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A SYSTEM-DYNAMICAL MODEL FOR EXPLORING THE QUALITATIVE BEHAVIOR OF BIOFUEL PRODUCTION BY ALGAE IN OPEN RACEWAY PONDS

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Abstract: Analysis of the economic viability of algal biofuel as an alternative energy source have relied on techno-economic models to analyze the effects of capital costs, operating costs, and depreciation on algae biofuel production in open bioreactors. While these models have been relatively successful in analyzing the economics of biofuel production, their predictive power is limited due to the following characteristics: (1) They are not mathematically rigorous, with most techno-economic models relying on simple, rule-based stochastic simulations to explore the effects of techno-economic input variables on biofuel production. (2) Most techno-economic models lack a system-dynamic component that allows them to analyze the effects of variables and internal dynamics generated by feedback between biotic components in open bioreactors on biofuel production. In this paper, I give a general overview of algae production in open raceway ponds, and describe a novel ecological modeling framework within which current research aimed at predicting pathways for increasing small and large-scale biofuel production could occur. Idiscuss how the exclusion of a system-dynamic component and empirically-based biological information about feedback between organisms in open bioreactors renders present techno-economic models inflexible, reducing the potential number of pathways that can be explored for increasing biofuel production. In this review, I highlight the general details behind a system dynamic ecological model currently under development to predict pathways for increasing large-scale biofuel production in open raceway ponds. Lastly, I comment on the ecological model's operationality, and ways to improve methods for comparing simulation results with empirically derived data.

INTRODUCTION

While terrestrial crop production and harvesting have a long developmental history, the use of algal biofuels as an alternative energy source is a burgeoning field having made extensive progress from the 1970s to 1990 (Sheehan et al. 1998). However, many scientists in the biofuel field concluded in the mid-1990s, that it was not economically viable to produce biofuel from microalgae because, even under best case scenarios of photosynthetic productivity, the price of cultivation and harvesting was two times the cost of generating a

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similar quantity of petroleum based gasoline (Scott, S.A., 2010). Since this time, gasoline prices have more than doubled (Scott, S.A., 2010), and as a consequence, biofuels derived from algae are now considered a viable alternative to petroleum-based energy. However, some caveats still remain, including unrealistic assumptions that other factors, including the price of materials needed for algae cultivation, harvesting, and biofuel extraction have remained constant, when in fact there has a marked increase in their price in the past fifth teen years (Scott, S. A., 2010; Sporalore, P. et. al, 1997)

In recent years, economists have developed techno-economic (TE) models as a tool to determine the effects of capital costs (CAPEX), operating costs (OPEX), and depreciation associated with cultivation, harvesting and extraction of biofuel from algae to predict pathways for minimizing costs and maximizing revenues from large-scale bioreactor systems, including open raceway ponds.

To date, most TE models are limited by the fact that they are not mathematically rigorous, relying on simple, rule-based stochastic simulations to explore the effects of TE input variables on algae production. These rules are used to determine if the algae population is viable or nonviable in terms of biomass yield at the time of harvest. Hence, the fate of an algae species determines total biofuel revenues for a given harvest period. Most importantly, the majority of TE models lack a system-dynamic component (but see Kenny and Flynn, 2014) that allows them to analyze the combined effects of multiple TE variables (TEVs), non-cost related environmental input variables (EVs), and random external input variables (RVs) on biofuel production. Moreover, most TE models cannot explore the effects of coupling between TEVs, EVs and RVson internal biological responses within large-scale bioreactor systems, which often exhibit nonlinear phenomena like sudden algae population crashes (ref). In most cases, this type of observed phenomena can be generated by feedback amongst internal response variables (IRVs) including feedback caused by interactions amongst single algae species (e.g. increased intra specific competition driven by overcrowding (allelopathic interactions) (Kenny and Flynn, 2014). Moreover, feedback amongst the internal components of an open bioreactor system can be amplified or dampened by the individual or combined effects of external input variables, dramatically affecting algae production.

Additional nonlinear phenomena that non-system dynamic based TE models are unable to explore include the effects of time delays (e.g. delays in increasing algae growth rates due to micronutrient limitation and internal feedback among algae and invasive species

(Borowitzka, 2013). The invasion of open raceway ponds by deleterious organisms is a commonly observed phenomena, where species including algae grazers (e.g. herbivorous zooplankton including Paraphysomonas sp. and diatom competitors (e.g. Amphora sp.) compete indirectly for pond resources with biofuel producing algae. (Chavis et. al, 2014). These organisms invade the ponds in response to environmental perturbation caused by increases in pond temperatures, variation in external wind patterns, and variation in seasonal rainfall (Chavis et. al, 2014).

In this paper, I focus on ecological dynamics generated by interactions between invasive species and biofuel producing algae in open raceway ponds. I highlight the general details behind a system dynamic ecological model (ECO) that predicts pathways for efficient biofuel production and argue that the inclusion of a system dynamic component and empirical biological information about species interactions within open raceway ponds makes the TE model more ill suited to predict pathways for efficient, large-scale biofuel production.

Open Raceway Ponds

Algae biomass production predominantly occurs in three main types of photo bioreactor (PBR) systems that are commercially applied today: open raceway ponds, tubular PBRs (open or semi-closed) and flat panel PBRs (Scott, S.A. et. al, 2010). Models discussed in this review are directed towards predicting biofuel production in open raceway ponds. Raceway ponds are shallow, ring-channel systems, in which the depth is maintained at no less than 0.2 m. This results in low algae biomass densities (0.02-0.3 g dry wt m^{-2} day^{-1}). To provide uniform mixing and reduce overcrowding, the algae culture is circulated with a paddle wheel at varying velocities (typically 0.25 ms^{-1}) (Borowitzka, M.A., 2013). While the day to day operational costs of raceway ponds require less energy for mixing than the two other reactor designs, they generate considerably less biomass per unit area per day, and harvesting costs are considerably greater than the two other PBR systems (Tilman D., D. et. al, 1996). In addition, open raceway ponds are highly susceptible to contamination by deleterious species (e.g. grazers, diatom competitors, viruses, and bacteria) that can cause algae population crashes, where existing biofuel producing algae populations go extinct or exhibit boom-bust behavior – high productivity followed by large losses in biomass over time (Brännström A. and Sumpter D.J., 2005; Smith, V.H. et. al; Downing A. L. and M.A. Leibold. 2002).

Throughout the southwestern United States, environmental conditions including brackish water and abundant light promote the use of open raceway ponds for industrial algal production of multiple algae species including Chlorella, Nannochloropsis, and Spirulina

(Chavis, A. et. al, 2014). Engineering designs and operating procedures for cultivating and harvesting these organisms in unmixed ponds and stirred raceways have been studied extensively (Borowitzka 2005)[10]. Shallow water depths of 7-8 inches (0.2–0.3m) are typically used, with areal dimensions ranging from 0.5 to 1ha for open raceway or central pivot ponds (circular ponds incorporating centrally pivoted rotating agitator), to greater than 200 ha (Greenwell, H.C., et. al 2009).

Water management procedures vary according to the intensity of operation and may include direct CO_2 addition under automated pH-stat control in shallow raceways. The algal biomass may be harvested by flocculation or centrifugation (del Campo et al. 2007)[11]. While algal productivities will inevitably be submaximal in open raceways (typically < 1.0 g dry wt m^{-2} d^{1} (ref)), it is generally accepted that these types of bioreactor systems will form the basis of large-scale algae production required for biofuels, owing to their simplicity and low costs (Sheehan et al. 1997). However, raceway configuration and operating procedures have not yet been optimized for those algal species short-listed for oil production (Rodolfi et al. 2009).

The Modeling Framework

Data-driven ECO computer models may be used in many ways to enhance protocols for the cultivation, harvesting, and extraction of biofuel from algae cultivated in open raceway ponds. While empirically based research often requires copious amounts of time and resources, ECO models are often a more efficient way to predict large-scale biofuel production in open raceway ponds (Smith, V.H. et. al, 2010). However, like every model, these models are only more efficient if they are able to accurately simulate reality (Smith, V. H. et. al, 2010; Ptacnik R., A. et. al, 2008). Ideally, ECO model output will include information to determine the optimal size and location for an algal biofuel reactor and processing facility, and whether multiple, small-scale distributed bioreactors or large-scale integrated systems for algal growth, dewatering and extraction are better.

ECO modeling techniques are of potential importance in the following areas: 1. Increasing algal growth and production of specific end products. 2. Optimization of bioreactor design and operation. 3. Production facility operation. 4. Coupled operation and financial modeling and risk analysis. ECO models provide important qualitative and quantitative information that enables researchers to understand the impact that raceway pond ecology has on optimizing biofuel production.

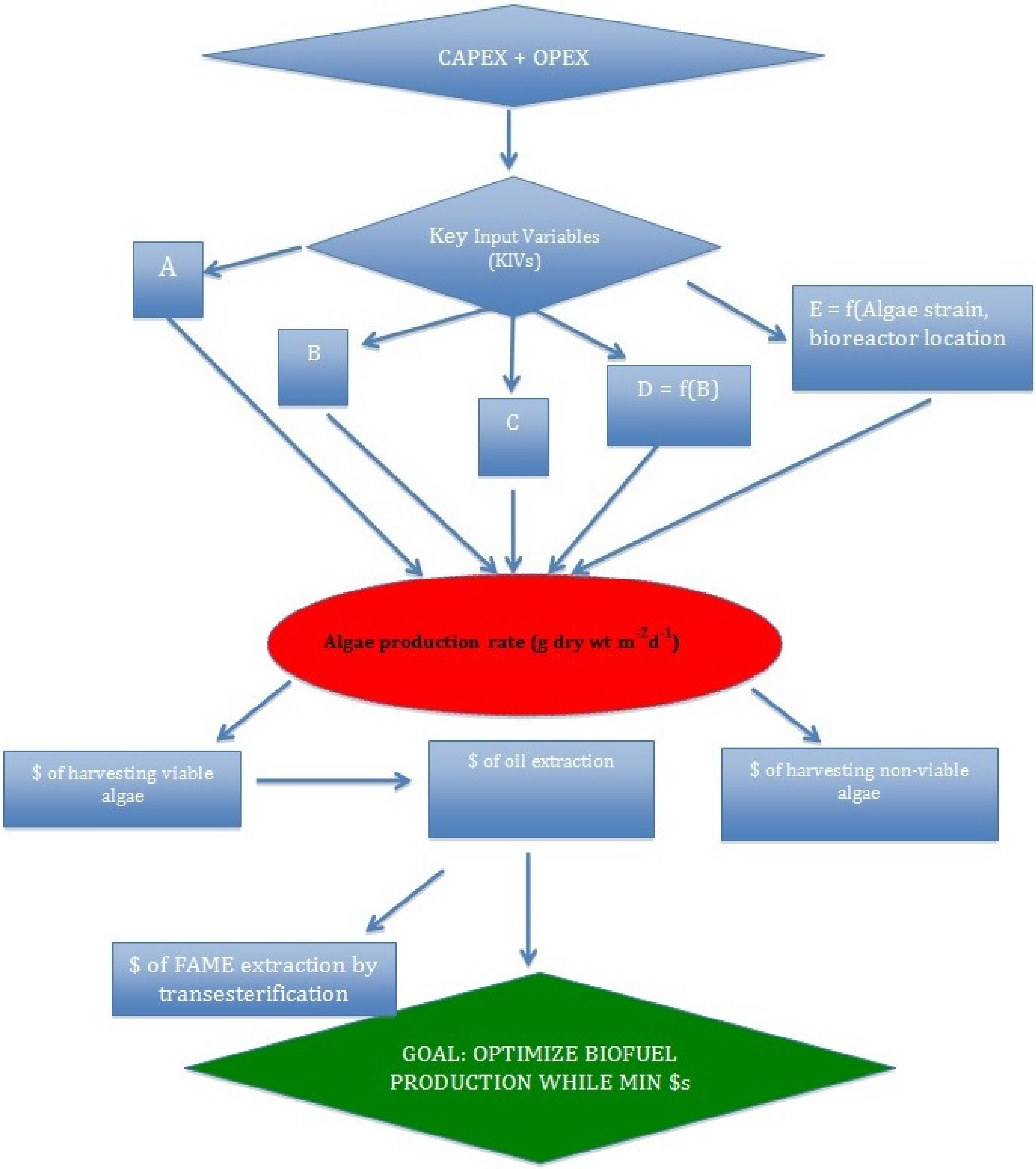

Fig 1. Conceptual diagram for general TE modeling framework for analyzing the economics of algae biofuel production in open bioreactors. KIVs: A = $ of micronutrients, B = H_20 depth, C = $ of CO_2, D = $ of H_20 replacement after evaporation, which is a function of the $ of H_20 evaporation, E = $ of bioreactor operation, which is a function of the type of algae strain and bioreactor location. Over a harvest period, algae production is determined by stochastic simulations (non-dynamic).

The standard TE modeling framework is composed of the following stages: Stage 1 consists of estimating CAPEX, OPEX and depreciation costs for process inputs over a harvest season. Costs are reported as a range of values for this preliminary analysis estimate. The impact of uncertainties in key design parameters on the calculated costs is usually examined using sensitivity analysis. In Stage II, a more detailed process design and economic evaluation is undertaken to estimate a minimum fuel-selling price for the designed process (Michael A. Borowitzka, 2013*)*. Figure 1 illustrates the general modeling framework within which TE models are developed and tested.

Raceway Pond Ecology and Biofuel Production: Feedback, Time Delays and Nonlinear Behavior

Because outdoor ponds are open to the environment, they contain diverse assemblages of natural algae and zooplankton; their behavior and operation is both subject to, and informed by, known ecological principles that define the system-dynamic properties of the system. Ecologists can therefore make critical intellectual contributions to the development of algal biofuels, using first principles from biochemistry, bioengineering, economics, and genetics. Unfortunately, to date, there has been limited exchange of ideas between researchers working in these fields, particularly amongst ecologists and economists. Clearly, communication between researchers in these two fields is necessary for the successful development and implementation of a TE model with strong predictive power.

In general, the ecological dynamics of an open raceway pond system reflect the amount of energy that goes into the system, organism composition within the system, whom eats whom, and how much energy is generated from each component within the system. Within the context of this review, energy is a measure of algal biomass generated over a specific time interval, oil extracted, and biofuel produced (Philip Kenny and Kevin J. Flynn, 2014). Thus, for the large-scale generation of biofuels from algae, open pond-based production facilities must be treated as complex, bioengineered ecosystems that obey the known principles of ecology (Smith et al., 2010) similar to the freshwater ecosystems in which algae naturally grow.

Empirical observations of open-pond production emphasizes that the ecological principles that underlie these systems are analogous to an open ecological system composed of predator–prey interactions (Brännström A. and Sumpter D.J., 2005). Outbreaks of plant-eating insects, for example, threaten agricultural crops and cost billions of dollars annually in pest control across the globe. Similarly, tiny, naturally occurring, herbivorous zooplankton that graze on the microalgae growing in raceway pond water can invade and become established within any open cultivation system. Because these ponds ultimately develop diverse communities containing both algae and zooplankton, they tend to exhibit oscillations in population numbers (common in predator–prey dynamics and resembling those of insect pests that reduce crop yields in standard agriculture). However, a solution to this dilemma comes from the now well-known concepts of bio manipulation and top-down ecological control (Smith, V.H. et. al, 2010). Similarly, open-pond systems are exposed to invasion by a wide variety of other organisms, some of which are undesirable because they can greatly reduce algal biomass yields.

Ecological theory predicts that pond bioreactors will that only contain communities of biofuel producing algae, will be susceptible to invasions by herbivorous zooplankton (protozoa, rotifers and micro crustacean) and diatom competitors, thereby creating a 3-species trophic level food web within the raceway pond system. However, a 3-level food web structure can potentially exhibit strong day-to-day variance in algal biomass due to temporal variations in grazing activities and levels of indirect diatom competition. For example, fishless, 2-trophic level systems tend to become dominated by large-bodied herbivores such as Daphnia, which can grazealgal biomass down to extremely low levels (Smith, V.H. et. al, 2010). Similar food web dynamics occur in HRAPs and sewage oxidation ponds: strong oscillations have been observed between Daphnia and microalgae in aerated sewage lagoons, HRAPs, and other wastewater-fed systems, with algal biomass concentrations that can exceed 1 mg L^{-1} as chlorophyll a (Philip Kenny, and Kevin J. Flynn. 2014).

From a biofuel production standpoint, high amplitude predator–prey oscillations can lead to algal biomass ‘‘crashes,’’ causing large and unpredictable reductions in biodiesel production. For example, microalgal biomass peaks as high as 0.33 mg L^{-1} chlorophyll a were observed in a Luxembourg lagoon when Daphnia were rare in the water column; in contrast, microalgal biomass declined by more than two orders of magnitude to only 0.001–0.002 mg L^{-1}during periods of maximum Daphnia abundance and grazing intensity (Smith, V.H. et.al, 2010).

Empirical studies of raceway species in the southwest United States indicate that increasing temperatures during the spring and summer months are a catalyst for invasion of the ponds by multiple organisms that are detrimental to the growth of algae targeted for biofuel production (Scott, S. A. et. al, 2010). Some of these organisms include predatorial grazers (e.g. rotifers) and various species of diatoms that compete indirectly for resources with the biofuel producing algae. Invasive species can reduce algal concentration and production to low levels within just a few days (Smith, V.H. et.al, 2010). For example, rotifers at high densities (>10 L^{-1}) were shown to reduce algal concentrations by 90% within 2 days (Smith, V. H. et.al, 2010). Fungal parasitism and viral infection can also significantly reduce the pond algal population within a few days and trigger changes in algal cell structure, diversity and succession (Smith, V. H. et.al, 2010).

System Dynamics of Open Raceway Ponds

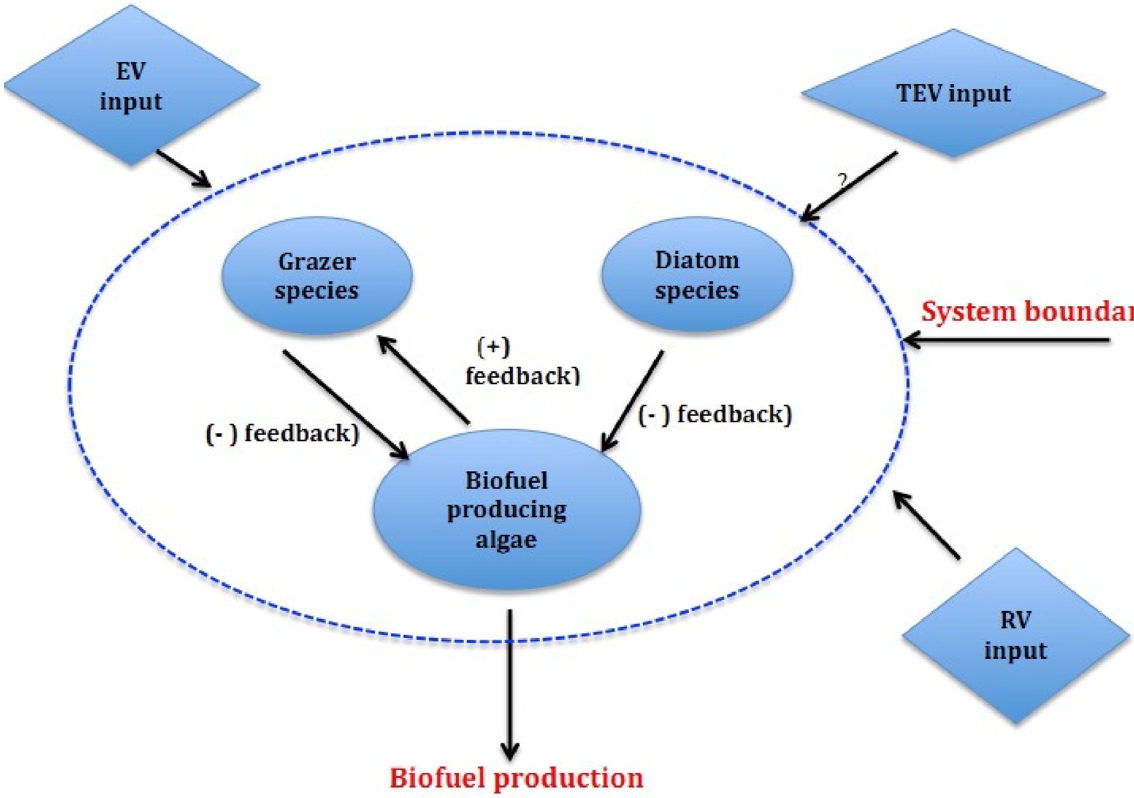

Fig 2. Conceptual diagram for a general ECO modeling framework for an open raceway pond composed of 2 invasive species (1 grazer species and 1 diatom species (indirect competitor)) and biofuel producing algae. Environmental (E), techno-economic (TE), and Random noise (R) variables are fed into the system and affect internal feedback dynamics generated by species interactions. Negative feedback reflects reduction in biomass production as a function of grazer and diatom biomass. Positive feedback reflects increased grazer biomass as a function of available biofuel producing algae. The system boundary separates the internal raceway pond environment from external input. The question mark over the arrow that connects input of techno-economic variables (TEVs) reflects the question as to how the TE information can be placed within the ECO model framework. This is a question for future research and is not emphasized in this review.

The open raceway pond is a dynamical system, with multiple external and internal variables that interact over time, generating feedback within the system that can lead to nonlinear behavior. Within a raceway pond, functional biotic groups represent biofuel producing algae and the species they interact with throughout the cultivation and harvesting process. An intra specific interaction of the algae functional group occurs within a specific range or boundary for each environmental variable (EV) and TE variable. This boundary represents separation of the internal pond environment from external input variables. Figure 1 is a conceptual diagram illustrating an open raceway pond system composed of biofuel producing algae and two invasive species. The diagram highlights the system dynamic components that drive interactions within the pond, and those interactions may generate nonlinear behavior (e.g. algae population crashes) that effects biofuel production.

The ECO model

Based on empirical evidence, the economics (i.e. production) of algae in raceway ponds is intimately linked with raceway pond invasion. Hence, this critical review highlights continued progress in the development and analysis of a data driven ECO model that considers the effects of ecological variables (EVs) and random variables (RVs) on large-scale biofuel production by Nannochloropsis salina sp. (1776) in an open raceway pond. The pond is composed of three interacting organisms: biofuel producing 1776, a 1776 grazer species, and a diatom species that competes indirectly with 1776 for pond resources. Here, RVs are parameters that take into account the effects of external noise (i.e. environmental noise) on algal biofuel production.

Simulations of the ECO model are being used to generate testable predictions of strategies for optimizing biofuel production for aviation by 1776 over the course of a typical harvest season in a raceway pond running in a Southwest United States-like environment. In this review, I highlight the basic architecture of the model with the STELLA®(HPS, 1998) modelling environment, and briefly describe some EVs and RVs, and ecological response variables in the model, including seasonal light, seasonal temp, CO_2, pH, and nitrogen, and the system-dynamic ordinary differential equations (ODEs) that describe growth of all species within the raceway pond. In addition, I define the functional forms of key EVs, and RVs in addition to ecological response variables.

TheECO model is composed of three functional groups (equations 1-3): Nannochloropsis salina sp. (1776), a diatom competitor species and a 1776 grazer species. A priori assumptions of the ECO model include: 1. Increased productivity of each functional group occurs within a specific range or boundary for each EV and RV. Loss of biomass (g m^{-2} d^{-1}) is modelled as a senescence of a constant proportion of standing stock biomass (i.e. the size of the initial inoculate); additionally, removal of 1776 biomass can occur through blowout (supersaturated media). 3. The mathematical constraint for each functional group consists of a logistic growth equation that predicts, under optimal conditions, an expected increase in biomass over time of that group within a giving volumetric area (e.g. 1000L raceway pond).

$$\frac{dG}{dt} = \left[\gamma G\left(\frac{aA}{b+A} + \frac{bD}{c+D} - \mu\right)\right] - G(G_{nd} + RV) \pm GEV \quad (1)$$

$$\frac{dD}{dt} = \left[\beta G\left(\frac{dA}{e+A} - \delta\right) - \frac{bG}{c+D}\right] - D(D_{nd} + RV) \pm DEV \quad (2)$$

$$\frac{dA}{dt} = \left[\alpha A\left(1 - \left(\frac{A}{A_k}\right)\right) - \frac{aAG}{b+A} - \frac{dAD}{e+A}\right] - A(A_{nd} + RV) \pm AEV \quad (3)$$

where A = Nanochloropsis salina (1776) biomass (g L^{-1}) G = Preadatorial grazer biomass ((#cells L^{-1}), D = Diatom competitor (#cells L^{-1}). $\gamma, \beta, and\ \alpha$ are the grazer growth rate (d^{-1}), diatom growth rate (d^{-1}), and algae growth rate (d^{-1}), respectively. A_k = equilibrium biomasss of A in the absence of G and D. μ = consumption rate needed to sustain and replace 1 G per unit time. δ = consumption rate of external micronutrients in pond needed to sustain and replace 1 D per unit time. b and e are the ½ saturation constants. G_{nd}, D_{nd}, and A_{nd} represent the natural death rates for each species in the model (% biomass lost d^{-1}), and RV is the random environmental noise (deviate sampled from a normal distribution).The effects of *EVs* (e.g. pond salinity, CO_2 concentration) are either subtracted or added to the time derivative for each species.

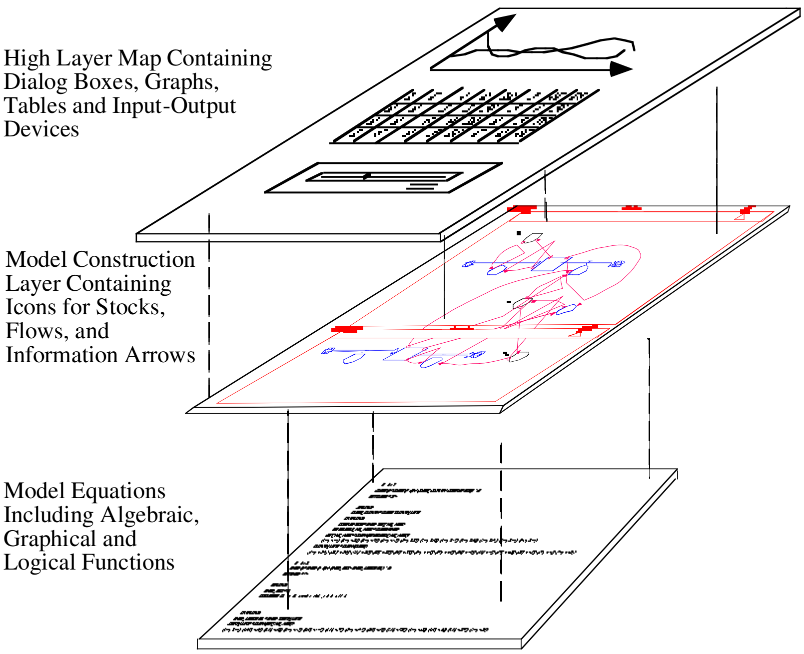

Figure 3. STELLA Modeling Environment ***(From Costanza and Ruth, 1998)***

Figure 3. Flow diagram showing the basic architecture of the ECO model within the STELLA© modeling environment. Within the bottom layer, data for growth responses of functional groups to input variables is used to define the functional form of the production

function (equation 1). The middle layer contains information about the flow of EVs and RVs, into the race way pond environment, which amplifies or dampens nonlinear behavior driven by feedback amongst *1776*, grazers and diatom competitors (e.g., the internal functional groups). The first layer contains qualitative and quantitative information generated by model simulations. This information is used to analyze the sensitivity of model behavior to system variables and ideally, to determining pathways for increasing biofuel production.

Initial results from ECO model Simulations

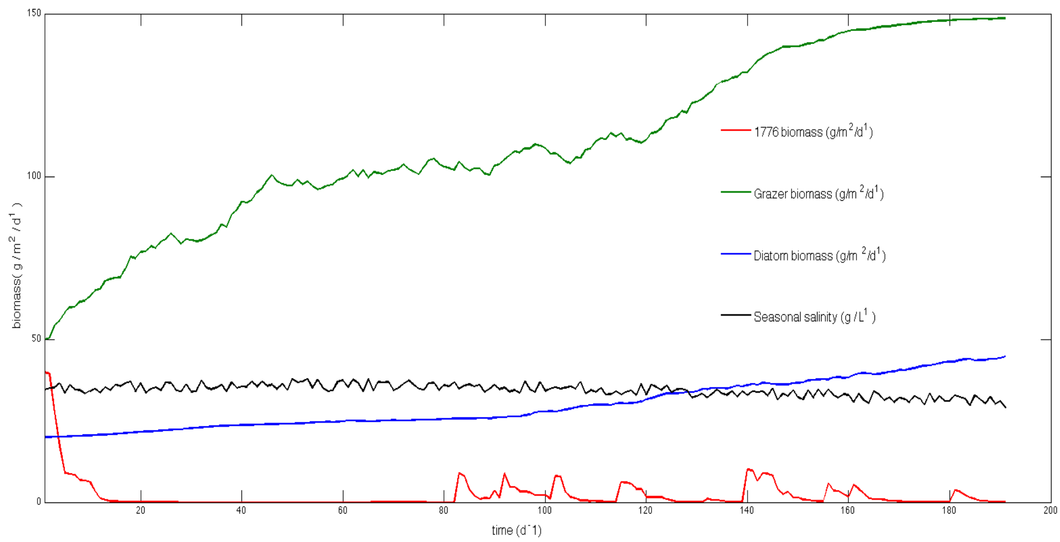

Figure 4. The inclusion of salinity (RV) and resulting population dynamics generated by the model (equation (2)-(4)). It is observed that 1776 exhibits boom-bust population dynamics as a function of increased growth in grazers and diatoms.
Parameter values: A = 45, D = 35, G = 50, $\gamma = \beta = \alpha =$ .01, A_k = 100, μ = 1.1, δ = 1.5, b =e = 5, G_{nd}, = D_{nd} =A_{nd} = 1.2, RV = 0.5, EV = 0.9.

Simulations of the ECO model (figure 4) are being used to generate testable predictions of strategies for optimizing biofuel production by *1776* over the course of a typical harvest season in a raceway pond running in a New Mexico-like environment. Presently, I am using sensitivity analysis to test which input variables subject to variation (change in initial value at start of simulation) have the greatest impact on inhibiting *1776* production by invasive species. Table 1 lists key EVs and RVs and their functional forms. Figure 4 illustrates the growth responses of *1776* as a function of some EVs and RVs listed in Table 1. One important note of mention is that the ECO model can be modified to be purely deterministic, so that one may compare results to the stochastic version of the model (null model comparison method).

Table 1.0. EVs and RVs used in equations (2-4)

Variable	Parameter	Units	Form
A	Algae biomass	mg L^{-1}	$\frac{dA}{dt} > 1^{*}$
D	Diatom density	# cells L^{-1}	$\frac{dD}{dt} > 1$
G	Predator density	# cells L^{-1}	$\frac{dG}{dt} > 1$
Salinity	Salinity of Raceway pond	% L^{-1}	% L^{-1}

*Indicates that the neither A, D, nor G will grow if the time derivative is not greater than one. If the time derivative is equal to one, this results in direct replacement each generation (i.e. zero growth).

Discussion

Steady progress is being made towards determining appropriate functional forms for all EVs, RVs, and internal response variables in the ECO model. Functional forms for environmental inputs are being determined and adjusted through extensive literature reviews and analysis of data from raceway ponds at New Mexico State University and other ponds located throughout the United States. More data is needed from team members working on raceway pond systems. Functional forms for TE inputs are being determined and adjusted through extensive literature review, and will be integrated into the ECO model as they become available.

The purpose of this review was to analyze the qualitative dynamics of an ECO model that takes into account, not only interactions amongst species within the raceway pond, but also the effects of RVs (salinity) on system dynamics.

Model Operationality

The operationality of the model presented here, can only be quantified by determining how well its dynamics compare with empirical data derived from raceway ponds. As more information that is empirical becomes available, researchers can compare theoretically and empirically derived data, and adjust the model to have greater predictive power. Clearly, the model presented in this paper is sparse with respect to the number of EVs that were used. The inclusion of CO_2, N, light levels and other EVs will increase the realism of the model, and allow comparisons to empirically derived data.

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