435f An Integrated Photosynthesis Model for the Biological Production of Hydrogen Using Microalga

Wonjun Park and Il Moon

This paper suggests the practical modeling for the photosynthesis in which the biological production of hydrogen is involved. The objective of modeling is to find the optimal condition and to describe the manual operation which is required to produce hydrogen effectively. The dynamic modeling with discrete events is developed for the hydrogen production using microalgae. The dynamic optimizations for the operation schedule as well as the optimal condition are performed simultaneously.

The microalgae are believed to produce hydrogen under controlled circumstances. Even thought their metabolic pathway does not produce much hydrogen at the normal condition. *Chlamydomonas reinhardtii* is known as a good strain to make hydrogen with the sulfur deprivation. The oxygen is the powerful inhibitor of hydrogenase which is a main enzyme to convert proton to hydrogen. Removing sulfur from the culture media results in the decline of oxygen but it does not influence on the function of mitochondria. Therefore, the oxygen which is produced during the photosynthesis is consumed by respiration. The reversible anaerobic process under illumination makes hydrogenases activated and hydrogen is produced with sulfur deprivation. Photosynthetic process is consisted of three major components inside the microalgae. The photosystem II (PSII) is the part responsible for adsorption of light and conversion of light into the activated electrons. The electrons pass throughout the cytochrome b_6f (Cyt) and photosystem I (PSI) deliveries them to the hydrogenase finally. The objects for the modeling is based on these distinguished parts and their functions.

The modeling is constructed by dynamic modeling to describe the biochemical reaction based on the electron pathway with metabolites. The discrete event with binary variable shows the manual operation of sulfur deprivation. The components in the photosynthetic process are explained by state variables. The additional modeling parts for the light adsorption and macroscopic population modeling with growth rate are also included. The integrative between biochemical modeling and macroscopic modeling is done with discrete event and variables.

Parameter Estimation for the simulation is performed with constrained multivariable methods. Metabolic flux analysis sets the range of constraints combined with modification of partial equations. The steady state assumption gives the initial quantitative values and the formulated dynamic model is arranged with algebraic equations. The hard constraints are derived from the enzymatic kinetics. The initial model is calibrated by the experimental data by iterative learning optimization with back propagation steps. The back propagation is originated from the neural network technique which takes a reasonable solution when the multivariable is under estimated. Finally, parameters are estimated with minimized error with the sets of experimental data. The final model fitted with data explains biological behaviors such as declines of the hydrogen after a certain time. And the biological pattern of cell population is analyzed depending on the light intensity. The manual operation with discrete event is applied as a rigorous model. The internal metabolites are analyzed as a meaning of metabolic flux from the results of dynamic simulation. The sensitivity analysis verifies the primary metabolites which are associated with photosynthetic process.

The optimal condition of light intensity is identified as $298\mu E/m^2 s$. The profiles for the cell population and metabolites such as ATP are described by simulation. The biological meaning is evaluated by intracellular metabolites. The dynamic optimization for the schedule of sulfur deprivation suggests the design factors and the configuration of sustained process for the hydrogen production using microalga. Several performance indexes are introduced to check the operability of suggested process. This paper suggests the framework for the phototrophic production of hydrogen using algae to develop the sustained process of hydrogen. The practical modeling for the biotechnological process of microalga is constructed considering the continuous variables and discrete variables as well. The suggested modeling methodology and related technique provides the fundamentals for the potential bioprocess.