Chapter 42
In Silico Models on Algal Cultivation and Processing:
An Approach for Engineered Optimization

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ABSTRACT

In modern system-level metabolic engineering, genome-wide metabolic reconstructions are used as a systems-based framework for integrating and analyzing large "omics" data sets as well as for assessing cell design molecular and bioinformatics approach "in silico". Microalgae growth processes are based on the concurrent interaction of micronutrients (Mg, Fe, Zn, etc.), macronutrients (N, C, P), and environmental parameters (temperature and light). Blackbox models or macroscopic models give the reliable interrelationship amidst the growth kinetics of microalgae and its potential of lipid and starch accumulation in response to any of the growth restraining factors. This chapter provides an insight into the different in silico models for the growth and cultivation of microalgae. Various factors such as light intensity/distribution, the temperature during cultivation, and nutrient concentration are considered. The chapter also summarises the role of different photobioreactors (PBRs) in optimising algae-based products using genome-scale models.

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INTRODUCTION

The attention given to algae in different commercial applications for biofuels, vital nature components production, etc. make it necessary to develop system-level metabolic engineering. The bioinformatics tools in understanding and guidance of the metabolic pathway and algal bioactive components regulation, as microalgae are considered as bio-cell factories. Therefore, a synergistic approach to *in silico* analysis and then conditioning *in vivo* will improve robustness and enhance the marketability of carbon-neutral fuels from algae (Banerjee *et al*., 2020).

In silico analysis and tools have been developed in the field of genome scale metabolic reconstructions (GEMs) and microbial metabolic engineering, which give a clear prediction of algal genes, sequences and allow driving the pathway to produce high contents of a certain compounds such as triacyl-glycerides (TAGs), the precursor for biodiesel (http://genome.jgi-psf.org/Chlre4/Chlre4.home.html). Despite, there is no available genome scale reconstruction (GEMs) for algae, several studies aimed the improving of *in silico* analysis and 'omics' databases (Dal'Molin *et al*., 2011). *Chlamydomonas reinhardtii* was used as a first trial remodel a large metabolic reconstruction of algae, which demonstrated 484 reactions and 458 metabolites sited in the chloroplast, cytosol and mitochondria (Boyle and Morgan, 2009; Herrera-Valencia *et al*., 2012).

This chapter provides an insight into the different *in silico* models for the growth and cultivation of microalgae. Various factors such as light intensity/distribution, the temperature during cultivation and nutrient concentration are considered. The chapter also summarises the role of different Photobioreactors (PBRs) in optimising algae-based products using genome scale models.

Background

In 2007, the first nuclear genome of *C. reinhardtii* was published, followed by *Thalassiosira pseudonana*, while *Nannochloropis gaditana* was in 2012 (Salehi-Ashtiani *et al.*, 2015). Modern approaches progress the microalgae metabolic modeling, which has been called genome-scale metabolic models. This makes a clear focus on special genetic targets to enhance certain compounds productivity such as lipids and carbohydrates for biofuel production. In addition, phenotypes behavior can be elucidated under the dynamic growth conditions. The bioinformatics approaches help in detection of the functional annotations and associating genes, or multiple genes with specific biochemical reactions, which generate the gene-protein-reaction (Salehi-Ashtiani *et al.*, 2015).

Algae are an active source of biofuel precursor, such as TAGs for biodiesel and sugars for bioethanol production. The biofuel production from algae require optimization and cultivation under certain conditions to increase the synthesis of TAG and polysaccharides. So this needs a deep understanding of algal metabolomics, fluxomics, genomic, and proteomics. Algae can produce valuable secondary metabolites which have a wide interest in food, pharmaceutical, and cosmetics industries (Reijnders *et al.*, 2014). Nowadays, some *in silico* tools are available to help in understanding of algal metabolic pathways, transcriptomics, genomes, and proteomics.

Algal diversity faces a great variance in habitat types and climatic changes. The classical identification methods by using cell morphology is not sufficient, other data on biochemical and genomic sequences must be included. In addition, the survival rate of species may be affected by sampling time and their transferring to the laboratory. A technique of using environmental DNA and genomic fragments that released by broken cells depends on "soil memory effect" (Foucher *et al*., 2020). By using the *in silico*