Title: Agent-Based Modeling of Algae Reveals Impact of Self-Shading on Metabolism

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Project Goals:

The overall research objective is to develop an experimentally validated multi-paradigm multi-scale modeling framework that will enable the most advanced and predictive metabolic modeling of diurnally grown photosynthetic organisms to date. The genome-scale metabolic model of C. zofingiensis will be embedded into an agent-based modeling framework to allow modeling of diurnal growth; the model will also be able to simulate intracellular fluxes, cell-to-cell interactions, cell-to-environment interactions, metabolite diffusion, and spatial distribution. This modeling approach will allow us to simulate metabolic shifts that occur due to diel cycles and generate rational engineering strategies to design production strains that are not impacted negatively by this natural phenomenon.

Abstract Text:

Economical algae production requires growth under outdoor light, but the diel nature of sunlight complicates modeling efforts. This poster documents a solution for that: a fully functional three-dimensional agent-based model, capable of simulating algal growth under diurnal conditions. By rendering light rays on a sub-micron scale, this model captures the self-shading effects of cell density and culture depth. It also includes diffusion, gas transport, and the carbonate equilibrium, making it straightforward to see the impacts of increasing gas-phase carbon dioxide concentrations. The agents themselves use diurnal transcriptomic data to dynamically adjust their individual metabolic constraints, an approach which successfully predicts phenotype from genotype. A typical simulation involves thousands of individual agents, each of which tracks its own metabolism over the length of the simulation. The combination of these advances results in a model capable of simulating physically relevant culture densities of cells, embedded in a water column of physically relevant length and under economically relevant light regimes.

One significant finding of this research is that commonly used culture densities are extremely effective at absorbing light over surprisingly short path lengths. Even under full sunlight, algal ponds need to strike a balance between culture density and functional volume; attempting to increase productivity of a given pond by making it deeper will only produce benefits at very low cell densities. Given that a deeper pond also requires more energy to aerate and mix, it is likely that very shallow ponds can produce algae more effectively.

This phenomena occurs because of the self-shading aspect of photosynthetic growth. Because total light energy scales off area, any given frontal area has a maximum quantity of energy associated with it. The cells nearest the surface receive the largest share of the light, and the energetic availability decreases with depth, as the remaining light is progressively absorbed by cells further down. At a critical depth, the average cell will encounter only a small fraction of the original light – sufficient to keep itself alive, but *not* enough to grow larger. Increasing the depth below that point is therefore counter-productive; the cells occupying that additional volume don’t contribute any additional biomass growth to the culture, and indeed may actually *decrease* it.

It is worth noting that this critical depth is a function of both algal density and total light. The more dense the culture is, the shallower the depth will be, as the increased quantity of cells will absorb more light. However, the stronger the light is, the deeper the critical depth will be; more energy will be available at every depth, even if the fractions of total energy remain the same. By rendering light rays and simulating their intersections with individual cells, this model is able to identify the energetic availability as a function of depth for *any* given culture density and light condition.

Since it is built off a metabolic model, this simulation can also be used to model the impacts of all features normally associated with constraint based metabolic models, but on a physically relevant scale. For instance, it can project the total nutrient needs of an algal pond, by summing uptake amounts across all cells – or, it could be used to compare productivity differences between reactor configurations. Adjusting the simulation parameters allows for changes in density, depth, light amount, light composition, and genotype. Finally, the model is – if the data is available – species agnostic; any constraint based model of a similar algal species with the same set of species-specific data can be used.

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