OptiBiU: an optimisation model to explore the Optimal Biomass Use in a circular biobased economy

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Optimizing the use of biomass in the bioeconomy may help to replace fossil-based products, and contribute towards limiting global warming, reduction of leakages and decrease of dependency on finite resources. However, judging the optimal use of biomass is currently hard. To be able to improve this understanding of optimal biomass use, a model of production of biobased products will be developed. The set up of this model is described in this report in terms of production of biobased products, in terms of conversion of biomass sources, including re-use and recycling as after-life options of products.

Keywords: optimization, biomass, bioeconomy, biobased

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1 Introduction

In the biobased economy fossil non-renewable sources are replaced by renewable biomass to produce materials and energy. The transition from our current mainly linear fossil-based economy towards this circular biobased economy leads to a number of questions. Among these are: which biomass is suitable for which material and/or energy, can biomass be used for multiple purposes (e.g. in a biorefinery approach), is enough biomass available to fulfill our needs (food, feed, energy, materials) and what are the consequences of redirecting biomass sources currently used, from their original towards new destinations? The main reasons for making this transition are to limit global warming, reduce harmful leakages to the environment, and end our dependency on finite resources. This means that the contributions to these goals need to be thoroughly assessed in the bioeconomy, while also taking into account that biomass use in the bioeconomy can compete with biomass needs for other purposes, such as food, biodiversity, soils and landscape. Currently it is not clear what the optimal use of biomass is on the system level, given objectives of e.g. maximizing production, limiting global warming, reduction of leakages and decreasing dependency on finite resources, and taking into account the options of cascading.

To address these challenges, one of the objectives of a project, entitled: "Exploring new connections and potentials for biomass in the bioeconomy" (KB-34-002-003), is to develop a model that can be used to explore the potential of replacing fossil-based products in a circular biobased system to mitigate global warming, to reduce nutrient losses and to decrease dependency on scarce natural resources.

In this document, the structure of OptiBiU is presented. OptiBiU is a mathematical programming model, that describes the production of biobased products, in terms of conversion of biomass sources, including re-use and recycling as after-life options of products. The goal of this model is to investigate the optimal use of biomass in the bioeconomy by addressing the following questions:

given primary¹ biomass availability and taking into account optimal cascading, how to

- "maximize" production of biobased products? (maximize between quotation marks because production can be measured in multiple ways)
- maximize replacement of fossil sources (taking into account current biomass uses)?
- maximize potential carbon sequestration?
- minimize greenhouse gas emissions?
- minimize residual waste?
- minimize other "harmful leakages"?

given product demands and taking into account optimal cascading, how to

- minimize primary biomass demand?
- minimize land use?
- maximize potential carbon sequestration?
- minimize greenhouse gas emissions?
- minimize costs?
- minimize residual waste?
- minimize other "harmful leakages"?

how does such "optimized" system compare to the current system with respect to

- demand for fossil sources
- land use
- carbon sequestration
- greenhouse gas emissions
- residual waste reduction

¹ Primary biomass here refers to both dedicated primary biomass and residues that are thus newly produced from agricultural production.

- use of finite resources
- C storage (i.e. removal of CO₂ from the atmosphere)
- socio-economic aspects
- implementability
- circularity, by means of a circularity score (Elbersen et al., 2022)

The initial intended use of the model is to shed light on the above questions, which may help to provide guidance towards optimal use of biomass sources. The model itself will initially not be developed as a publicly available tool, but to such development may be decided in a later stage.

2 The biomass valorization system

The conversion of biomass sources to products can be visualized as a sequence of steps from biomass sources, through processing, to products (Figure 1). These products are then used for a certain time, after which they can be reused, (partly) recycled, or end-up as unusable waste or loss. Reusing refers to using the product again with the same purpose ('refurbished'), whereas recycling refers to using intermediate products as a secondary biomass source for new products. Waste, in our description, solely refers to situations were products are not reused or recycled, but wasted without being useful for the economy, for example because products end up in the environment or in a landfill. The term loss is used when products decompose and carbon is emitted (lost) to the atmosphere, as is the final destination of carbon in Soil Organic Matter (SOM) or fuels. SOM and fuels themselves are interpreted as biobased products in the model to be able to take their uses and their demands explicitly into account when searching for optimal biomass use. They are examples of 'end-use' because most of the organic matter in SOM and fuels cannot be reused or recycled any more for another product in the system. Products that end up in waste incineration from which electricity and/or heat is used, are not converted to waste in our description, but to a product that can be interpreted as a type of fuel. Once burnt, part of the matter is lost in the form of carbon dioxide, but part, for example in the form of mineral ashes, may still be recycled.

Figure 1 Visualization of production of biobased products.

2.1 Mathematical formulation

To describe the model mathematically, we first describe the indices, decision variables, parameters and some auxiliary variables, and then explain the equations below.

In the optimization model, the following indices and sets are used:

- *i* ∈ *I* set of possible products
- *j* ∈ *J* set of intermediate products
- *k* ∈ *K* set of primary biomass sources
- *l* ∈ *L* set of intermediate product to product conversion processes
- $m \in M$ set of biomass to intermediate product conversion processes
- *n* ∈ *N* set of product to intermediate product conversion processes

The decision variables used in the model are:

- *Wⁱ* amount of product *i* annually produced (ton/year)
- *Xj,l* amount of intermediate product *j* annually processed in process *l* (ton/year)
- *Yk,m* amount of biomass *k* annually processed with process *m* (ton/year)
- *Zi,n* amount of product *i* annually processed in process *n* (ton/year)

The following are auxiliary variables that have no role in the optimization but help to explain the system:

- *Qⁱ* quantity of products *i* in the system (ton)
- *A^j* amount of intermediate products *j* annually produced (ton/year)
- *B^k* amount of primary biomass *k* annually produced (ton/year)
- P_v total value of production, which can be monetary or any other value of products ([unit]/year)
- *P^e* total emissions of production ([unit])
- U total land use of all primary biomass sources (km^2)

Parameters² used in the model are:

- *aijl* conversion factor from intermediate product *j* to product *i*, through process *l* (ton product/ton intermediate product)
- *bjkm* conversion factor from biomass type *k* to intermediate product *j*, through process *m* (ton intermediate product/ton biomass)
- *cijn* conversion factor from product *i* to intermediate product *j,* through process *n* (ton intermediate product/ton product)
- *maxbm^k* maximum production per biomass source *k* (ton/year)
- *maxprⁱ* maximum production per product *i* (ton/year)
- *minprⁱ* minimum production per product *i* (ton/year)
- *recⁱ* fraction of products *i* suitable for recycling at end of lifetime (-)
- *reuⁱ* fraction of products *i* suitable for reuse at end of lifetime (-)
- *rⁱ* fractions of annually reused products *i* (year-1)
- *sⁱ* fractions of annually recycled products *i* (year-1)
- d_i fractions of products *i* annually turning into waste or loss (year⁻¹)
- *vⁱ* lifetime of products *i* (year)
- *prdⁱ* dry matter content of product *i* (kg dm/ton)
- *imd^j* dry matter content of intermediate product *j* (kg dm/ton)
- *bmd^k* dry matter content of primary biomass type *k* (kg dm/ton)
- *prcⁱ* carbon content of product *i* (ton C/ton)
- *imc^j* carbon content of intermediate product *j* (ton C/ton)
- *bmc^k* carbon content of primary biomass type *k* (ton C/ton)
- *lu^k* land use per primary biomass source *k* (km² /ton/year)
- *qv, i* value of product *i*, which can be monetary or any other value ([unit]/ton)
- *yef, k* emission factor of production of primary biomass type *k* ([unit]/ton/year)
- *bef, j,k,m* emission factor of processing biomass type *k* into intermediate product *j* through process *m* ([unit]/ton/year)
- *aef, i,j,l* emission factor of production of product *i* from intermediate product *j* through process *l* ([unit]/ton/year)
- *uef, i* emission factor of use phase or product *i* ([unit]/ton/year)
- *ref, i* emission factor of making product *i* suitable for reuse ([unit]/ton/year)
- *def, i* emission factor of emissions resulting from waste of product *i* ([unit]/ton/year)
- *cef, i,j,n* emission factor of recycling product *i* into intermediate product *j* through process *n* ([unit]/ton/year)

² When not explicitly indicated, ton can refer to both ton dry matter or ton fresh matter, depending on available data. N.B. conversion factors a, b, and c should be consistent with the used units.

The amount of products produced per year consists of products made from new biomass (so-called primary biomass), products made from intermediate products originating from recycling and products made by reusing (parts of) existing products. The annual stock change of products can be described by a differential equation:

$$
\frac{dQ_i}{dt} = W_i - r_i Q_i + r_i Q_i - s_i Q_i - d_i Q_i = W_i - s_i Q_i - d_i Q_i \qquad \forall i
$$
\n(1)

The total quantity of each product (Q) is calculated from its annual production (W) and the average service lifetime of a product (equation 2), which represents the average period of a product from the moment of its production till the moment it is reused, recycled, wasted or lost.

$$
Q_i = v_i W_i \tag{2}
$$

For optimization purposes, we assume an equilibrium situation, equating equation 1 to 0. This means that annually as much new products should be produced as are recycled, wasted and lost. The optimal equilibrium can then be found by for example maximize the biobased production under a given amount of primary biomass availability (equation 3), or minimize production of primary biomass under a given product demand (equation 4).

$$
\max \sum_{i} W_i \tag{3}
$$

$$
\min \sum_{k} \sum_{m} Y_{km} \tag{4}
$$

This optimization is subject to the following constraints regarding production and recycling:

Equation 5 matches the conversion of intermediate products, to produced products, equation 6 matches the conversion of primary biomass and recycling of products, to produced intermediate products, and equation 7 matches the amount of recycled products to available stock. Due to the assumed equilibrium condition, the annual productions of intermediate products equal the annual conversions of these intermediate products into products. So, their net change is also zero, similar to the situation with the products. Further, production is constrained by minimum (8) and maximum (9) product demands as well as maximum biomass production (10).

In addition to the basic equations, the description of the system can be extended by describing how parameters in the system can be inferred from other data that may be more easily available, and how the system links to several emissions and other impacts.

3.1 Dependence of r, s and d on lifetime of a product

Each year, the fraction of products that reach the end of the lifetime (*v*) is given by the inverse of the lifetime (v^{-1}). At that moment, three options exist: reuse (r), recycling (s) and waste or loss (d). This leads to the following relations for *r, s* and *d*.

$$
r_i = rev_i r_i
$$

\n
$$
s_i = rec_i v_i r_i
$$

\n
$$
d_i = (1-rec_i-reu_i) v_i
$$

\n(12)

3.2 Production value

Total value of production (P_v) depends on value per product (q_v) and amount of products annually produced:

$$
P_v = \sum_i q_{v,i} W_i \tag{14}
$$

3.3 Production emissions

Production emissions (*Pe*), such as greenhouse gas emissions, is the sum of emissions in each stage of the production of a product:

 $P_e = \sum_{k,m} y_{ef,k} Y_{km} + \sum_{j,k,m} b_{jkm} b_{ef,jkm} Y_{km} + \sum_{i,j,l} a_{ijl} a_{ef,ijl} X_{jl} + \sum_i u_{ef,i} v_i W_i + \sum_i r_{ef,i} r_i v_i W_i + \sum_i d_{ef,i} d_i v_i W_i + \sum_{i,j,n} c_{ef,ijn} c_{ijn} Z_{in}$ (15)

3.4 Land use

Assuming that land use is only required for the production of primary biomass, and not for other parts of the production process, the calculation of land use is a special case of the first term in equation 15.

 $U = \sum_{k} \sum_{m} l u_k Y_{km}$ (16)

4 Optimization objectives

Describing the system according to equations 1-16 facilitates optimization of multiple objectives. Optimization objectives include maximizing production value of production, given primary biomass supply, minimizing carbon emissions, and minimizing land use. These three objectives are listed below as examples but several of the other objectives described in the introduction may be analyzed in similar ways. Depending on the objective, different variables may be maximized or minimized, under different additional sets of constraints.

4.1 Maximize production value of biobased products

Production value (*Pv*) may be expressed in various units, including monetary value. Maximization of product value, given primary biomass supply can be described as follows.

Objective: maximize *P^v*

4.2 Minimize emissions or land use

The objective of minimizing emissions, such as greenhouse gas emissions, or land use, given minimum and maximum production quantities per product can be described as follows.

Objective for emissions: minimize *P^e*

Objective for land use: minimize $\sum_k \sum_m l u_k Y_{km}$

5 Operationalizing the model

For a truly optimal system, all linked biomass sources and products should be included in the model, to find the real optimal connection of biomass and products. However, this would require collection of data of a large number of biomass sources and related products, which would take a considerable effort. More useful would be to have a scalable system that is already useful with a limited number of biomass sources and products included. However, the risk of setting such system boundaries is that it hides potential burden shifts or shows configurations that are optimal in the model, but would not be optimal in the real bioeconomy. For example, system boundaries restricting the biomass sources that are used to produce textiles, and for example excluding cotton, could put a high pressure on producing textiles to fulfill the demand for textiles, while in reality part of the demand would be fulfilled by the production of cotton. To deal with this, we assume that when biomass sources, such as cotton, are excluded, the product demand that is taken into account, is the product demand excluding current demand for products based on the excluded biomass sources.

Working with such system boundaries, allows to build an operational system step by step, because data can collected step by step for individual biomass sources. Data to be collected includes the availability and potential of biomass sources such as fiber hemp, fiber flax, straw or grass cuttings, the products that can be produced from it, and the production process in such a way that intermediate products can be distinguished.

5.1 Software

The model will initially be implemented in FICO Xpress, a commercial solver of excellent performance. This software is relatively user-friendly, is accessible, and targeted at optimization, and therefore preferred over GAMS, Python and R.

6 Data requirements

To run OptiBiU all parameters specified in section 2.1 should be provided. This requires good insights in modelled processes and available biomass streams. Minimum production *minpr* can be derived from current use of products sourced from within the modelled system (country). Maximum production *maxpr* can be derived from current use of products sourced globally.

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