The International Journal of Life Cycle Assessment (2020) 25:73–88
https://doi.org/10.1007/s11367-019-01665-z

LCA OF WASTE MANAGEMENT SYSTEMS

A process-oriented life-cycle assessment (LCA) model for environmental and resource-related technologies (EASETECH)

Concetta Lodato[1] · Davide Tonini[2] · Anders Damgaard[1] · Thomas Fruergaard Astrup[1]

Received: 11 March 2019 / Accepted: 11 July 2019 / Published online: 26 July 2019

Abstract

Purpose In life-cycle assessment (LCA), environmental technologies are often modelled as "black-box processes", where inputs and outputs are typically not linked through physical and/or (bio) chemical relationships. This limits transparency and usability of environmental modelling of resource systems for which the conversion of materials and chemical substances in the materials is essential for the environmental performance. We introduce an advanced "process-oriented" modelling framework allowing quantitative and parameterised physical-chemical relationships between input material composition, conversion process units and subsequent output products, promoting mass and substance balanced conversion modelling and environmental assessment.

Methods A dedicated LCA model, EASETECH, has been used to provide a user-friendly platform for performing advanced LCA of complex technologies, without the need for additional software/tools. In the modelling framework, the technology is subdivided into individual unit processes. In each process, the characterisation of the input feedstock material into biochemical, physical, chemical and nutritional properties is taken into consideration in each multi-output production flow. For each unit process, the processes governing the mass/energy/substance transition and transformation are described by mathematical equations (i.e. relationships between inputs and outputs) through the use of parameters. A range of new operators were developed to establish these relationships that allow for non-linear responses whereby changes in one flow can give a non-linear response in other flows. The modelling framework and the involved operators are explained and applied to a biorefinery case study.

Results and discussion The model facilitates "tracking" of the feedstock material properties from the input to the final products, by establishing mass, substance and energy balances for each conversion unit process. In addition, the process-oriented modelling framework appropriately represents material/substance transition and transformations. The choice of process parameters has considerable importance for the overall results. This was illustrated by one-at-a-time changes in parameter values in two different biorefinery unit processes (i.e. hydrolysis, and fermentation and distillation). In addition, the relevance of feedstock characteristics for the performance of the individual unit processes was proved with fixed parameter sets with different feedstocks. The biorefinery case study demonstrated that the LCA model can be applied to technology cases with different process configurations (e.g. different efficiencies) and different input feedstock properties, where it automatically adjusts to these changes in properties.

Conclusions The advanced process-oriented modelling framework offers more flexible modelling of the conversion technology than previously available, improved options for technology development in view of environmental performance, and potentially more accurate results. This provides a significantly improved basis for environmental modelling and decision-making in relation to resource systems.

Keywords Biorefinery · EASETECH · Environmental assessment · Life-cycle assessment · Material flow analysis · Resource recovery · Technology modelling · Unit process

Responsible editor: Shabbir Gheewala

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s11367-019-01665-z) contains supplementary material, which is available to authorized users.

✉ Concetta Lodato
conlod@env.dtu.dk

1 Department of Environmental Engineering, Technical University of Denmark, Bygningstorvet, 115, 2800 Kgs. Lyngby, Denmark

2 European Commission, Joint Research Centre, Edificio Expo, Calle Inca Garcilaso, 3, 41092 Seville, Spain

Abbreviations

CT	Composite transformer
FD	Fraction distributor
FG	Fraction generator
FH	Fraction hub
FT	Fraction transformer

GW Global warming
LCA Life-cycle assessment
LCI Life-cycle inventory
MD Material distributor
MF Material flow
MG Material generator
NG Natural gas
RED Renewable Energy Directive
RF Residue flow
SD Substance distributor
SG Substance generator
SH Substance hub
ST Substance transformer

1 Introduction

Life-cycle assessment (LCA) represents a standardised and systematic methodology for assessing the environmental performance of technologies and technology systems (ISO 2006a, b; EC-JRC 2010). In the transition to a more resource efficient and sustainable society, e.g. represented by circular (bio) economy initiatives (European Commission 2017; Zabaniotou 2018) and the European sustainability targets (e.g. European Parliament and the Council of the European Union 2009), appropriate management and utilisation of waste materials and residual resources in society are critical in order to minimise losses, maximise environmental savings and avoid suboptimal solutions at societal level. Waste and residual resources represent complex and heterogeneous materials with a wide range of physical and (bio) chemical properties. Recovery and conversion of such materials into secondary raw materials and new valuable products rely on the specific characteristics of these materials, and the environmental benefits associated with potential management solutions are highly affected by the material properties themselves (Bisinella et al. 2017). LCA modelling of residual resource systems, therefore, should not only account for the resource characteristics but also reflect relationships between input material properties and the output products for a wide range of different conversion technologies and process configurations. This puts considerable demands on LCA modelling of resource systems to ensure transparency and flexibility in modelling.

A wide range of (non) commercial LCA models is available for environmental assessment (e.g. SimaPro 2019; Thinkstep Gabi 2019; TEAM 2019; Umberto NXT LCA 2019; for a more complete list, see EPLCA 2019). While most of these modelling tools are primarily targeted environmental assessments of products and manufacturing, rather than systems comprising several technologies involving material flows and conversion of material resources through physical, chemical and biological processes, the majority of these tools follow a so-called black-box modelling approach where embedded data inventories represent individual technologies with a fixed list of inputs and outputs. This means that the user is limited to the technology assumptions "embedded" in the inventories. As differences in modelling assumptions (e.g. technical assumptions, technology type and the inventories used) lead to differences in LCA results (e.g. Gentil et al. 2010), this is a crucial aspect that has particular importance in relation to resource systems and when the technologies themselves are in focus (e.g. Astrup et al. 2018; Henriksen et al. 2018). A few LCA models are specifically designed to evaluate material and resource flow systems (e.g. Jain et al. 2015), with EASETECH being a notable example for LCA of environmental technologies (Clavreul et al. 2014). Using principles from material flow analysis (MFA), EASETECH keeps track of mass, substance and energy flows throughout a system of processes and technologies represented by a scenario (Clavreul et al. 2014). However, EASETECH is focused on modelling of linear material and substance flows, but does not allow accounting of interactions between individual materials and substances nor the transformation of substances themselves. This interaction is needed in case of technologies involving conversion of substances and materials, and where flows and transformations are linked to the amount of specific materials entering a process. As such, there is a need for LCA modelling frameworks allowing constraints, non-linear relationships and new substances to be created as a result of biological and chemical reactions, while maintaining the overall mass, substance and energy balance of the model.

Black-box models can be defined as a combination of one or more single-operation unit processes aggregated into a fixed list of inputs (energy, materials and chemicals) and outputs (products, emissions and residues) with no direct relationship between inputs, outputs and process operations (EC-JRC 2010). The evolution from product LCA to process LCA has taken time seeing the process as black-box, thus limiting the analysis of unit processes within complex systems (Jacquemin et al. 2012). Recently, this challenge has been highlighted by Maes et al. (2015) who explained how black-box modelling approaches present considerable limitations to application of the EU renewable energy guidelines (European Parliament and the Council of the European Union 2009) when applied on complex production sites, mainly because black-box models cannot appropriately represent the individual unit processes and therefore do not identify the impacts associated with these unit processes. For resource conversion technologies such as biorefineries, this means that no specific links exist between the input feedstock composition, the subsequent transformation of feedstock properties occurring within the individual unit processes, and the final outputs and emissions from the biorefinery. This is in contrast to real processes in which all these aspects are directly interlinked. As such, the LCA models cannot account for potential changes in feedstock composition between case studies, nor for changes in performance of the involved unit processes. Limiting LCA models to fixed technology aggregations and inventory data, thereby significantly limits the applicability of the LCA model, but also reduces the transparency of the model and requires new inventory datasets to be developed for each case study.

To overcome the need for implementing inventory datasets according to the specific technological, geographical and temporal scope of an assessment, several approaches have been applied in literature: (a) relatively simple MFA methods for determination of material flow and emission partitioning within technologies and across a system of technologies (e.g. Mancini et al. 2015; Turner et al. 2016), and (b) more advanced process simulation tools (ASPEN 2019; ProSim 2019; ProMax 2019; CHEMCAD 2019) to evaluate individual biological, physical and chemical unit processes within a technology (e.g. Tumilar et al. 2016). While these approaches and tools certainly have merits, the definition of the technology inventories remains separated from the LCA modelling itself. A few studies (e.g. Arora et al. 2016; Brunet et al. 2012; Gaha et al. 2017) have attempted to combine LCA modelling with the process simulation tools mentioned above and/or with mathematical programming tools (e.g. MATLAB). While this potentially allows a more detailed process-oriented approach (as opposed to black-box datasets), these models are typically not integrated with the LCA tool and need to be run separately, often requiring specific insights in the programming itself (i.e. limited user-friendliness) (Asprion and Bortz 2018). While such integration is desirable, so far, we are not aware of tools that allow modelling of unit processes of complex technologies and concurrently performing a full LCA.

To further advance and facilitate LCA modelling of more complex and integrated resource management technologies and systems, LCA models should allow the establishment of quantitative relationships between input feedstock composition, unit processes, and subsequent outputs of products and emissions. This means "opening-up" the black-box models and allows the definition of useful relationships between inputs, outputs and process configurations. While subdivision of complex technologies into unit processes is supported by current LCA guidelines (EC-JRC 2010), such a modelling approach is here termed "process-oriented" LCA modelling. Modelling of residual resource technologies like biorefineries requires detailed data of the input material (e.g. water content, energy content), the transformations of materials or substances during processing, and the transition of mass from one flow to another. To enable transparent and flexible adjustment of the model to a specific case study, the involved model parameters should reflect subdivision in relevant unit processes (e.g. for a biorefinery: pre-treatment, hydrolysis, fermentation and distillation, separation and recovery of the solid and liquid fractions). In an integrated technology system with several flows associated to multiple product outputs, working with parameterised unit processes and input-output process relationships allows to change a specific production flow and have a non-linear response in other flows such as increasing or decreasing their production and associated emissions. Currently, no existing publically available LCA model offers such process-oriented modelling approach relevant for resource-centric technologies and systems, although some models enable interaction with external software to allow users some degree of taking these aspects into account.

The aim with this study is to advance LCA modelling of integrated technologies and technology systems targeting environmental assessment of resource management by implementing advanced "process-oriented" LCA modelling. The following specific objectives are addressed: (i) provide a framework for process-oriented LCA modelling of multi-output conversion technologies, (ii) define the needed operators and implement these in the software EASETECH, (iii) demonstrate the applicability of the modelling framework on a simplified biorefinery case study, focusing on global warming impacts in combination with the importance of feedstock characteristics and unit process parameters (e.g. conversion efficiency) under specific operating conditions, and finally on this basis (iv) evaluate the perspectives and implications of the proposed advanced process-oriented modelling approach. The outcome of the study represents the methodological basis for advanced mass, substance and energy balanced LCA modelling to resource technology systems in EASETECH.

2 Material and methods

2.1 Principles of process-oriented LCA modelling

The characterisation of the input feedstock into individual fractions, each with associated biochemical, physical, chemical and nutritional properties, is the point of departure of a process-oriented LCA. Subdividing a material flow according to properties enables modelling of the conversion (or "fate") of these properties within a specific process, technology or an entire system of several technologies, and linking the input feedstock to the associated outputs generated by the involved processes. These material properties thereby represent an extension of the substances used within MFA (Allesch and Brunner 2015; Brunner and Rechberger 2016), e.g. carbon is a chemical element and cellulose is a compound; both of them are properties of the biomass feedstock: the carbon content takes into consideration the carbon content of cellulose, representing a part of the total carbon in the biomass. Conversion of the input feedstock is associated with either transition or transformation of feedstock properties. Transition occurs when a specific amount of a material or fraction or substance (and thereby share of material properties), usually expressed in percentages, is transferred from an input to an output of a process. The transition within a process can be partial (less than 100% of a material flow is transferred) or total when the entire material flow is transferred. Transformation of the input feedstock material occurs when one or more fractions or one or more substances has a change in its composition within a process. Thus, some fractions/substances may cease to exist, while new ones may be introduced. Also, in this case, the transformation can be total, when a fraction or substance is entirely used in a transformation, or it can be partial when only a defined quantity of a selected substance/fraction is involved in the conversion process. Consequently, the original material prior to the transformation does not exist anymore because a different material is generated departing from it, however maintaining the overall mass, energy and substance balance of the process. Moreover, mass transition and transformation within a system are linked to environmental exchanges that subsequently are converted into environmental impacts. For example, in a process where mass and energy are given by the material conversion of the process itself, considering emission factors during the characterisation phase (after the inventory) allows emissions to be quantified according to the availability of the substance/mass/energy involved in different material flows within the considered unit process. In addition, in the process-oriented model, the technology is subdivided into individual unit processes. For each unit process, the (bio) physical processes governing the mass/energy/substance transition and transformation are identified and described by mathematical equations. These equations allow the establishment of relationships and interdependencies between the input feedstock material properties and the (unit) process outputs. Parameters can be applied to allow adjustments of material flows and process performance to specific cases. If a parameter is in an equation, it can directly affect its result, and thus the conversion process, the substance/mass/energy flow and the respective emission. Furthermore, the proposed framework allows for non-linear responses whereby changes in one flow can give a non-linear response in other flows.

Figure 1 illustrates the generic black-box vs process-oriented technology modelling: in the black-box modelling approach (Fig. 1a), the technology is described by an input and several outputs represented by $Input_1$, the products P_1, P_2, P_3 and the emission E_1.

Any relationships and interdependencies between the input feedstock material and the output products are not represented by the model. In addition, the technology is not subdivided into unit processes and relationships/interdependencies represented by equations containing parameters are not included. On the contrary, in the process-oriented modelling approach, the technology (Fig. 1b) is described through input feedstock material properties (e.g. In_1, In_2, In_3), relevant unit processes (process *A*, *B*, *C*, *D*), and relationships between input feedstock material properties and process outputs using equations with parameters. In Fig. 1b, the output product P_B is partially transferred to process C, i.e. P_B has an associated conversion efficiency (eff_1) in the transition from process B to C. ($1\text{-}eff_1$) represents what is left, i.e. residue, of P_B subsequently transferred to process D. An example of total transition is represented by the product P_C, totally transferred to process D together with the residues of process B. P_2 and P_3 are two products of process D generated through two equations ($P_2 = P_C * par_1/par_2$; $P_3 = Residues * par_3$). These equations are two examples of relationships between inputs and outputs within process D and par_1, par_2 and par_3 are the three associated parameters. As an example, Fig. 1c illustrates this modelling approach implemented on a second-generation biorefinery where the lignocellulosic input feedstock is converted into bioethanol, a solid and liquid fraction, and CO_2. The feedstock is characterised according to relevant biochemical, chemical, physical and nutritional properties (e.g. cellulose, proteins, carbon content, energy content, water content, digestibility, etc.). The overall biorefinery technology is represented by a range of unit processes: (1) pre-treatment, (2) hydrolysis, (3) fermentation and distillation and (4) recovery. In the entire biorefinery system, both transitions and transformations occur, and the relationships between the input feedstock properties and the output products are identified and described by appropriate equations involving adjustable parameters (e.g. conversion efficiency of C6 sugars, eff_{C6}, into ethanol production, thereby facilitating flexible adaption of the model from one case study to another). An example of material transformation is given by the hydrolysis, where polysaccharides, such as cellulose, pectin, hemicellulose, starch and sucrose, are converted into simple sugars with five and six carbon atoms (C5 and C6 sugars). While one substance (polysaccharides) thereby is transformed into another substance (monosaccharides) and thus cease to exist, the overall mass and substance balance of the technology is maintained and the flows are trackable. In the Electronic Supplementary Material (ESM) (Sections S2 to S6), these biorefinery unit processes are thoroughly described including the transformation equations used.

The process-oriented modelling approach allows users to establish models with all the necessary unit processes involved, to clearly define the feedstock conversion and to include appropriate modelling parameters and assumptions. This is useful particularly in studies that wish to base the assessment on pre-developed models reproducing specific technologies such as lignocellulosic biorefineries, but intend to apply case-specific process performance data and/or update the model to reflect assumptions more relevant for the case study in question.

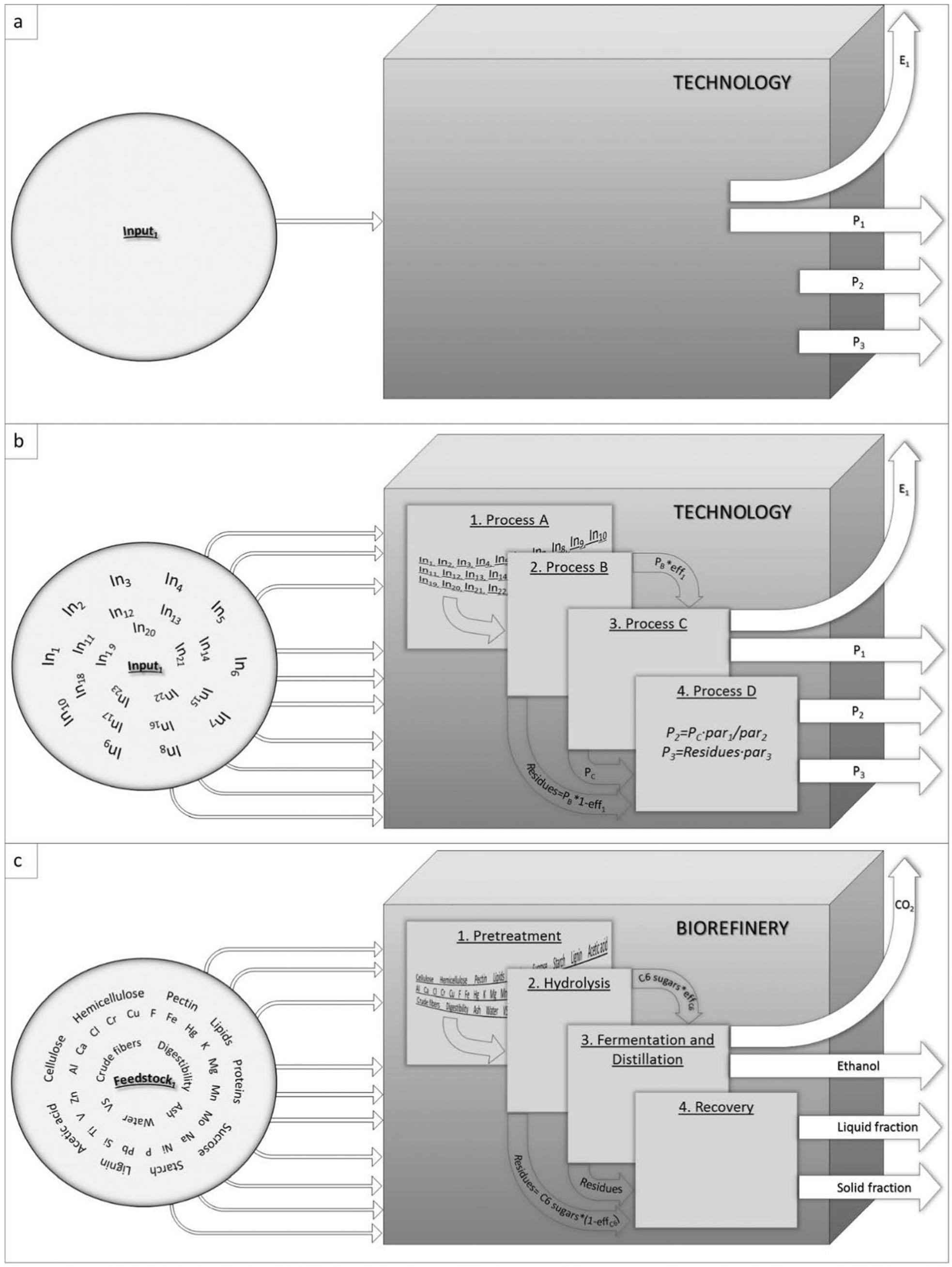


Fig. 1 **a** Black-box modelling approach applied to a generic technology; *Input₁* is the input process; P_1, P_2 and P_3 are the output products and E_1 is an example of technology emission. **b** Process-oriented approach applied to the same generic technology; same input, final output products and emission (i.e. $Input_1$, P_1, P_2, P_3, E_1); the input properties (e.g. In_1, In_2) are considered. In addition, relationships/interdependencies are established between the technology unit processes (i.e. *Process A*, *B*, *C, D*) and described with equations containing parameters (Eq. 1: $P_2 = P_{A2} \cdot par_1/par_2$ and Eq. 2: $P_3 = P_{B1} \cdot par_3$, with par_1, par_2 and par_3 as parameters). **c** Process-oriented approach applied to the case of a second-generation biorefinery. The unit processes considered are *pretreatment*, *hydrolysis*, *fermentation and distillation*, *recovery*. The input is $Feedstock_1$, having properties (e.g. cellulose, Ca). Relationships/interdependencies are described through equations with parameters; the final whole-system output products are *ethanol*, *liquid fraction* and *solid fraction*. CO_2 represents an example of emission

2.2 EASETECH modelling features supporting process-oriented modelling

To facilitate process-oriented LCA modelling in EASETECH, a range of new “operators” were developed following the principles of domain-specific language illustrated in Zarrin and Baumeister (2014). The new operators allow a domain expert (a person with the relevant technological and systemic expertise) to establish the relationships between input and output for the individual unit processes, described in the previous section. In EASETECH, LCA scenarios are characterised by a number of “process modules” that are connected with arrows indicating material flows between the processes (see Section 2.3 for further details). Process modules may represent individual unit processes or entire technologies and can be nested, i.e. a number of “unit-process modules” may be “packed” into another process module. As such, the scenario building in EASETECH follows the overall principles of MFA; for details, see Clavreul et al. (2014) and Allesch and Brunner (2015). These principles are also applied to the unit processes modelled involving the new operators and subsequently implemented into EASETECH. Table 1 provides an overview of all new operators, while the remainder of this section explains the key features of the operators. Further

Table 1 Operators available in EASETECH and their application for the modelling of processes within technologies and systems

Operator	Application
Material flow [MF]	MF transfers material from a source element to a target element. It is allowed using more than one MF from the same source element
Residue flow [RF]	RF transfers what is left in a source element (residue). It is allowed using only one RF from the same source element
Fraction distributor [FD]	FD extracts a fraction from a material
Fraction generator [FG]	FG generates a fraction in a material
Fraction hub [FH]	FH groups fractions from an input material
Fraction transformer [FT]	FT transforms a fraction into another one within a material. As a consequence, the previous fraction does not exist anymore
Material distributor [MD]	MD extracts a material
Composite transformer [CT]	CT groups more than one operator. It allows iterating a sequence of transformations and transitions
Primitive parameter	It generates a parameter (numeric or string)
Data table parameter	It generates a table of parameters; it may contain one or more data columns
Data column	It generates columns into a data table parameter; each column refers to a parameter
Material generator [MG]	MG generates a material that may contain one or more material fractions
Input	It contains all the initial inputs (starting point)
Output	It contains all the final outputs (ending point)
Substance distributor [SD]	SD extracts a substance within a fraction
Substance hub [SH]	SH groups substances from fractions
Substance transformer [ST]	ST transforms a substance into another one; consequently, the previous substance does not exist anymore
Substance generator [SG]	SG generates a substance

details describing the individual operators applied for the modelling of the biorefinery case study (see also Section 2.3) unit processes can be found in the ESM, Sections S2.7, S3.1, S4.1, S5.1 and S6.1.

The following three macro levels are considered in the model: materials, fractions and substances. Materials, following the MFA definition, contain both substances and goods. In this case, goods represent fractions, "entities" that share common characteristics, i.e. substances. As such, "grass", "branches" and "wood" may all represent fractions in a material called "garden waste", while substances represent chemical, nutritional, physical and biochemical properties (e.g. cellulose, proteins, lower heating value, methane potential, digestible energy). Some of the substances may be correlated, e.g. the energy content of a fraction is a function of the content of cellulose, proteins, etc. Physical, chemical, nutritional and biochemical properties are assigned to the substance level, although they are not necessarily substances as such (e.g. energy is not a substance, but it is modelled using the same operators as for substances).

For the individual process module, there is at least one input and one output. There are three possible input types: (i) an output from another process, (ii) a material consisting of several fractions or (iii) a single fraction. The anaerobic digestion of organic waste is an example of the first case; it generates biogas and digestate as final outputs: the digestate may then be used as input to a subsequent fertilisation process. For the second case, e.g. a material (e.g. garden waste) with multiple fractions (e.g. grass, wood), the operator that generates the input feedstock material is *material generator* (MG); then, a *fraction generation* (FG) is needed for generating each fraction within the input material. Thus, we are generating the material composition. The last case, when the input is a single fraction (e.g. grass), only an FG is applied to generate the fraction. Lastly, a *substance generator* (SG) is used to specify each input material property, i.e. chemical, biochemical, physical and nutritional. Each of these properties is modelled as substances within a fraction. A range of physico-chemical relationships, represented by mathematical equations, are applied when a substance or a fraction is "transformed" within a process, e.g. one or more substances are converted into a specific product (e.g. glucose to ethanol) that may be the final output of a process or an intermediated product subsequently used in another conversion flow. The following operators are used for this purpose: *substance transformer* (ST) and *fraction transformer* (FT) when the transformation is related to a substance and a fraction, respectively. With these operators, a selected substance or fraction involved in the conversion process can be specified not to exist anymore while another substance or fraction is generated in its place, i.e. transformation from one entity into another. However, a transformation may also represent a modification of the substance or fraction content by changing only its amount while still preserving the substance or fraction itself. It is possible to change the content of a substance: the substance is the same and its amount is different (e.g. decreasing the water content of 50% of the original value).

Furthermore, each material/fraction/substance within a system or a technology may be transferred from one process to another, i.e. interprocess transition, or within a single process from inputs to outputs, i.e. intra-process transition. The interprocess transition represents cases when a process output is transferred to a subsequent process input, e.g. when sugars produced during hydrolysis are used in fermentation to generate ethanol and CO_2; thus, the transition is from hydrolysis to fermentation. The intra-process transition is when specific properties are involved in the generation of process outputs, e.g. when in hydrolysis, cellulose is depolymerised into C6 sugars and this transition occurs from the hydrolysis input to the hydrolysis output. The carbon content of cellulose (here classified as a substance) contributes to the generation of C6 sugars (classified as substance). To model these two types of transitions, one needs to be able to separate and "extract" a single material/fraction/substance from the remaining materials/fractions/substances. Extracting means isolating the material/fraction/substance and considering it as a single independent element to be subsequently used in other conversion flows. Operators that allow this extraction are *material distributor* (MD), *fraction distributor* (FD) and *substance distributor* (SD). Considering the example of garden waste, an FD may be applied in the example where only grass (a fraction within garden waste) is addressed in a specific (unit) process. Thus, grass may be extracted from the other fractions composing the garden waste and routed to a different flow for modelling purposes. An example of using SD is the separation of non-biodegradable matter such as lignin within an organic feedstock. With SD, the lignin representing a feedstock's biochemical property may be extracted and routed to a combustion process for energy utilisation. In cases when more than one fraction or substance are routed to a new flow, these fractions and substances need to be grouped: a *fraction hub* (FH) is used for grouping fractions while a *substance hub* (SH) is for substances. *Material flows* (MF) are represented by an arrow and are used for the transition of materials, fractions and substances from a source element to a target element. Within a process, conditional statements can be associated with individual MFs, e.g. water content > 0, to ensure a flow continues as long as the given condition is true. A *residue flow* (RF) is applied to close mass balances, i.e. to "catch" and transfer any remaining mass (residues) after transformation operations. Also, RF is represented by an arrow and is used for transitions. While it is possible to have more than one MF from a source element (e.g. an operator), only one RF can be used to close the mass balance. If the residues are transferred to a target element within the process, no other residue exists.

In addition to the above-mentioned methods to transform, divide and group materials, fractions and substances, a range of calculations may be done on these entities by a *composite transformer* (CT). In a CT, calculations may be grouped and if necessary combined with more operators relevant for the material, fraction or substance "level" in question. These calculations are performed using mathematical equations with parameters. *Primitive* parameters represent single values, such as a constant (e.g. conversion efficiency of C6 sugars, $eff_{C6} = 88\%$). *Data table parameter* is used when an element has more than one parameter associated. Each column of the data table represents a parameter, i.e. the values are elements in the table, and each row is a set of parameters. The data table is identified by a name. In order to build this table, columns need to be added for each parameter; this can be done with a *data column* (DC). For each parameter (column), the value type is specified (i.e. a number or string). For example, we model cellulose that has as a parameter mass in kilogrammes and conversion efficiency into sugars in percentage; since it has two parameters associated, we may have a data table parameter with three data columns, one for cellulose (substance), and a further two for the mass and the conversion efficiency. A process finishes with one or more outputs having all properties generated during the process modelling. This involves using one/more *output*(s) representing all the material properties transferred to it/them through MFs and/or RFs.

An example of a combination of more than one operator described in this section is presented in Fig. 2. This represents an illustrative example removing 10% of water (substance) from the grass (fraction) in garden waste (material). A way to accomplish this is first to define and generate the material garden waste through an MG; secondly, the generation of fractions within it, such as grass, wood, plants, branches, tree, and soil, stones and foreign objects, through FGs; thirdly, all these fractions are grouped in an FD, linked to a CT where the substances associated with each fraction are generated through SGs. Subsequently, the grass is extracted through an FD and the other fractions within the garden waste are sent to the final output through an RF. All the substances within grass are grouped in an SH. Water is extracted through an SD and its content is transformed (i.e. − 10%) in an ST. In the final output, water with the different content is sent through an MF linking ST with the final output. Additionally, the other substances (with the same content) are sent to the final output through an RF from SH.

2.3 Application of the process-oriented modelling approach to a biorefinery case

2.3.1 Description of the technology system

The case study evaluates a second-generation biorefinery using the above-mentioned operators within EASETECH. The biorefinery is composed of five main unit processes: *biomaterial generation*, *pre-treatment*, *hydrolysis*, *fermentation*

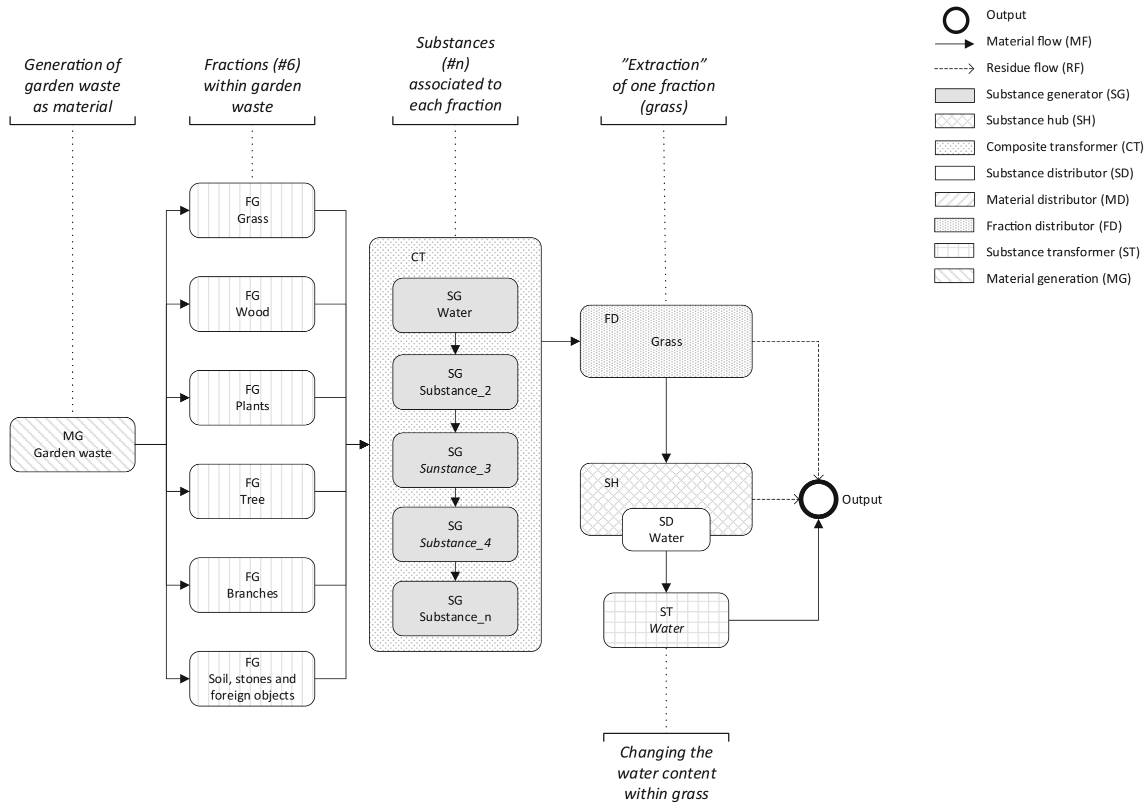


Fig. 2 Example of an application of operators for decreasing the water content (substance) of the grass (fraction) within garden waste (material)

and *distillation*, *recovery*. In biomaterial generation, the input feedstock is modelled considering all its properties (substances), such as biochemical (organic matter content), elemental (inorganic matter content), nutritional (i.e. the "feeding value" calculated based on the feedstock nutritional-energy content) and physical (e.g. water, ash, etc.), see Electronic Supplementary Material, Section S2 for details. For modelling purposes, biomaterial generation is considered as a process, although this does not represent the conversion of the feedstock but merely the relevant calculations of feedstock properties prior to the input to the pre-treatment process. Some properties (e.g. dry matter, nitrogen, oxygen, hydrogen, carbon, sulphur, energy content, methane potential, etc.) are stoichiometrically calculated based on the biochemical and physical contents of the feedstock; as such, these properties are correlated to other properties (Eq. S1 to S15, Electronic Supplementary Material – ESM). In the biomaterial generation, mathematical equations then recalculate some of the properties of the selected feedstock, with the advantage of correlating them (e.g. C with LHV, N with proteins, cellulose/hemicellulose/proteins/etc. with nutritional value and LHV). All the mathematical equations used in the biomaterial composition are explained in the ESM, Sections S2.1 to S2.6. In pre-treatment (Section S2 - ESM), energy in the form of heat is used to pre-treat the feedstock. The structure of the lignocelluloses is broken down to separate the lignin from the cellulose and hemicellulose and allow an efficient conversion into fermentable sugars. Pre-treatment may also result in some losses (e.g. when eventual mass is lost, the conversion efficiency to the pre-treatment output composition is lower than 100%) not routed further to the hydrolysis process. In hydrolysis (Section S4 - ESM), cellulose, starch, hemicellulose, pectin and sucrose are hydrolysed into C5 and C6 sugars. The non-hydrolysed biochemical properties represent the hydrolysis residues. In fermentation and distillation (Section S5 - ESM), the C5 and C6 sugars are converted to bioethanol, CO_2 and liquid molasses. The unconverted sugars are transferred to yet another output and passed on to a recovery process (Section S6 - ESM), which in addition to the fermentation residues receives the mixed solid and liquid residues from hydrolysis (hydrolysis residues); here, all residues are separated to maximise further utilisation.

Regarding the further utilisation of these output products, the liquid fraction was assumed to be converted into biogas, while the solid fraction was assumed to be incinerated with energy recovery. For both fractions, natural gas was assumed to be substituted for simplicity. In order to focus on the technology system modelling, we deliberately neglected the possible impacts from diverting the feedstock from its current use(s) and eventual land-use changes. This should be kept in mind when interpreting the results to avoid inconsistent und unfair comparisons with other studies. We briefly stress the importance of these aspects in Section 4.3.

2.3.2 Assessment scope, functional unit and system boundary

The primary goal with the LCA was to demonstrate the applicability of process-oriented modelling in EASETECH and illustrate potential learnings that can be achieved on this basis. In this perspective, the assessment focus was placed on a single biorefinery scenario without the range of scenario alternatives and sensitivity/uncertainty evaluations otherwise part of an LCA (see Negro et al. 2017; Serra et al. 2017; Wang et al. 2016). As such, the case study followed the principles of the relevant ISO standards (ISO 2006a, b), while not strictly complying with these. Two perspectives were evaluated with the case study: (i) the importance of unit process performance and choice of process parameters for the overall results, and (ii) the importance of feedstock characteristics for the performance of the individual unit processes at fixed parameter sets. For the first perspective, three types of input feedstock were considered: wheat straw, beet top and wild grass, while the second perspective was proved based on *Miscanthus*, brewer's grains and willow. The first set of biomasses was selected based on their different composition to test the biorefinery model and the expected different results. Table 2 presents key characteristics and properties. The second set of biomasses was selected according to their cellulose, hemicellulose and lignin content. These three organic molecules have high importance for the carbon pool available in the biorefinery; *Miscanthus* has the highest cellulose content, brewer's grain has the highest hemicellulose content and willow has the highest lignin one.

The functional unit represented "the valorisation within a biorefinery of one tonne (wet weight) of input-feedstock into three main output-products: bioethanol, solid, and a liquid fraction". While results were calculated for all the impact categories included in the IPCC 2013 method (IPCC 2013; 100-year time horizon was assumed), only results for global warming were discussed for the purpose of illustrating the functionality and applicability of the process-oriented modelling approach. Figure 3 illustrates a generic representation of the biorefinery process-oriented model.

To ensure simplicity, a "zero burden" approach was followed and no upstream burdens associated with the input feedstock biomass nor any indirect effects associated with the diversion from alternative uses of the biomass (counterfactual scenarios) were included. System expansion was applied to credit the system for avoided impacts associated with substituting and displacing conventional market products with the biorefinery output products. Ethanol was assumed to be used in vehicles, substituting gasoline; molasses, the liquid fraction from the biorefinery, was used in a biogas plant substituting the production and combustion of natural gas; solid biofuel, the solid fraction from the biorefinery, was used in an incineration plant that substituted the production and combustion of natural gas. The emission factor assumed for gasoline was 0.097 kg CO_2-eq MJ^{-1} and the emission factor for natural gas was 0.067 kg CO_2-eq MJ^{-1} from EASETECH database (Clavreul et al. 2014). The residual digestate after biogas production was assumed to displace conventional NPK fertilisers, according to the content of N, P and K. The substitution efficiency was assumed to be 40% for N according to current Danish legislation (Danish Ministry of Food, Agriculture and Fisheries 2018) and 100% for P and K. Air and water emissions arising from digestate and mineral fertilisers (avoided) spreading on-land were based on the work of Yoshida et al. (2016); particularly, the emission factors used to describe N_2O emissions from digestate and substituted mineral fertilisers were 2.78% and (2.32 × 0.40)%, respectively. The system boundaries included refinery operations, harvest of biomass, transportation (digestate and solid fraction) as well as final utilisation and management of all biorefinery outputs.

3 Results

3.1 Importance of unit process operational efficiencies

Figure 4 presents the results of global warming (GW) in kg CO_2-eq t^{-1}_{ww} for a biorefinery using wheat straw as feedstock. The biorefinery outputs are given in MJ t^{-1}_{ww} as a function of the efficiencies of the hydrolysis (Fig. 4a, b) and the fermentation (Fig. 4c, d) unit processes. Through the selection of parameters (e.g. yield, efficiencies, etc.), the model responds to variations in the performance of the individual unit processes and allows users to adapt a specific biorefinery configuration. Here, the environmental impacts of the entire technology systems were calculated by one-at-a-time changes in parameter values, from a low conversion efficiency (25%) to a complete conversion (100%). For example, for fermentation of C5 sugars, only the fermentation efficiency was changed with all other parameters unchanged; the parameter values (0%, 25%, 50%, 75% and 100%) were selected for illustrative purposes.

As the results demonstrate, process parameters play an important role: the user can modify the mass and energy balances (here represented by the process outputs) with a direct effect on the associated environmental impacts (here represented by GW). In this example, increased efficiency of cellulose hydrolysis leads to better GW performance (Fig. 4b); this is reflected by the increased production of liquid fuel (ethanol) and the decreased production of solid fraction (sometimes called solid biofuel) resulting in the decreased substitution of natural gas combustion. In addition, increasing the fermentation efficiency of C6 sugars leads to better GW performance (Fig. 4d); also in this case, fuel production was increased, but now the liquid fraction (sometimes called molasses)

Table 2 Characteristics and properties of wheat straw (feedstock 1), wild grass (feedstock 2) and beet top (feedstock 3), used as feedstock for the biorefinery case study

Bio_material_generation—parameters						
Subgroup 1	Biochemical properties	Description	Feedstock 1	Feedstock 2	Feedstock 3	Unit
1	Acetic acid*	CH3COOH	0.0	0.0	0.0	$\%_{DM}$
2	Cellulose	Cellulose parameter	34.7	29.1	11.2	$\%_{DM}$
3	Hemicellulose	Hemicellulose parameter	22.4	24.2	16.2	$\%_{DM}$
4	Lignin	Lignin parameter	17.7	3.0	8.2	$\%_{DM}$
5	Lipids	Lipids parameter	2.3	0.5	2.4	$\%_{DM}$
6	Pectin	Pectin parameter	0.0	0.0	8.2	$\%_{DM}$
7	Proteins	Proteins parameter	3.5	5.2	16.9	$\%_{DM}$
8	Starch	Starch parameter	0.0	0.0	3.6	$\%_{DM}$
9	Sucrose	Sucrose parameter	0.0	0.0	11.9	$\%_{DM}$
10	Other VS	Unspecified VS parameter	14.07	33.86	4.9	$\%_{DM}$
Subgroup 2	Elemental properties					
11	Al	Aluminium	0.0168	0.0000	0.0000	$\%_{DM}$
12	Ca	Calcium	0.2435	0.5500	1.3000	$\%_{DM}$
13	Cl	Chlorine	0.3876	0.8000	1.6000	$\%_{DM}$
14	Cr	Chromium	0.0003	0.0000	0.0000	$\%_{DM}$
15	Cu	Copper	0.0004	0.0007	0.0013	$\%_{DM}$
16	F	Fluorine	0.0011	0.0000	0.0000	$\%_{DM}$
17	Fe	Iron	0.0134	0.0220	0.0000	$\%_{DM}$
18	Hg	Mercury	0.0000	0.0000	0.0000	$\%_{DM}$
19	K	Potassium	0.9870	0.3300	4.8000	$\%_{DM}$
20	Mg	Magnesium	0.0439	0.1800	0.4100	$\%_{DM}$
21	Mn	Manganese	0.0020	0.0070	0.0090	$\%_{DM}$
22	Mo	Molybdenum	0.0001	0.0000	0.0000	$\%_{DM}$
23	Na	Sodium	0.0100	0.1500	0.9700	$\%_{DM}$
24	Ni	Nickel	0.0001	0.0000	0.0000	$\%_{DM}$
25	P	Phosphorus	0.0490	0.4000	0.1750	$\%_{DM}$
26	Pb	Lead	0.0003	0.0000	0.0000	$\%_{DM}$
27	S	Sulphur	0.0000	0.2100	0.2000	$\%_{DM}$
28	Si	Silicon	0.9300	0.0000	0.0000	$\%_{DM}$
29	Ti	Titanium	0.0005	0.0000	0.0000	$\%_{DM}$
30	V	Vanadium	0.0001	0.0000	0.0000	$\%_{DM}$
31	Zn	Zinc	0.0034	0.0000	0.0045	$\%_{DM}$
Subgroup 3	Feedstock					
32	Fraction name	Fraction	Wheat straw	Wild grass	Beet top	String
Subgroup 4	Feedstock amount					
33	Quantity	Input amount	1000	1000	1000	kg_{ww}
Subgroup 5	Nutritional properties					
34	Crude_Fibers_input	Crude fibres parameter	45.3	78	82	$\%_{DM}$
35	Digestibility_input	Substrate digestibility	44	24.9	12	$\%_{DM}$
Subgroup 6	Physical properties					
37	Ash	Ash parameter	5.4	4.1	16.5	$\%_{DM}$
38	VS	Volatile solid parameter	94.7	95.9	83.5	$\%_{DM}$
39	Water	Water parameter	12.2	78.8	76.7	$\%_{ww}$

*Acetic acid may be present in some biomasses as degradation product

decreased, thereby resulting in lower biogas production and lower substitution of natural gas combustion. In Fig. 4, for a cellulose hydrolysis efficiency of 0% the associated GW performance was − 269 kg CO_2-eq t_{ww}^{-1}; for an efficiency of 25%, the associated GW performance was − 339 kg CO_2-eq t_{ww}^{-1}; for an efficiency of 50%, the associated GW performance equalled − 409 kg CO_2-eq t_{ww}^{-1}; for 75%, it was − 479 kg CO_2-eq t_{ww}^{-1} and for 100%, it was − 549 kg CO_2-eq t_{ww}^{-1}. Such direct proportionality between the energy/mass balances and the GW impacts may not necessarily have a direct effect on full scenario results as also framework conditions may be important, e.g. type of substituted energy, system boundaries and process configurations. Furthermore, the linear results are due to the equations applied in the case example, the model could just as well have been used for cases with exponential changes, or more scattered results if conditions for flow properties were applied in the model. These aspects can, however, be captured by the process-oriented LCA model either by adjusting parameters, changing the mathematical relationships involving the functions introduced earlier, or choice of background process data and interactions with the background system. For further details of the biorefinery modelling results involving variations in parameter efficiencies and associated GW impacts, please see ESM, Section S7, Table S7.1, S7.2 and S7.3.

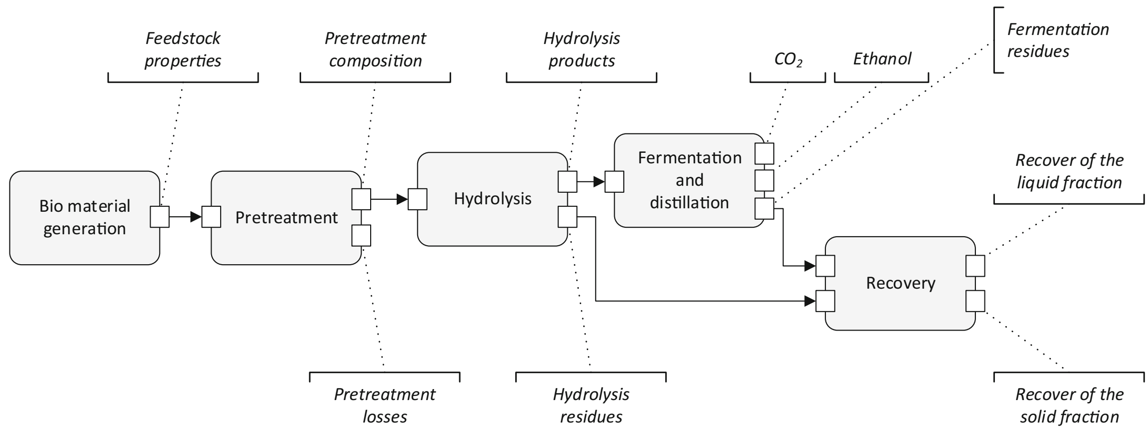


Fig. 3 Generic representation of the biorefinery process-oriented model in EASETECH with the intermediate and final outputs

Overall, similar results and trends were obtained for the two other feedstock types, beet top and wild grass, i.e. higher efficiencies provided larger environmental savings (see ESM, Section S8, Fig. S8.1 and S8.2 for the results). Differences in biochemical and physical properties between wheat straw, beet top and wild grass were reflected in the results by different "levels". With a cellulose hydrolysis efficiency of 0%, the associated GW performance for beet top was − 55 kg CO_2-eq t_{ww}^{-1} and for wild grass − 37 kg CO_2-eq t_{ww}^{-1}; for an efficiency of 25%, the associated GW performance for beet top was − 61 kg CO_2-eq t_{ww}^{-1} and for wild grass − 51 kg CO_2-eq t_{ww}^{-1}; for an efficiency of 50%, the associated GW potential was respectively − 67 and − 65 kg CO_2-eq t_{ww}^{-1}, while for 75%, it was − 73 and − 79 kg CO_2-eq t_{ww}^{-1}, and − 79 and − 93 kg CO_2-eq t_{ww}^{-1} in the case of 100%. While a similar trend in results can be expected, the model demonstrates the relative importance of the hydrolysis and fermentation steps for the three different feedstocks and thereby transparently explains the difference in results between the cases. This demonstrates that the model can be applied to technology cases with different process configurations (illustrated here by different efficiencies of unit processes and subsequent changes in material and substance flows) and can accommodate different input feedstock properties in a flexible manner.

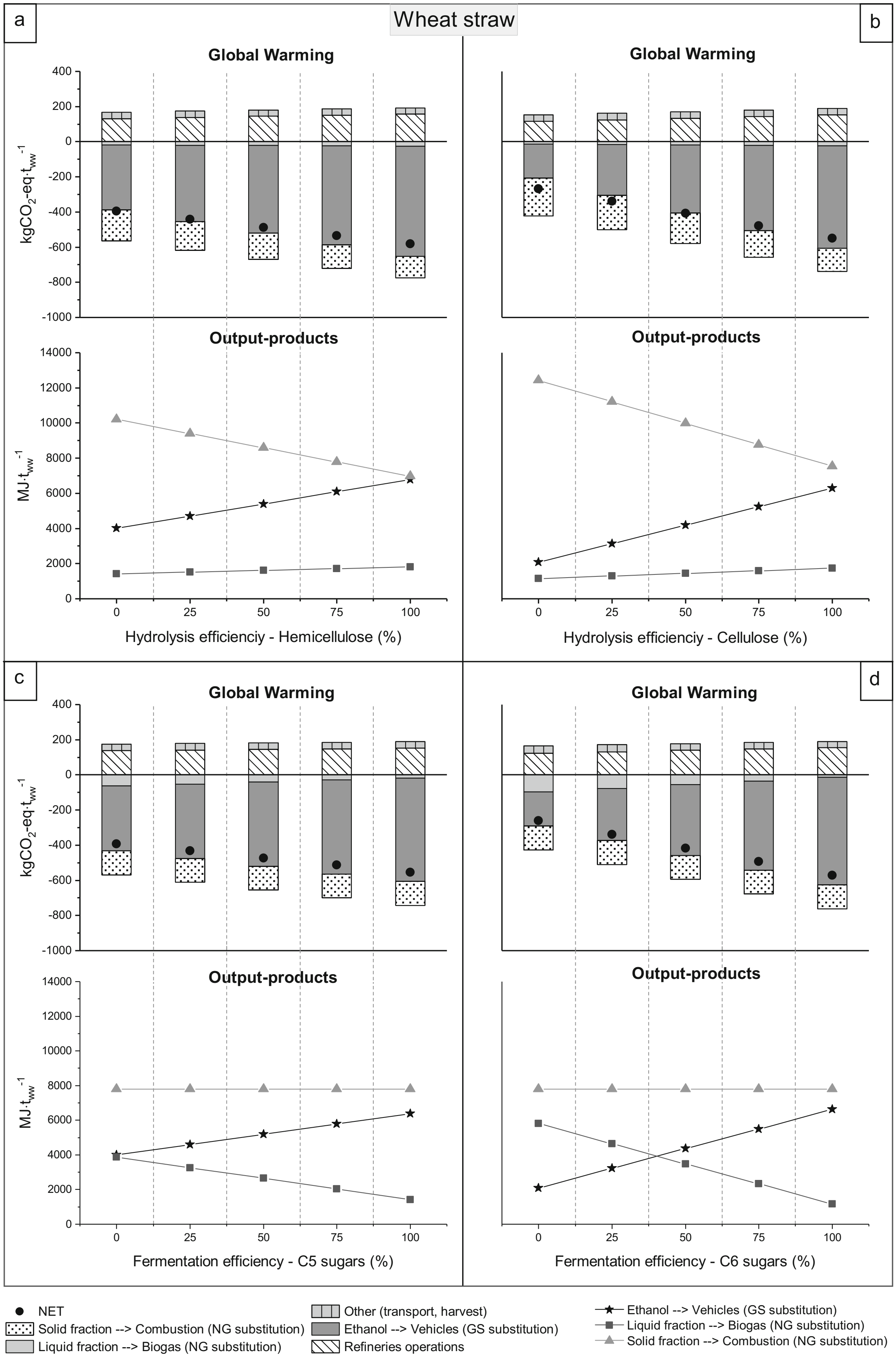
3.2 Importance of input feedstock characteristics

The feedstock characteristics play an important role for the biorefinery performance, both with respect to GW (kg CO_2-eq t_{ww}^{-1}) and output products (e.g. MJ·t_{ww}^{-1}) as illustrated in Fig. 5.

Among the three biomasses addressed here, *Miscanthus* has the highest cellulose content (CE = 47.6%$_{DM}$), brewer's grain has the highest hemicellulose content (HC = 29.5%$_{DM}$) and willow the highest lignin content (LG = 31.6%$_{DM}$). In Electronic Supplementary Material, Section S9, Tab S9.1 presents key characteristics and properties of these three biomasses. The cellulose, hemicellulose and lignin contents for these three biomasses are shown in Fig. 5. The conversion efficiencies considered were 95% and 75% for cellulose and hemicellulose respectively during hydrolysis, and for both C5 and C6 sugars, it was 88% during fermentation and distillation.

Considering the three main products of the biorefinery (ethanol, solid and liquid fraction), cellulose and hemicellulose affect mostly the production of ethanol and the liquid fraction as these molecules can be hydrolysed into chains of monosaccharides (e.g. glucose) used in the fermentation to produce ethanol and CO_2. Lignin represents the carbon pool that in a biorefinery leads to the formation of the solid fraction output unless pre-treatment is applied, together with non-hydrolysed material. With this in mind, based on the composition of the three feedstocks, *Miscanthus* generated more ethanol (7400 MJ·t_{ww}^{-1}), followed by willow (3500 MJ·t_{ww}^{-1}) and brewer's grain (1400 MJ·t_{ww}^{-1}). Considering the solid fraction, although willow has the highest lignin content, *Miscanthus* provided the largest solid fraction (7200 MJ·t_{ww}^{-1}), due to the larger amounts of unconverted sugars (dry basis). The liquid fraction is influenced mainly by the fermentation and distillation process. For this reason, *Miscanthus* provided the highest liquid output (1600 MJ·t_{ww}^{-1}) followed by brewer's grain (1000 MJ·t_{ww}^{-1}) and willow (960 MJ·t_{ww}^{-1}). In this illustrative example, the conversion of all three biomasses provided net GW savings as no upstream activities (e.g. production) and indirect effects (e.g. land-use changes) were included. The largest savings were obtained from *Miscanthus* due to its higher dry matter content. These results were in accordance with Parajuli at al. (2017), who showed that the high dry matter and energy yield of the input feedstock material can contribute to a better environmental performance. In addition, the relevance of conversion efficiencies of feedstock properties (e.g. carbohydrates) in the biorefinery processes was highlighted in Parajuli et al. (2017), in agreement with this study.

While the influence of feedstock choice on the LCA results has been evaluated previously in the literature (e.g. Bernstad


Wheat straw
a
b
c
d
Global Warming
Output-products
kgCO2-eq·t_ww^-1
MJ·t_ww^-1
400
200
0
-200
-400
-600
-800
-1000
14000
12000
10000
8000
6000
4000
2000
0
0
25
50
75
100
Hydrolysis efficienciy - Hemicellulose (%)
Hydrolysis efficienciy - Cellulose (%)
Fermentation efficiency - C5 sugars (%)
Fermentation efficiency - C6 sugars (%)
NET
Solid fraction --> Combustion (NG substitution)
Liquid fraction --> Biogas (NG substitution)
Other (transport, harvest)
Ethanol --> Vehicles (GS substitution)
Refineries operations
Ethanol --> Vehicles (GS substitution)
Liquid fraction --> Biogas (NG substitution)
Solid fraction --> Combustion (NG substitution)

◀ **Fig. 4** An overview of the process-oriented LCA model response, in terms of global warming, GW, (kg CO_2-eq kg_{ww}^{-1}) and mass/energy balance (MJ t_{ww}^{-1}), to (one-at-the-time) unit process performance variations (i.e. 0%, 25%; 50%; 75%; 100%). **a** Hemicellulose conversion efficiency in hydrolysis. **b** Cellulose conversion efficiency in hydrolysis. **c** C5 sugars conversion efficiency in fermentation. **d** C6 sugars conversion efficiency in fermentation. The feedstock considered is wheat straw. NG, natural gas; GS, gasoline

Saraiva 2017; Tonini et al. 2016a, b), the above process-oriented assessment approach demonstrates the added insight of the importance of individual unit processes (and potentially also parameter choices as illustrated in the previous section). Particularly, the inter- and intra-process transition, the material transformation due to the process specificities and the feedstock specificities (e.g. the importance of feedstock properties and their availability to be degraded or converted into different products), and their consequences in terms of environmental impacts.

4 Discussion

4.1 Novel insights from process-oriented modelling

The process-oriented approach focuses on the evaluation of process relationships through subdivisions of technologies into unit processes and appropriate linking of process material inputs with transformation and process outputs. In previous literature (e.g. Tonini et al. 2016a, b), these aspects have been demonstrated as critical for the LCA results and interpretation,

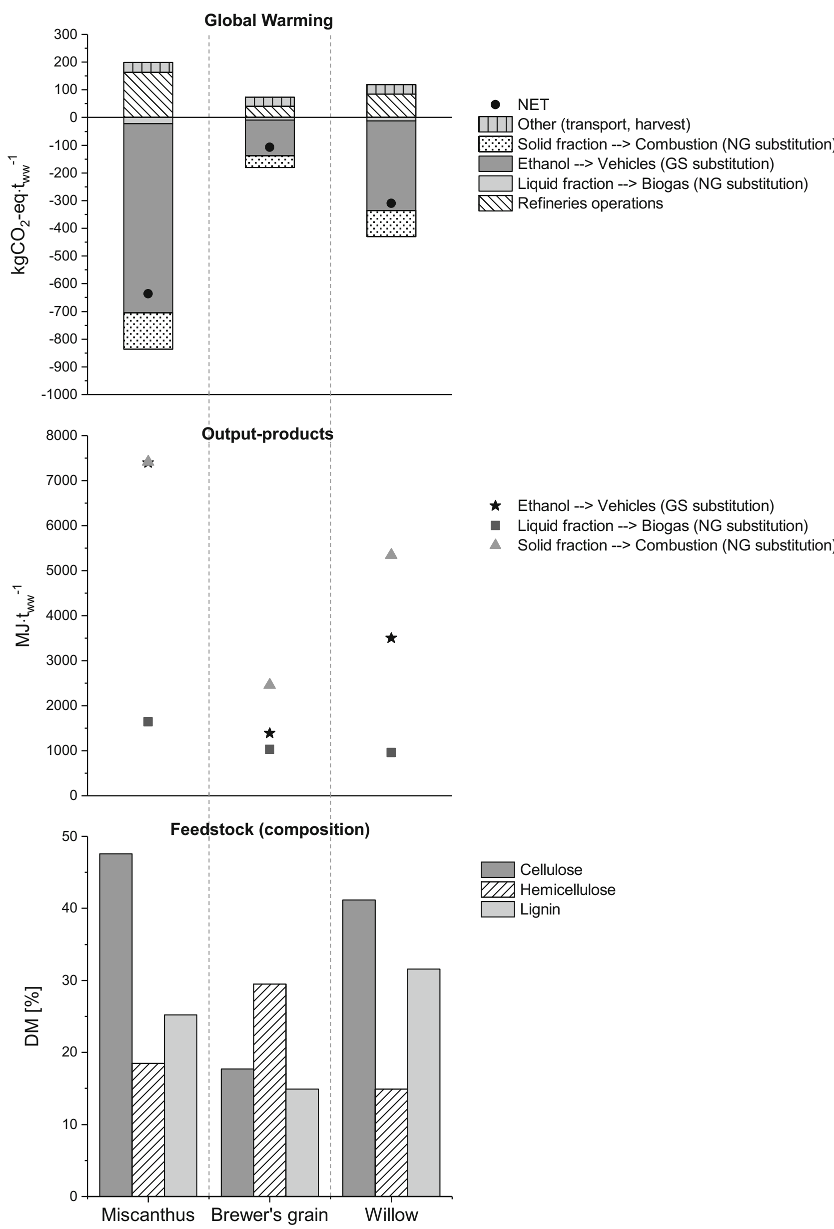


Fig. 5 Process-oriented LCA model response, in terms of global warming, GW, (kg CO_2-eq kg_{ww}^{-1}) and mass/energy balance (MJ t_{ww}^{-1}), to three different feedstocks (i.e. *Miscanthus*, brewer's grain and willow) having different shares of cellulose, hemicellulose and lignin. NG, natural gas; GS, gasoline. For these three biomasses, the values of the parameters used are in hydrolysis, a cellulose and a hemicellulose conversion efficiency of 95% and 75% respectively, and in fermentation and distillation, the conversion efficiency of 88% for both C5 and C6 sugars

in particular in relation to integrated technologies such as biorefineries where the feedstock characteristics and the biorefinery outputs are interdependent and further affect the downstream substitutions (e.g. energy, feed, materials). One of the most notable advantages of the process-oriented modelling approach is the possibility of implementing new (unit) processes by using operators in a single modelling tool such as EASETECH, rather than requiring a combination of several tools as illustrated by previous literature (e.g. in Tonini et al. 2016a, b, and Vadenbo et al. 2018, where a combination of Matlab, Gams, and SimaPro was applied).

Mathematical equations describing the input-output relationships are integrated within the model itself and default parameter values can be further adjusted by the users. The subdivision into unit processes is important for identification, quantification and evaluation of intermediate process outputs within the system. Further, the process parameters and associated mathematical relationships themselves may be selected to appropriately represent operational parameters that can be recognised by users and more easily adjusted to accommodate specific case studies and industry data. Quantification of the intermediate products linking individual unit processes allows evaluation of the environmental performance of these unit processes, which may further allow identification of technology hotspots at a much more detailed level than traditional "black-box" modelling approaches, both in terms of production and emissions. This is fully in line with existing recommendations, e.g. by ILCD guidelines (EC-JRC 2010) and strongly highlighted in Jacquemin et al. (2012).

The process-oriented modelling approach enables more control of the material, energy and substance flows within the analysed technologies. This is particularly important in relation to integrated technologies such as biorefineries or many waste technologies for which intermediate products affect the subsequent processing; an aspect that black-box approaches cannot capture (Maes et al. 2015). Modelling a biorefinery technology within EASETECH following the process-oriented approach offers an "active" material flow system represented by the established input-output relationships and parameters. This material flow system is linked to environmental emissions and output product substitutions associated with the LCA scenarios; thereby a direct link between input feedstock composition, process operation and environmental performance is established. For example, higher hydrolysis and fermentation efficiencies incur larger ethanol production with lower solid and liquid residue quantities, thereby increasing gasoline substitution and lowering natural gas substitution. Although purposely kept simple in this illustrative case study, interactions between the foreground and background systems can be easily modelled with appropriate selection of parameters. The conversion of biochemical properties of the feedstock into the biorefinery products depends on the type of feedstock and its degradability under the specific operating conditions of the technology. All such aspects can be addressed and evaluated by the proposed process-oriented modelling approach.

4.2 Implications for LCA

Subdividing the technology into relevant unit processes and establishing appropriate input-output relationships including operating parameter variations allow a direct response of the LCA model with respect to potential environmental impacts. While subdivision into smaller units has been suggested in previous literature, this has mainly been discussed from the perspective of Maes et al. (2015) rather than with the intention of Götze et al. (2014) and Papadokonstantakis et al. (2016) as suggested here for the process-oriented approach. Only few studies have discussed the potential of establishing operational relationships and more "technology relevant" parameters (e.g. Portha et al. 2010; Kikuchi et al. 2014). As previously indicated, the ability to "track" intermediates and conversion of individual input material fractions is essential for LCA modelling of multi-output technologies (e.g. Astrup et al. 2018), although relatively few LCA studies take this aspect seriously. With a black-box approach, where unit processes may be combined even if they are physically separated, relevant disaggregation of the environmental impacts associated with individual outputs may not be possible (e.g. Jacquemin et al. 2012). As the process-oriented modelling approach attempts to disaggregate technology and process elements into individual units reflecting the actual process flow and conversion steps, the process-oriented approach can facilitate easier compliance with the recommendations provided by current ISO standards and ILCD guidelines with respect to multi-functionality. In the case of LCA modelling of material and resource technology systems, we suggest that the process-oriented approach is a needed development from black-box approaches and that these cannot be considered state-of-the-art for such systems. We envision that further development of process-oriented inventories may offer a route to avoid the current challenges of multi-functionality associated with complex multi-output technologies.

LCA studies are also sometimes used to assess the environmental performance of technologies prior to commercialisation and full-scale implementation, e.g. prospective assessment of emerging technologies (Arvidsson et al. 2017). From a black-box modelling perspective, such assessments pose specific challenges with respect to data uncertainties, process configurations, potential performance improvements, etc. as these aspects are typically aggregated within the technology inventory thereby limiting transparency. Process-oriented modelling, on the other hand, allows disaggregation and establishment of appropriate data relationships. Thereby, the uncertainties and importance of individual process parameters may be evaluated directly and linked to the environmental performance of the technology in question. This makes process-oriented modelling particularly relevant for LCA assisted technology developments and upscaling activities, as the assessment results allow identification of process hotspots that may otherwise remain un-evaluated. We envision that these aspects are particularly important in relation to integrated and multi-output technologies as part of circular (bio) economy initiatives.

4.3 Further research and perspectives

As developed and implemented in this study, the process-oriented modelling approach represents a first attempt to demonstrate applicability and potential. Future research is intended to focus on improving the existing model and extending the process-oriented modelling approach to a wide range of material-centric technologies, e.g. anaerobic digestion, thermal pyrolysis and gasification, thermal combustion, and biomaterial production facilities. This requires identification and appropriate implementation of relevant process relationships between input resources and materials (e.g. chemicals, energy, etc.) and process outputs and emissions. While EASETECH offers a unique basis for this as the modelling is already based on material flows, implementation of new process-oriented technology models nevertheless requires considerable effort (see Electronic Supplementary Material as an example for a biorefinery). However, once a process-oriented model is established, subsequent adjustments can be achieved simply by changing the appropriate parameters (assuming the fundamental process configuration remains appropriate). As mentioned earlier (Section 2.3.1), to focus on the technology modelling, we deliberately excluded the upstream impacts associated with diverting the feedstock from its current use(s) or with land-use changes. Such impacts have been earlier estimated in the order of 19–88 kg CO_2-eq t_{ww}^{-1} for wild grass and wheat straw, 191–360 kg CO_2-eq t_{ww}^{-1} for perennial energy crops as willow and *Miscanthus,* and 265–287 kg CO_2-eq t_{ww}^{-1} for agro-industrial residues as beet top and brewer's grain (Tonini et al. 2016a, b). These figures should be added to the results quantified in this study to obtain a full picture of the Climate Change impact of the studied scenarios.

5 Conclusions

The study developed a process-oriented environmental life-cycle assessment modelling framework, implemented this in EASETECH and applied this on a biorefinery case study for illustrative purposes. The process-oriented modelling framework provides an improved representation of complex technologies allowing definition and evaluation of process relationships between inputs and outputs. This is particularly important for integrated technologies comprising individual unit processes, e.g. biomass conversion and management of residual resources. Traditional black-box modelling approaches, represented by most existing LCA models, do not offer similar possibilities for detailed evaluation of processes and technologies nor allow the same level of transparency with respect to inventory definition. The process-oriented modelling framework provided by this study allows consistent balancing of material, fraction and substance flows within the technology system and, through mathematical expressions, at the same time establishment of the process relationships that affect these flows through transition and transformation within each single unit process. Based on the biorefinery case study, the advantages of the modelling approach were demonstrated: input feedstocks and key process operational parameters can be adjusted easily in order to evaluate process performance and the importance of feedstock properties. This facilitates quantification of individual/intermediate (bio) product flows within unit processes; this has not been possible previously. The potential implications of process-oriented modelling are considerable, e.g. in relation to novel insights associated with uncertainty evaluation, technology upscaling and process optimisation.

Acknowledgements The authors wish to acknowledge funding from the Danish EUDP grant "SustEnergy" (grant no. EUDP 6417-0044).

Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

References

Allesch A, Brunner PH (2015) Material flow analysis as a decision support tool for waste management: a literature review. J Ind Ecol 19:753–764

Arora P, Hoadley A, Mahajani S, Ganesh A (2016) Multi-level modelling of sustainable chemical production: from CFD to LCA. In: Computer aided chemical engineering. Elsevier 38:499–504. https://doi.org/10.1016/B978-0-444-63428-3.50088-6

Arvidsson R, Tillman A-M, Sandén BA et al (2017) Environmental assessment of emerging technologies: recommendations for prospective LCA. J Ind Ecol 00:1–9

ASPEN (2019). https://www.aspentech.com/. Accessed 12 Feb 2019

Asprion N, Bortz M (2018) Process modeling, simulation and optimization: from single solutions to a multitude of solutions to support decision making. Chemie Ing Tech 90:1727–1738

Astrup TF, Pivnenko K, Eriksen MK, Boldrin A (2018) Life cycle assessment of waste management: are we addressing the key challenges ahead of us? J Ind Ecol 22:1000–1004

Bernstad Saraiva A (2017) System boundary setting in life cycle assessment of biorefineries: a review. Int J Environ Sci Technol 14:435–452

Bisinella V, Götze R, Conradsen K et al (2017) Importance of waste composition for life cycle assessment of waste management solutions. J Clean Prod 164:1180–1191

Brunet R, Cortés D, Guillén-Gosálbez G et al (2012) Minimization of the LCA impact of thermodynamic cycles using a combined simulation-optimization approach. Appl Therm Eng 48:367–377

Brunner PH, Rechberger H (2016) Handbook of material flow analysis. CRC Press, Taylor & Francis Group, Boca Raton 453 pp

CHEMCAD (2019) https://www.chemstations.com/. Accessed 20 July 2019

Clavreul J, Baumeister H, Christensen TH, Damgaard A (2014) An environmental assessment system for environmental technologies. Environ Model Softw 60:18–30

Danish Ministry of Food, Agriculture and Fisheries (2018) Plantedirektoratet Bekendtgørelse nr. 1008 af 02 juli 2018 om jordbrugets anvendelse af gødning og om plantedække i planperioden 2018/2019. Available at https://www.retsinformation.dk/pdfPrint.aspx?id=202375 (accessed 17 June 2019).

EC-JRC (2010) International Reference Life Cycle Data System (ILCD) Handbook—general guide for life cycle assessment—detailed guidance. Publications office of the European Union, Luxembourg. https://doi.org/10.2788/38479

EPLCA (2019) European Platform on Life Cycle Assessment. List of tools. Internet site developed by the European Commission JRC, Directorate D, Sustainable Resources. Retrieved from: http://eplca.jrc.ec.europa.eu/ResourceDirectory/faces/tools/toolList.xhtml. Accessed 12 Feb 2019

European Commission (2017) Horizon 2020 -Work Programme 2014–2015 9. Food security, sustainable agriculture and forestry, marine and maritime and inland water research and the bioeconomy. Retrieved from http://www.iuav.it/Ricerca1/BANDI/PROGRAMMI-/INTERNAZIO/HORIZON-20/WORKPROGR/Societal-c/h2020-wp1820-food_en.pdf. Accessed 20 Feb 2019

European Parliament and the Council of the European Union (2009) Directive 2009/28/EC of the European Parliament and of the Council of 23 April 2009. Off J Eur Union 140(16):16–62. https://doi.org/10.3000/17252555.L_2009.140.eng

Gaha R, Benamara A, Yannou B (2017) Proposition of eco-feature: a new CAD / PLM data model for an LCA tool. In: Haddar M, Chaari F, Benamara A, Chouchane M, Karra C, Aifaoui N (eds) Design and Modeling of Mechanical Systems—III. CMSM 2017. Lecture Notes in Mechanical Engineering. Springer, Cham, pp 763–770. https://doi.org/10.1007/978-3-319-66697-6_74.

Gentil EC, Damgaard A, Hauschild M et al (2010) Models for waste life cycle assessment: review of technical assumptions. Waste Manag 30:2636–2648

Götze U, Hertel A, Schmidt A, Päßler E (2014) Technology and manufacturing process selection. Springer London, London

Henriksen T, Astrup TF, Damgaard A (2018) Linking data choices and context specificity in life cycle assessment of waste treatment technologies: a landfill case study. J Ind Ecol 22:1039–1049

IPCC (2013) Climate change 2013: the physical science basis. In: Stocker TF, Qin D, Plattner G-K, Tignor M, Allen SK, Boschung J, Nauels A, Xia Y, Bex V, Midgley PM (eds) Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 1535 pp. https://doi.org/10.1017/CBO9781107415324

ISO (2006a) Environmental management—life cycle assessment—requirements and guidelines. ISO 14044, Geneva

ISO (2006b) Environmental management—life cycle assessment—principles and framework. ISO 14040, Geneva

Jacquemin L, Pontalier P-Y, Sablayrolles C (2012) Life cycle assessment (LCA) applied to the process industry: a review. Int J Life Cycle Assess 17:1028–1041

Jain P, Dyson B, Tolaymat TM, Ingwersen W (2015) A comparative analysis of life-cycle assessment tools for end-of-life materials management systems. U.S. Environmental Protection Agency, Washington, DC EPA/600/R-15/232

Kikuchi Y, Kimura S, Okamoto Y, Koyama M (2014) A scenario analysis of future energy systems based on an energy flow model represented as functionals of technology options. Appl Energy 132:586–601

Maes D, Van Dael M, Vanheusden B et al (2015) Assessment of the sustainability guidelines of EU Renewable Energy Directive: the case of biorefineries. J Clean Prod 88:61–70

Mancini L, Benini L, Sala S (2015) Resource footprint of Europe: complementarity of material flow analysis and life cycle assessment for policy support. Environ Sci Policy 54:367–376

Negro V, Ruggeri B, Fino D, Tonini D (2017) Life cycle assessment of orange peel waste management. Resour Conserv Recycl 127:148–158

Papadokonstantakis S, Karka P, Kikuchi Y, Kokossis A (2016) Challenges for model-based life cycle inventories and impact assessment in early to basic process design stages. In: Sustainability in the Design, Synthesis and Analysis of Chemical Engineering Processes. Butteworth-Heinemann, pp 295–326. https://doi.org/10.1016/B978-0-12-802032-6.00013-X

Parajuli R, Knudsen MT, Djomo SN, et al (2017) Environmental life cycle assessment of producing willow, alfalfa and straw from spring barley as feedstocks for bioenergy or biorefinery systems. Sci Total Environ 586:226–240. https://doi.org/10.1016/j.scitotenv.2017.01.207

Portha J-F, Jaubert J-N, Louret S, Pons M-N (2010) Life cycle assessment applied to naphtha catalytic reforming. Oil Gas Sci Technol – Rev d'IFP Energies Nouv 65:793–805. https://doi.org/10.2516/ogst/2010019

ProMax (2019) https://bre.com/. Accessed 20 July 2019

ProSim (2019) http://www.prosim.net/en/index.php. Accessed 20 July 2019

Serra P, Giuntoli J, Agostini A et al (2017) Coupling sorghum biomass and wheat straw to minimise the environmental impact of bioenergy production. J Clean Prod 154:242–254

SimaPro (2019) https://simapro.com/. Accessed 12 Feb 2019

TEAM (2019) https://ecobilan.pwc.fr/en/team.html. Accessed 12 Feb 2019

Thinkstep Gabi (2019) https://www.thinkstep.com/. Accessed 12 Feb 2019

Tonini D, Hamelin L, Astrup TF (2016a) Environmental implications of the use of agro-industrial residues for biorefineries: application of a deterministic model for indirect land-use changes. GCB Bioenergy 8:690–706

Tonini D, Hamelin L, Alvarado-Morales M, Astrup TF (2016b) GHG emission factors for bioelectricity, biomethane, and bioethanol quantified for 24 biomass substrates with consequential life-cycle assessment. Bioresour Technol 208:123–133

Tumilar A, Sharma M, Milani D, Abbas A (2016) Modeling and simulation environments for sustainable low-carbon energy production—a review. Chem Prod Process Model 11:97–124

Turner DA, Williams ID, Kemp S (2016) Combined material flow analysis and life cycle assessment as a support tool for solid waste management decision making. J Clean Prod 129:234–248

Umberto (2019) https://www.ifu.com/en/umberto/lca-software/. Accessed 12 Feb 2019

Vadenbo C, Tonini D, Burg V, et al (2018) Environmental optimization of biomass use for energy under alternative future energy scenarios for Switzerland. Biomass and Bioenergy 119:462–472. https://doi.org/10.1016/j.biombioe.2018.10.001

Wang Q-L, Li W, Gao X, Li S-J (2016) Life cycle assessment on biogas production from straw and its sensitivity analysis. Bioresour Technol 201:208–214

Yoshida H, Nielsen MP, Scheutz C et al (2016) Long-term emission factors for land application of treated organic municipal waste. Environ Model Assess 21:111–124

Zabaniotou A (2018) Redesigning a bioenergy sector in EU in the transition to circular waste-based bioeconomy—a multidisciplinary review. J Clean Prod 177:197–206

Zarrin B, Baumeister H (2014) Design of a domain-specific language for material flow analysis using Microsoft DSL tools. In: Proceedings of the 14th Workshop on Domain-Specific Modeling - DSM '14. ACM Press, New York, pp 23–28

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.