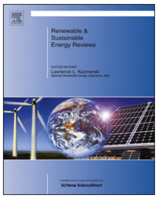
Renewable and Sustainable Energy Reviews 43 (2015) 530–544

Contents lists available at ScienceDirect

Renewable and Sustainable Energy Reviews

journal homepage: www.elsevier.com/locate/rser



# Mathematical modeling of production and biorefinery of energy crops

Lijun Wang [a,*], Samuel A. Agyemang [b], Hossein Amini [b], Abolghasem Shahbazi [a]

[a] *Biological Engineering Program, Department of Natural Resources and Environmental Design, NC, United States*
[b] *Department of Computational Science and Engineering, North Carolina Agricultural and Technical State University, 1601 E. Market Street, Greensboro, NC 27411, United States*

## ARTICLE INFO

*Article history:*
Received 22 August 2013
Received in revised form
6 October 2014
Accepted 3 November 2014

*Keywords:*
Crop growth kinetics
Biorefinery
Mathematical modeling
Computational fluid dynamics
Life cycle assessment
Geographical information system
Biomass supply logistics

## ABSTRACT

Mathematical models have been widely used to simulate all aspects of bioenergy production systems including the growth kinetics of energy crops, conversion processes, production economics, supply logistics and environmental impacts. There is limited commercial experience to produce and process energy crops at a large scale around the world. Those models can provide powerful tools to design a bioenergy system and evaluate its technical feasibility, economics and environmental impacts. A crop growth model can be used to estimate the yields of energy crops in a region under different growth conditions. A geographical information system (GIS) model can be used to maximize the energy production of energy crops by indentifying suitable land to grow them based on their specific characteristics and the current use of the land. A combination of process models and reaction kinetics provides advanced computational tools for the design and optimization of various biomass conversion processes. The biomass supply chain consists of multiple harvesting, storage, pre-processing and transport options. Mathematical models have been developed to analyze and optimize complex biomass supply systems. A life cycle assessment (LCA) model can be used to compare the environmental impacts of different biomass production and conversion technologies. Various mathematical models applied to bioenergy systems were reviewed. The challenges in mathematical modeling of bioenergy systems which include the difficulty in generalizing a bioenergy system, the lack of physical and chemical properties of various biomass, the complexity of multi-scale processes and the validation of the models were then discussed.

## Contents

---

* Corresponding author. Tel.: +1 336 285 3833; fax: +1 336 334 7270.
*E-mail address:* lwang@ncat.edu (L. Wang).

http://dx.doi.org/10.1016/j.rser.2014.11.008
1364-0321/

## 1. Introduction

Lignocellulosic biomass is an abundant renewable energy source. Energy crops such as switchgrass, sweet sorghum and microalgae have been widely investigated to fulfill the future energy and chemical demands. Biorefineries which integrate different conversion processes including thermochemical, chemical and biological conversion are required to convert various biomass feedstocks into different energy products such as alcohols, biodiesels, syngas and hydrogen. A bioenergy system involves the interaction between chemical and physical processes at a multi-scale of molecular, reactor and system levels. A bioenergy supply chain typically has five major components of biomass production, biomass logistics, biomass-to-product conversion, product distribution and product end use [1].

There are few commercial bioenergy systems in operation. The design and analysis of a bioenergy system is challenging due to the complexity of the system, and the lack of data and knowledge. Experiments at a large scale are often expensive and complicated. Mathematical models can provide economical and powerful tools for the design and optimization of a bioenergy system. There are four basic groups of mathematical modeling techniques applied in bioenergy systems: (1) biomass production models [2], (2) biorefinery processing models [3], (3) economic models of bioenergy supply chains [4,5], and (4) life cycle assessment models of bioenergy systems [6,7].

This article was to review the various mathematical models that have been developed to simulate bioenergy systems including production of energy crops, conversion of biomass into different energy products, biomass supply logistics and environmental impacts of a bioenergy system. The challenges in mathematical modeling of bioenergy systems were then discussed.

## 2. Mathematical modeling of the production of energy crops

### 2.1. Modeling of energy crop growth kinetics

Energy crops such as switchgrass, sweet sorghum and microalgae have been widely investigated. However, there is limited commercial experience to produce energy crops at a large scale around the world [2]. The yield of energy crops is an important parameter to assess their production cost. A crop growth model can be used to estimate the yields of energy crops in a region under different situations. van den Broek et al. [2] developed an energy crop growth model to estimate potential and water-limited yields for a certain region on the basis of solar radiation and daily data for precipitation and pan-evaporation. The potential growth rate of an energy crop at a specific region where temperature, fertilizers and water are not limiting growth factors was calculated by [2]:

$$G_p = \varepsilon \phi f_{PAR}\left(1 - e^{-k \cdot LAI}\right) HI \tag{1}$$

where $G_p$ is the potential rate ($g_{\mathrm{dm}}/\mathrm{m}^2\mathrm{day}$), $\varepsilon$ is the crop radiation utilization coefficient ($g_{\mathrm{dm}}/\mathrm{MJ_{PAR}}$), $\varphi$ is the solar radiation ($\mathrm{MJ/m^2day}$), $f_{PAR}$ is the amount of photo-synthetically active radiation ($-$), LAI is the leaf area index ($m^2_{leaf}/m^2_{ground}$), $k$ is the canopy extinction coefficient ($m^2_{ground}/m^2_{leaf}$) and HI is the harvest index ($-$). The input data for the growth of *Eucalyptus camaldulensis* in Nicaragua are given in Table 1 [2].

The temperature, nitrogen and water-limited growth rate can further be calculated as a function of the potential growth rate by taking into account of individual limiting factors, which was given by [2,8]:

$$G_l = f_T f_N f_W G_p \tag{2}$$

where $f_T$, $f_N$ and $f_W$ are limiting factors for temperature, nitrogen availability and water in the soil. The limiting factors can be determined by [8]:

$$f_T = \frac{(T - T_{\min})}{(T_{\max} - T_{\min})} \tag{3}$$

$$f_N = \frac{\left(\mathrm{N}_{leaf} - \mathrm{N}_{leaf,\ \min}\right)}{\left(\mathrm{N}_{leaf,\ \max} - \mathrm{N}_{leaf,\ \min}\right)} \tag{4}$$

$$f_W = \frac{E_t}{E_{tp}} \tag{5}$$

where $T$ is temperature, N is nitrogen, $E_t$ is the actual transpiration in the soil and $E_{tp}$ is the potential transpiration in the soil.

The use of a crop growth model requires input data such as meteorological data, soil data, and crop characteristics, which can be determined at a reference location. However, the interactions between site-specific properties such as climate, available soil water and nutrients and crop growth are complex. Therefore, the above model assumes that the nutrient conditions and yield reduction by weeds, pests and diseases at a specific location and reference location are the same [2]. The predictions showed that the potential and water-limited yields for the growth of *Eucalyptus camaldulensis* in Nicaragua, the Netherland were 35 t dry mass/(ha year) and 23 t dry mass/(ha year), respectively. The actual yield was 13 t dry mass/(ha year), which was about 58% of its water-limited yield [2].

**Table 1**
input data for the growth of *Eucalyptus camaldulensis* in Nicaragua [2].

| Parameter | Value | unit |
|---|---|---|
| $\varepsilon$ | 2.2 | $g_{\mathrm{dm}}/\mathrm{MJ_{PAR}}$ |
| $k$ | 0.5 | $m^2_{ground}/m^2_{leaf}$ |
| $\varphi$ | 57 | TJ/(ha year) |
| HI | 0.85 | – |
| LAI | 0.8–3.2* | $m^2_{leaf}/m^2_{ground}$ |

* The leaf area index depends on the growth year and rotation.