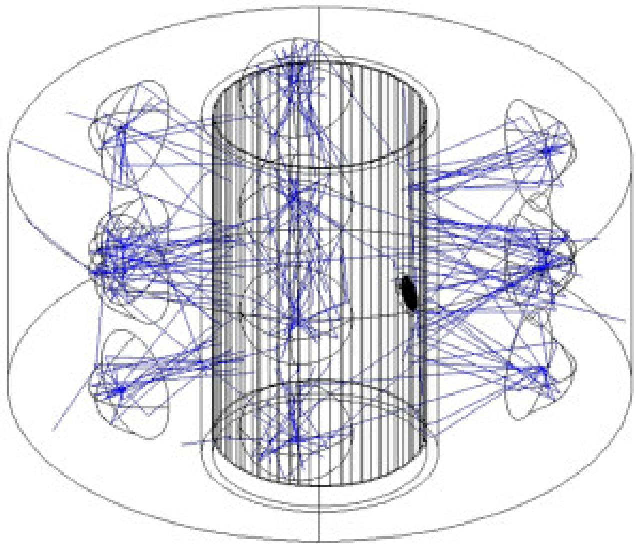

Fig. 2. Optical ray tracing simulation of the photobioreactor setup to quantify the amount of light energy which is accessible for the phototrophic bacteria.

For the first time, an optical design software tool (ZEMAX) was used to simulate the trajectories of light rays towards the photobioreactor surface (Figure 2). The optical simulation provided information about the physical behavior of light rays and quantified the light energy which enters the interior of the photobioreactor and can be used by the cells to perform the bioreaction.

The distribution of light intensity across the bioreactor was modeled by a simple empirical approach and was visualized for different process conditions. An important part of this work was the simulation of the fluid flow and fluid velocities which are dependent on the stirrer performance and induce the cellular movement. The “Computational Fluid Dynamics” module and “Particle Tracing” module of COMSOL Multiphysics were used to analyze the fluid flow conditions within the bioreactor and follow the tracks of individual cells. Thereby, an optimum average cellular time cycle illumination of 1.5 Hz was identified yielding the highest continuous produced rate of hydrogen (170.5 mL L^{-1} h^{-1}) so far.

Summarizing, a comprehensive consideration of all parameters influencing the light access of phototrophs is necessary to achieve an efficient bioprocess development of sustainable photobiotechnological processes.

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