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An environmental assessment system for environmental technologies

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Abstract

A new model for the environmental assessment of environmental technologies, EASETECH, has been developed. The primary aim of EASETECH is to perform life-cycle assessment (LCA) of complex systems handling heterogeneous material flows. The objectives of this paper are to describe the EASETECH framework and the calculation structure. The main novelties compared to other LCA software are as follows. First, the focus is put on material flow modelling, as each flow is characterised as a mix of material fractions with different properties and flow compositions are computed as a basis for the LCA calculations. Second, the tool has been designed to allow for the easy set-up of scenarios by using a toolbox, the processes within which can handle heterogeneous material flows in different ways and have different emission calculations. Finally, tools for uncertainty analysis are provided, enabling the user to parameterise systems fully and propagate probability distributions through Monte Carlo analysis.

Keywords

EASETECH; Life cycle assessment; waste; LCA model; uncertainty; flow modelling
Software availability

Name: EASETECH (Environmental Assessment System for Environmental Technologies)
Developer: DTU Environment and DTU Compute (Technical University of Denmark)
Contact: corresponding author or www.easetech.dk
Programming framework: .NET
Language: English
Availability and online documentation: See www.easetech.dk
Year first available: 2013

1 Introduction

Over the last 30 years, life cycle assessment (LCA) has developed as a major tool for quantifying the environmental impacts of products and systems. Detailed guidelines such as the ILCD Handbook (European Commission, 2011) and ISO standards (2006) have been developed to guide the users in how to carry out the LCA. To facilitate the actual modelling more than 50 models are available today to help practitioners in their LCA projects (EPLCA, 2013), to meet the demand of more and more complex modelling needs (Hilty et al., 2014). As these models have developed with increasing functionality and database sizes, there has been a split between generic models intended for the modelling of all types of products and systems and models that specialise in certain types of products or systems.

1.1 Generic versus specialized LCA models

An example of specialised areas for the application of LCA is the assessment of solid waste management systems. Whereas product-based LCA usually follows a single product from cradle-to-grave, a waste-LCA will assess the handling of a very heterogeneous material consisting of a number of different waste fractions (end-of-life products in the waste mass) from end-of-life to grave or remanufacturing. These waste fractions have significant variability in their physical and chemical properties (Riber et al., 2007), and their optimal handling varies greatly among fractions (e.g. handling of food waste versus a plastic bottle). Splitting the waste into several flows, e.g. by source separation, and keeping track of masses and substances in the subsequent treatment schemes are key issues in modern waste management.

Generic LCA tools, such as SimaPro (2013) or GaBi (2013), do not allow for the modelling of a reference flow consisting of a mix of materials. To make up for this, “add-on” models have been developed that can take into account these very heterogeneous reference flows. An example of this is the waste management models developed by Doka (2009) for waste treatment technologies such as landfills and waste incineration facilities. Users can input data corresponding to their waste input flow in the add-on models, and the results of these models can then be imported into the generic LCA models.
The LCA models dedicated to waste management (WM) are built to cope with these specificities and to handle parallel flows through complex systems (Damgaard, 2010). The main difference in comparison to generic LCA models is that the LCA and treatment process modelling are directly integrated into one model. This means that the LCA practitioner can more easily evaluate the influence of various parameters of the waste management scheme (composition of reference flow, options for sorting, changes in technologies etc.) on the resulting environmental impacts, as variations in these parameters will have direct impact on any linked process. This also means that a user can easily track the impacts back to find the material in the heterogeneous reference flows that caused the impact, since the impacts are directly related to the chemical and physical properties of each material.

In a review of more than 200 waste-LCA studies, Laurent et al. (2014) showed that in approximately half of the studies practitioners preferred using dedicated waste-LCA models rather than generic LCA models. This confirms the recognition of a need for dedicated tools which help the practitioner keep track of multi-fraction flows.

1.2 Waste LCA models and EASETECH

For waste LCA models, the approach has thus far involved developing dedicated tools targeted at WM experts, which follow waste from its generation to emissions in the environment, provide specific treatment processes adapted to waste management and use parameters with which WM experts are familiar and for which they can provide data. Several waste-LCA models have been developed over the past decade. These models are either very specific targeted models for single technologies such as Boesch et al. (2014), or larger more complex models covering full waste management systems. Gentil et al. (2010) presented a review of nine full models, showing how the different models learned and evolved from previous models while incorporating new knowledge and functionality. The work and research carried out with these models provided a valuable holistic understanding of how these waste systems worked and how different processes and flows interacted. In the meantime, systems have become increasingly more complex in terms of management (e.g. combined treatment of different waste streams) and technologies (e.g. new thermal processes), therefore there is a need for more flexible models, that give the user the ability to design better process models and to expand all possible flow paths. Additionally, sensitivity and uncertainty analysis with regards to system parameters is crucial, to assess the robustness of results. To cope with these new requirements, we decided to develop a new LCA model, based on experience gained from the development of EASEWASTE (see Figure 1). The only other model included in the review by Gentil et al. (2010) still being developed and externally released is the DST model (Weitz et al., 1999). This model has just been released in a new version called the Solid Waste Optimization Life-cycle Framework (SWOLF) (Levis et al.,
Figure 1:

The first model developed at the Technical University of Denmark was EASEWASTE, which was initially released in 2004 (Kirkeby et al., 2006) and followed by updated versions in 2008 and 2012. The model handles a flow of fractions that have different physical properties (e.g. moisture content, heating value) and chemical compositions (e.g. carbon, nitrogen, mercury). These flows are thus handled as a matrix of waste fractions and material properties, and each fraction can be handled independently or grouped based on general similarity (e.g. PE bottle and plastic waste) in different processes. For each flow the user can define the collection system, transport mode and treatment in a defined number of processes. The purpose of EASEWASTE is to provide inventories of waste management technologies to users which can be used in LCA modelling. All of these processes are based on published research, making use of the findings of different research projects, assessing for example waste-to-energy (Riber et al., 2008), landfilling (Manfredi and Christensen, 2008; Damgaard et al., 2011) and biological treatments (Boldrin et al., 2011) (see EASEWASTE (2013) for a full list).

EASETECH has been developed to allow modelling of a range of different environmental technologies from a systems perspective, using a toolbox of processes (as explained in 3.1.2). The model is currently used by DTU researchers to model wastewater treatment (Yoshida et al., under review), sludge treatment (Gable et al., 2013) and renewable energy technologies (Turconi et al., 2013) which was not possible in the former model.

The objectives of this paper are to present this new model, called EASETECH, and in particular:
- to explain how the new LCA EASETECH model was developed (Section 2);
- to show the important novelties in this model as a result of this development (Section 3.1);
- to describe the software in terms of data input (Section 3.2), calculation structure (Section 3.3) and uncertainty propagation (Section 3.4) and
- to present a case study implemented in EASETECH (Section 4).

2 The development process
This section describes the development process and does not include any description of the modelling. The EASETECH model was developed through several steps. The first step consisted in the development of a conceptual model to ensure the feasibility of the model. The objective of this phase was to rethink the design
of the previous model, identify the core features of waste treatment technologies and exploit similarities between the different technologies.

This conceptual model was developed as a computational prototype in the programming language Ruby (Flanagan and Matsumoto, 2008), using an agile software development method (Abrahamsson et al., 2002). To specify each new feature, a user story was written, describing what the user provides as input values for the different technologies and which outcomes are expected from the computations. All user stories were entered into the FitNesse Wiki (FitNesse, 2013), an automated testing tool which uses the Framework for Integrated Tests (Fit) (Mugridge and Cunningham, 2005) to evaluate all user stories in the context of the developed conceptual model. This process ensures that the conceptual model always models the correct computations. A user story example is presented in the supplementary information.

Overall, 73 different user stories were implemented to test the various computations in the conceptual model, from simple material flow transformations to LCA calculations including computations with uncertainty. The conceptual model resulted in a toolbox of generic processes which could be combined to model the different treatment technologies.

Based on the experiences learned from the conceptual model and some first concepts of user interfaces, the EASETECH model was developed from 2011 in the .Net Framework. The development followed an agile software development method called ‘Scrum’ (Schwaber, 2004), wherein the client specifies small incremental features to be implemented during a time period of two weeks, called a ‘sprint’. The software was first released in January 2013. All major features are explained in detail in Section 3.

3 Program description

3.1 Specificities and novelties of EASETECH

In this section the two key features that make EASETECH unique compared to other LCA software are described, namely the use of material fractions and a toolbox of modules that can be combined freely.

3.1.1 Modelling flows of material fractions

A main feature of EASETECH is the use of material fractions when defining the reference flow of a system. In most LCA programs the reference flow is defined as a single material (e.g. plastic polymer or a coffee maker), but when modelling environmental treatment technologies, reference flows can consist of a very heterogeneous mix of materials. It is thus critical to keep this information during the whole modelling. Therefore in EASETECH the reference flow it is not defined as a single material, but as a composition of a number of different fractions, and the fate of each single fraction is tracked throughout the system. This is a main difference in comparison to traditional LCA and MFA tools such as SimaPro (2013), GaBi (2013), openLCA (2013) and Umberto (2013). This is very important because different materials have different chemical compositions, and the optimal treatment for one material fraction might be suboptimal for another fraction. It is therefore critical that the starting point of the modelling process is a composition matrix where
each material fraction is specified in terms of chemical composition (e.g. carbon or mercury content), as well as fraction-specific parameters (i.e. water content, heating value, methane potential). An example of a composition matrix is provided in Figure 2.

![Figure 2:](image)

This means that in EASETECH the focus is on tracking substances in the different fractions of material flows, from their generation to their release into the environment. The flows thus consist of a matrix of material properties specified for an unlimited number of material fractions, which is maintained as the input and output in each module into which it enters. This setup not only allows the user to track the different substance flows over the full system, but also to create Sankey diagrams as known from material flow analysis (Brunner and Rechberger, 2004) and to relate emission inventories to the different material flows throughout the model.

### 3.1.2 A toolbox of material processes

The basis for building the different technologies in EASETECH lies in the use of a toolbox of template material processes. As explained in more detail in Section 3.2.9, the processes that handle flows in EASETECH are called “material processes”. Flows need to be handled in different ways, so 17 templates have been created in EASETECH version 1.0 and are listed in Table 1. The toolbox offers a set of generic process modules to create, modify and split flows. In addition to this, more specific material processes have been developed to model anaerobic digestion, landfill gas generation, leachate generation and the application of processed waste on agricultural land, as the initial focus of this model was on waste management. In the example of landfill gas generation, a specific module was developed which models first order degradation of organic matter and whose output details the landfill gas composition over time. The option to be able to add specific material processes whose output compositions can be related to any desired parameter of the input flow is an important strength.
<table>
<thead>
<tr>
<th>Template name</th>
<th>Description</th>
<th>Material transfer function in flow calculation layer</th>
<th>Input-specific emissions added to the LCI calculation layer *</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material generation</td>
<td>Create a material flow (two possible data input methods: using a library of material fractions or direct input)</td>
<td>Create a flow</td>
<td>Upstream impacts can be included</td>
</tr>
<tr>
<td>Energy generation</td>
<td>Create an energy flow (with associated mass and substances)</td>
<td>Create a flow</td>
<td>Upstream impacts can be included</td>
</tr>
<tr>
<td>Basic process</td>
<td>Keep the flow unchanged</td>
<td>Equal</td>
<td>-</td>
</tr>
<tr>
<td>Water content</td>
<td>Modify the water content of the input flow</td>
<td>Modify the flow</td>
<td>-</td>
</tr>
<tr>
<td>Change of energy content</td>
<td>Modify the energy content of the input flow</td>
<td>Modify the flow</td>
<td>-</td>
</tr>
<tr>
<td>Addition of substances</td>
<td>Add substances to the input flow</td>
<td>Modify the flow</td>
<td>-</td>
</tr>
<tr>
<td>Mass transfer</td>
<td>Split the input flow according to total mass</td>
<td>Transfer material fractions to outputs</td>
<td>-</td>
</tr>
<tr>
<td>Substance transfer</td>
<td>Split the input flow according to different properties (two possible data inputs: fraction specific or default)</td>
<td>Transfer substances to outputs</td>
<td>Possible emissions of substances to environment compartments</td>
</tr>
<tr>
<td>Mass transfer over years</td>
<td>Split the input flow according to years</td>
<td>Transfer year fractions to outputs</td>
<td>-</td>
</tr>
<tr>
<td>Anaerobic digestion</td>
<td>Produce a gas and a digestate out of an anaerobic digester</td>
<td>Produce gas and digestate</td>
<td>-</td>
</tr>
<tr>
<td>Landfill gas generation</td>
<td>Degrade organic matter according to exponential first-order decay, creating a landfill gas and remaining waste</td>
<td>Produce gas and remaining waste</td>
<td>-</td>
</tr>
<tr>
<td>Leachate generation</td>
<td>Define leachate generation and remaining waste</td>
<td>Produce leachate and remaining waste</td>
<td>-</td>
</tr>
<tr>
<td>Use on land</td>
<td>Distribute C, N and P from the input flow and create an avoided flow</td>
<td>End or create an avoided flow</td>
<td>Emissions of C, N and P compounds to air, water and soil compartments</td>
</tr>
<tr>
<td>No output</td>
<td>Has no output</td>
<td>End</td>
<td>-</td>
</tr>
<tr>
<td>Emissions to the environment</td>
<td>Translates input flow into release into an environmental compartment</td>
<td>End</td>
<td>Emissions of substances to environment compartments</td>
</tr>
</tbody>
</table>

*: All templates have basic process exchanges (elementary exchanges and external process use) contributing to the material process’s LCI.

Currently new specific material processes are added by the developers, and in the future an external editor will be developed to allow the user to define new template processes with specific material transfer functions. Indeed, because the matrix format forces the inputs and outputs of all material processes to be
defined based on the same pattern, it is relatively easy to add new template processes to the software. This allows for more flexibility, as new research needs might require new functionalities in the material processes.

All templates can be used to form new technologies by applying project-specific data. They can also be conceptualised as sub-technology-level processes which can be combined and grouped together to form whole treatment technologies. The grouped processes can be saved in the library of material processes and used in any scenario. An example of such a combination is given in Figure 3. While landfilling was modelled in EASEWASTE as one large process containing the modelling of gas and leachate generation and handling, it is regarded in EASETECH as a combination of different material processes whereby two specific material processes modelling landfill gas and leachate generations are followed by different generic processes to model, for example, gas collection and the transfer of gas pollutants into the environment. This new way of defining processes from the detailed level up to the full process makes the software flexible in the sense that small processes can usually be found in various treatments; for instance, a gas engine can be found to treat gas produced in an anaerobic digester but also in a landfill. Similarly, leaching processes can be modelled in landfills and in the use of processed waste in unbound layers in roads, which allows users to easily model new possible processes by combining parts of already existing ones.

![Image of Figure 3](image-url)

Figure 3:

The software is provided with a predefined set of technologies for all commonly used treatment options for solid waste. Most of these technologies consist of grouped material processes to form the actual treatment process. Table 2 provides an overview of the technologies provided in the current database and the material process they use. All of these technologies have been documented in published scientific research.
Table 2: Overview of the technologies for waste management provided in the current database. Each technology is built by combining several modules (as illustrated in Figure 3). The number in the cell is the amount of modules of each type used for one technology. Footnotes refer to article examples.

<table>
<thead>
<tr>
<th>Technologies</th>
<th>Modules</th>
<th>Basic</th>
<th>Substance transfer</th>
<th>Mass transfer to outputs</th>
<th>Change of energy content</th>
<th>No output</th>
<th>Water content</th>
<th>Addition of substances</th>
<th>Emissions to the environment</th>
<th>Mass transfer over years</th>
<th>Landfill gas generation</th>
<th>Leachate generation</th>
<th>Anaerobic digestion</th>
<th>Use-on-land</th>
</tr>
</thead>
<tbody>
<tr>
<td>Collection¹</td>
<td></td>
<td>1</td>
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<td>Transport²</td>
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<td>Material recovery facility</td>
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<td>Material recycling²</td>
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<tr>
<td>Thermal treatment³</td>
<td></td>
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<td>1</td>
<td>1</td>
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<tr>
<td>Mixed waste landfill⁴</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td>1</td>
<td>5</td>
<td>2</td>
<td>1</td>
<td>1</td>
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<tr>
<td>Mineral waste landfill⁴</td>
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<td>1</td>
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<tr>
<td>Composting plant⁵</td>
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<tr>
<td>Anaerobic digestion plant⁶</td>
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<tr>
<td>Application on farm land⁶</td>
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<td>2</td>
</tr>
</tbody>
</table>

¹ Larsen et al. (2009), ² Merrild et al. (2008), ³ Riber et al. (2008), ⁴ Manfredi and Christensen (2009), ⁵ Boldrin et al. (2011), ⁶ Boldrin et al. (2010)

3.2 Data input in EASETECH

Two types of data can be identified in EASETECH: “background” data, which the user is not expected to modify very often (considered as being stored in “catalogues”), and data that the user will edit to model specific scenarios (considered as being stored in “process libraries”). Figure 4 shows how EASETECH utilises the different data storage types when creating scenarios and how the different catalogues, process libraries and scenarios are connected.
Figure 4:

The section gives a short description of all catalogues, process libraries and scenarios, describing what they consist, which data are provided in EASETECH version 1.0 and how the user can modify data using the graphical user interface presented in Figure 5. Additional screenshots of the interface are provided in Part II of the Supplementary Information (SI).

Figure 5:
3.2.1 Material fractions

The material fractions catalogue consists of a list of material fractions for which material properties have been defined. These material fractions are used in the processes of material and energy generation at the start of any scenario. Seventy material fractions are provided to the user in version 1.0, based on several waste characterisation studies (Boldrin and Christensen, 2010; Eisted and Christensen, 2011; Riber et al., 2009), but the user can always add more material fractions, if required.

3.2.2 Elementary exchanges

This catalogue contains all the elementary exchanges that can be used in the program. The ecoSpold (v2) format (ecoinvent Centre, 2013) was adopted to define these elementary exchanges. This nomenclature is used by the ecoinvent database v3 and in a number of other LCA programs, so this choice will ensure data exchange compatibility with many databases and software applications. In addition, a converter developed by the openLCA project (openLCA, 2013) enables the conversion of datasets between the ecoSpold v1, ecoSpold v2 and ELCD data formats (EC, 2010). EASETECH version 1.0 is provided with the 3,700 elementary exchanges contained in the ecoSpold v2 format, but new elementary exchanges can also be added.

3.2.3 Impact categories

This catalogue contains all the impact categories and associated characterisation factors that are used in LCIA methods to evaluate the impacts of a system. Each impact category consists of a list of elementary exchanges (from the catalogue of elementary exchanges) and their associated characterisation factors with regard to this particular impact category. The unit of the characterised result is also specified therein. EASETECH version 1.0 is provided with the impact categories of the LCIA methods EDIP97 (Wenzel et al., 1997), EDIP2003 (Hauschild and Potting, 2004), ReCiPe (Goedkoop et al., 2009), CML (CML, 2013), USEtox (Rosenbaum et al., 2008) and IPCC 2007 (Solomon et al., 2007). New impact categories can be created through the manual input of characterisation factors, or they can be imported as xml files following the ecoSpold v1 and v2 data formats.

3.2.4 LCIA methods

This catalogue contains all LCIA methods which are used for the impact assessment of scenarios in EASETECH. Each LCIA method consists of a selection of impact categories (from the catalogue of impact categories). Associated normalisation references and weighing factors can be added for each of these impact categories. The LCIA methods cited in the previous section are provided in EASETECH version 1.0, together with their most recent normalisation factors published in the literature. The user can create new LCIA methods manually or import them as xml files.

3.2.5 Interfaces

This catalogue is utilised to link the physical flow of a substance with receiving environmental subcompartments. Thus, when a user sets the transfer coefficient of a substance to a receiving compartment
in a material process, the model knows how to convert the mass of substance in the material input to an elementary exchange. For example, a flow of fossil carbon (e.g. in plastics) which is combusted and released through a stack into the air as carbon dioxide will be linked to the elementary exchange “Carbon dioxide, fossil; non-urban air or from high stacks” and multiplied by a conversion factor of 44.01/12.00 to include the weight of oxygen in the final compound.

3.2.6 Constants and parameters
The catalogue of constants contains all constant values that can be used in all data input fields. Examples of constants provided in EASETECH version x are the molar mass of carbon (“M_C”), the lower heating value of methane (“LHV_CH4”) and the molar volume of an ideal gas at a standard temperature and pressure (“volume_gas”).

Parameters, which are similar to constants but specific to one scenario, are used to perform uncertainty analysis and are explained in more detail in section 3.4. The list of parameters attached to a scenario can be accessed by right-clicking in the background of this scenario.

3.2.7 Material properties
All the material properties that are included in the calculations are found in the material catalogue. The user can also select the material properties to be included in the different display modes (named “default”, “gas”, “liquid” and “soil”) when asking for material composition.

3.2.8 External processes
While all catalogues are accessed from the menu bar (“4” in Figure 5), process libraries are located in the left pane (“3” in Figure 5). The library of external processes (“3b” in Figure 5) includes all “second-level processes” that can be used in material processes (which are considered as “first-level processes”). The basic idea behind EASETECH is to follow a flow through several material processes. The modelling of these material processes includes the use of auxiliary materials and energy, the production of which produces emissions called “upstream impacts”. The processes fulfilling these services are called “external processes” in EASETECH. Each external process contains all elementary exchanges related to the production of one functional unit of material or energy (e.g. the production of 1 kg ammonia, or 1 kWh of Electricity, at the consumer, based on coal power). Besides defining elementary exchanges related to the production of the material, it is also possible to add the use of another auxiliary material or form of energy in the production of the external processes themselves. However, this adds the risk of creating a loop function, whereby material A uses material B, whose production again uses material A (for example: Coal extraction → Energy Production → Coal extraction). To avoid the model staying in this loop, the model sets a number of iterations through which it should run before cutting off the loop.

Users can define their own processes as well as import LCIs of processes in the ecoSpold (v1 and v2) format. Additionally a number of external processes are already included in EASETECH version 1.0, these
processes are based on publicly available reports. Metadata and sources are provided together with the data for transparency and consistency check. Data input is carried out in the tabs “Process exchanges” and “Documentation”, presented in Figure 5 as “2b” and “2c”, respectively).

3.2.9 Material processes – templates and predefined material processes

The library of material processes (located in “3a” in Figure 5) contains two types of modules: templates and predefined material processes. Templates are single empty material processes which can be used as a basis for creating new processes, as described in section 3.1.2. Predefined processes are processes already made by users to model processes for handling and treating a material. Both kinds of processes can be used directly in a scenario, where a user can then modify them further, if needed, for the specific intended use.

Predefined processes can be either single material processes or groupings of material processes, as presented in Section 3.1.2. When saved in the process library, grouped processes are seen as a single material process and can be used in scenarios. The user has the option to expand this grouped process at a later time, in order to see all sub-processes in the procedure.

Material processes can be edited once they are dragged into the main window (“1” in Figure 5) and can be stored in the library of material processes (“3a” in Figure 5). Data for material processes are input into the tabs “Material transfer”, “Process exchanges” and “Documentation” (“2a”, “2b” and “2c” in Figure 5). Material transfer data explain how the process’s outputs are computed based on the inputs. As explained in section 3.1.2, material transfers are specific for each template module. Substances can also be transferred to subcompartments (e.g. to air or surface water), following which the resulting emissions are referred to as “input-specific”, as they are related directly to the input composition. Process exchanges data contain all elementary exchanges and external processes used in the material process. Direct emissions included in the “Process exchanges” tab are called “process-specific”. The documentation tab contains detailed information on how the data were gathered and handled before being entered into EASETECH, and also assigns scores for the quality of the data. This ensures that other users of the dataset understand the underlying assumptions and intended use.

3.2.10 Scenarios

The straightforward creation of scenarios is undertaken by dragging and connecting material processes from the library of material processes over into the scenario window (“1” on Figure 5). A scenario always starts with a material or energy generation process which covers the functional unit for the scenario (i.e. amount of material/energy and composition of this amount in fractions). From this point the user keeps connecting outputs to inputs, until all output boxes are connected and no more flows need to be handled. The final process can either be in the form of a final storage material process (e.g. mixed waste landfill) or in the form of a conversion process where the material crosses the system boundary (e.g. material recycling of scrap steel into new steel that can be used for new products outside the system).
3.3 Calculations and modelling structure in EASETECH

The structure of computations in EASETECH is presented in Figure 6. The program uses data contained in catalogues and in the scenario to compute results in five different layers: material flow compositions, life cycle inventory (LCI), characterised, normalised and weighted impacts. Layer computations are consecutive, i.e., results of the first layer are used in the calculation of the second layer, and so on. The results from these five layers are presented in the tabs shown as “2d”, “2e”, “2f”, “2g” and “2h” in Figure 5.

![Figure 6:](image)

The first layer – the flow layer – keeps track of all the mass and substance flows, as described in Section 3.1.1. Each material process template has a specific material transfer function that defines how output(s’) composition(s) are calculated based on the data input by the user (always defined in tab “Material transfer, “2a” in Figure 5). The different material transfer functions are explained briefly in Table 1 and in more detail in the SI. The results of this first calculation layer constitute flow compositions, presented in tab “2h” in Figure 5.

The second layer involves calculating the LCI of all material processes by using the results from the flow layer and the LCI data from the material process. The computation of an LCI involves determining, for each elementary exchange $i$, the quantity $Q_i$ of emissions or resource consumption. Therefore, an LCI is a collection of pairs $(i; Q_i)$. Like in other LCA tools, elementary exchanges originate either through the use of a material or energy production process (external process) or from an emission from the process itself. In the first case, for each external process $k$ in the tab “Process exchanges” (“2b” in Figure 5), the list of
elementary exchanges $LCl_k$ is the product of the LCI of the process $k$, the amount of $k$ used in the material process and the amount of the associated substance in the input flow.

Concerning emissions, EASETECH distinguishes between two types: process- and input-specific emissions (cf. Section 3.2.9), which are specified by the user in two distinct parts of the material process and have slightly different calculation modes:

- For process-specific emissions, quantity $Q_i$ is quantified for each elementary exchange $i$ specified in the “Process exchange” tab (“2b” in Figure 5) as the product of the emission of $i$ in the process by the amount of the selected substance in the input flow.

- Input-specific emissions are elementary exchanges resulting from transferring substances of the flow composition to environment subcompartments. These kinds of emission are specified in the “Material transfer” tab (“2a” in Figure 5) and LCI calculations are specific to each material process template. Details for each material process are given in the SI (Section III, part 3).

Therefore the LCI of a material process is defined as the sum of all external process contributions, process-specific emissions and input-specific emissions:

$$LCl_{Material\ process} = \sum_{k=external\ process} LCl_k + LCl_{process-specific} + LCl_{input-specific}$$ (1)

An example is used to explain the calculations of process- and input-specific emissions. Figure 7 shows an example of how an incineration plant was modelled by using the “Substance transfer – per fraction” template. The “process exchange” tab shows the process-specific emissions happening on-site, in addition to the use of external processes (Figure 7b). This results for example in an emission of carbon monoxide of $3.3 \times 10^{-5}$ kg / kg TWW. In the “material transfer” tab, transfer coefficients are specified for different substances, which induce input-specific emissions. For example, Figure 7a shows the distribution of mercury among the different combustion outputs: this result in an emission of 0.007475 kg mercury to the “air – unspecified” subcompartment per kg mercury input to the process.
Figure 7:

The third layer contains the calculations of the characterised impacts of all processes, based on the LCI results and the use of the characterisation factors contained in the applied LCIA method (Equation 2). Characterised impacts are presented in two tables in the tab “Charact. Imp.” (“2e” in Figure 5), both of which show the characterised impact of the full process (or scenario) in the different impact categories (columns). While the first table presents the contributions of the different elementary exchanges to the characterised impact, the second table shows the contribution of the various sub-processes. The fourth layer calculates the normalised impacts using Equation 3. Finally, the weighted impacts are calculated in the fifth layer using Equation 4. Normalised and weighted impacts are presented respectively in tabs “Norm. Imp.” and “Weight. Imp.” (respectively “2f” and “2g” in Figure 5), in the two same forms of tables as in the tab “Charact. Imp.”.

\[
IP(j) = \sum_i Q_i * CF(j),
\]

(2)

\[
NIP(j) = \frac{IP(j)}{NF(j)}
\]

(3)

\[
WIP(j) = NIP(j) * WF(j)
\]

(4)

where: \( IP(j) \) is the impact potential for impact category j, 
\( Q_i \) is the quantity of elementary exchange i inventoried,
CF\(j\), is the characterisation factor of elementary exchange i for impact category j,

\(NIP(j)\) is the normalised impact potential for impact category j,

\(NF(j)\) is the normalisation factor for impact category j,

\(WIP(j)\) is the weighted impact potential for impact category j and

\(WF(j)\) is the weighting factor for impact category j.

### 3.4 Tools for uncertainty analysis

It is important to evaluate the uncertainty of the obtained results. Tools implemented in EASETECH, to make uncertainty analysis easier, are based on the recommended method for uncertainty analysis provided by Clavreul et al. (2012).

EASETECH allows the use of parameters or formulas using parameters in all input fields. For each parameter the user can specify one value, a list of values or a probability distribution. When computing with lists of values, the result will also be shown as a list of values. For example, when a parameter called “elec_rec” has the list of values [0.2, 0.3, 0.4, 0.7], the resulting LCI for carbon dioxide is shown as a list of values, e.g. [4, 6, 8, 14]. This allows the user to test for different assumptions (sensitivity analysis).

To compute the uncertainty of the obtained LCA results, the implemented tools involve representation of parameter uncertainties as probability distributions and propagation by Monte Carlo simulation (Clavreul et al., 2012). The user can define, for each parameter, a probability distribution of uniform, triangular, normal or lognormal shapes. For a Monte Carlo simulation, the calculation involves sampling all distributions to obtain a list of values for each parameter (the length of which equals the number of runs) and then running the model with this list of values. To acquire a first rough impression of the results of the Monte Carlo simulation, results are first run with a list of 100 sampled values for each distribution. The result of this first run is thus imprecise but quick to calculate, which allows the user to gain immediate feedback on the effect of using the distributions. Instead of showing the list of sampled values in the result, which can be very long, the result is presented as a distribution with the average and standard deviation of the list of values, shown as “\(D(\text{average, standard deviation})\)” in the results fields. In addition, the user may want to obtain more precise results, e.g. for certain impact categories’ impacts, and run the simulation with a larger list size, e.g. 10,000 runs. This can be done by clicking on the result and typing in the sample size one would like to use, i.e. “10,000”, which will then run the Monte Carlo simulation 10,000 times and will copy the list of resulting values into the copy buffer, which can then be pasted into Excel for further analysis.

While it is important to assess uncertainty in the impacts from single scenarios, it is even more valuable to assess the uncertainty of the difference between two scenarios’ impacts. This analysis, known as “discernibility analysis” (as introduced by Heijungs and Kleijn, 2001), is a crucial step in uncertainty analysis, as several parameters may be used in both scenarios. For example the carbon footprint of an electricity production mix may have uncertainty (e.g. between 0.8 and 1.1 kg CO\(_2\)-eq/kWh) which will
induce uncertainty in the results of two electricity-consuming scenarios (getting e.g. respective impacts of [1.6-2.2] and [2-2.75] kg CO₂-eq). Based on this, the modeller might conclude that there is uncertainty in the designation of a scenario as the best, but when calculating the difference between the two scenarios the results will show in this example that the second scenario always emits more, meaning that there is no uncertainty in the final decision. Discernibility analysis can be performed easily by using the same list of values for each parameter in the two scenarios, extracting all results into Excel and then computing in Excel the difference between the scenarios for each run. An example of discernibility analysis is presented in the following section.

4 Case study
A case study was implemented to show how process datasets can be added in the EASETECH model and which kinds of results can be extracted therefrom. The case study investigated the environmental impacts of two organic waste treatments: incineration and anaerobic digestion (AD). The functional unit is the collection and treatment of one tonne of organic kitchen waste from households in Denmark in 2011. The case study is presented in more detail in Clavreul et al. (2012), where modelling was performed in EASEWASTE.

The waste composition data originate from a sampling campaign undertaken by Petersen and Domela (2003). The hypotheses were that organic waste was source-sorted with a 60% efficiency while 5% of other combustible and non-combustible fractions were missorted and thus ending in the organic kitchen waste. The resulting waste composition used as an input for this study is presented in Figure 2 and contains 12 waste fractions.

Figure 8 shows an overview of the implementation of the two systems in the EASETECH model. Eight different templates are used to model the various treatment processes through which the waste travels. For example, transportation processes are modelled using the basic template (where input equals output), while
the combined heat and power (CHP) gas engine is modelled using the “Emissions to the environment” template (e.g. specifying fugitive emissions of methane and the conversion of methane to energy). All the processes used in this modelling procedure are presented in the SI (Part IV, Section 1).

Once the system is set up, the analysis can start. A first possibility is to visualise the composition of the different flows, e.g. to analyse whether or not the digestate produced after anaerobic digestion fulfils the requirements for application on agricultural land. Figure 9 shows an example of a Sankey diagram for mercury, in which it can be seen clearly that the mercury in the incinerator is volatile and has been captured in the air pollution control system, from which it ends up in fly ash that is sent to final storage. In the AD scenario, as mercury is volatile, 40% of it follows the biogas in the AD and is emitted into the air from the gas engine (based on Earle et al., 2000). This Sankey diagram thus highlights to the user the importance of controlling the amount of mercury in the AD technology.

![Figure 9:](image)

Normalised impacts, which were calculated using the LCIA methods recommended by the ILCD (European Commission 2011, and the SI, Part IV, Section 2), are presented in Figure 10. They are presented in person-equivalents (PE) so that each scenario’s impacts are compared to the impacts from one person in one year. The results show that the incineration scenario performs better in the impact categories of global warming (20% greater benefits), acidification (it is beneficial while the AD scenario is not), terrestrial eutrophication (40% less emissions) and on the three toxic impacts categories. The AD scenario performs better in photochemical ozone formation (40% less emissions), freshwater eutrophication (seven times more benefits) and particulate matter (10% greater benefits). The impacts on ozone depletion were considered as negligible (impacts lower than $10^{-3}$ PE), and the two scenarios compared equally with regards to resource depletion (less than 5% difference).
Uncertainty propagation was performed for global warming impacts through Monte Carlo analysis, in which the two systems were parameterised by using 24 parameters. Screenshots showing how this is done in EASETECH are provided in the SI (Part IV, Section 3). Uncertainty distributions, which were defined for each of the parameters, are presented in Table S2 of the SI. Figure 11a presents the frequency distributions of both scenarios’ impacts. The normalised impacts of the incineration scenario have a standard deviation of 13 mPE around their mean of -42 mPE, while the AD scenario impacts have a standard deviation of 11 mPE around their mean of -32 mPE. The discernibility analysis is presented in Figure 11b, in which the frequency distribution of the difference between the incineration scenario and AD scenario impacts is plotted. This analysis shows that in 87% of the cases the incineration scenario obtained a better score than the AD scenario, underlining the fact that this is a better solution regarding impacts on global warming.
5 Discussion and conclusion

The main objective of this research was to develop a new holistic framework that would allow for the modelling of highly heterogeneous material flows with large variations in physical parameters and chemical properties. The new software allows the user to model flows of materials and the impacts of treatment technologies until release into the environment. Flexibility has been achieved (1) by creating a framework whereby processes can be connected easily to form scenarios, without the limitations of system size and complexity, and (2) by providing a toolbox of processes that the user can use to model very different types of treatments and management options.

The opportunity to model at the sub-process level is also offered in other LCA models, but what makes EASETECH unique is its focus on allowing the simultaneous modelling of a large amount of heterogeneous materials (made of various fractions). This new model concentrates on substance tracking and the assessment of flows at the substance level, which is particularly important when assessing the performance of environmental technologies.

At the same time, special effort has been applied to usability. Indeed, increasing flexibility may lead to an increase in complexity of use, but we believe the model is quite easy to start with and to use in general, for different reasons: (1) a fixed structure has been maintained throughout the processes in the model, where tabs are clearly defined for data input and calculation outputs, (2) the same matrix structure is maintained for all flows, (3) the handling of large scenarios is facilitated by an easy-to-use graphical interface which allows the user to drag and drop processes into scenarios and (4) a set of processes based on published research is provided, which enables the user to model scenarios and visualise results quickly and efficiently.
The model requires a considerable amount of data to model treatment systems, which implies that it is important to be able to assess the robustness of the results. The model allows for this assessment through the use of parameters in lieu of fixed input values at the data input place. Therefore, the robustness of results can be explored by carrying out sensitivity and uncertainty assessments in the model through parameter variation and Monte Carlo simulation.

In EASETECH we have chosen to store data in the ecoSpold v2 data format, which will entail easy data exchange with other models. This means that a user can easily import required data into the model when they are not readily available in the accompanying database. In the future, the goal is to make the model’s results directly recordable in an aggregated ecoSpold v2 format so that the user can use it in other software models.

In this first version of the model, the focus has been on processes allowing the user to model waste management systems. Nevertheless, the model has been developed with the intent and flexibility to be used in other environmental areas, and we are currently working on expanding it to allow for the modelling of energy systems also consisting of heterogeneous flows. In the near future, it will also be explored how the model can contribute to modelling in other environmental treatment fields (waste water, soil remediation, water supply, bioenergy production). Finally, future developments of EASETECH will also focus on improving the facilities concerning uncertainty analysis, offering parts of the analysis, e.g. showing the resulting distribution as a histogram, directly without having to use Excel.

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References


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Figure captions

Figure 1: Historical development of LCA models at the Technical University of Denmark.

Figure 2: Example of material composition computed in the flow layer. The figure only shows an excerpt of the chemical elements and fractions available in EASETECH.

Figure 3: Modelling of landfilling in the EASETECH model. Each box is an independent module. Grey boxes are explanations of actual processes.

Figure 4: Interactions between the different data catalogues. An arrow going from box A to box B indicates that an element in catalogue A can be used in an element in catalogue B. In the table in each box are given examples from the database. The catalogues are all explained in detail in this section.

Figure 5: EASETECH user interface (1: main window; 2: data input and results display; 2a: material transfer; 2b: process exchanges; 2c: documentation; 2d: LCI; 2e: characterised impacts; 2f: normalised impacts; 2g: weighted impacts; 2h: flow composition; 3: libraries; 3a: material processes; 3b: projects and scenarios; 3c: external processes; 4: catalogues; 4a: material fractions; 4b: elementary exchanges; 4c: impact categories; 4d: LCIA methods; 4e: interfaces; 4f: constants; 4g: material properties). Additional screenshots of the interface are provided in Part II of the Supplementary Information (SI).

Figure 6: Data and calculations in the different results’ layers. Arrows show the flows of information needed for calculations. The different layers represent the parallel calculations. * Input-specific emissions are specific to each of these material process templates: substance transfer, emissions to the environment and use-on-land.

Figure 7: Graphical overview of the two scenarios modelled in EASETECH. The blue boxes are the material processes. Blue arrows are composition flows between processes. Orange arrows depict a transfer from the composition layer to an environmental compartment (i.e. air, soil, water). Red crosses represent the degradation or removal of a compound (e.g. evaporation of water).

Figure 8: Data input in the incineration process (based on the template “Substance transfer – default”). a: Material transfer tab (shown only for mercury), b: Process exchanges.

Figure 9: Sankey diagram of mercury flows in the two scenarios.

Figure 10: Normalised impacts of the incineration (Inc) and anaerobic digestion (AD) scenarios in PE (GW: global warming, OD: ozone depletion, POF: photochemical ozone formation, AC: acidification, EU: terrestrial eutrophication, fEU: freshwater eutrophication, PM: particulate matter, HT: human toxicity (c: carcinogenic, nc: non-carcinogenic), ET: Ecotoxicity, RD: resource depletion)
Figure 11: Results of the Monte Carlo analysis (1,000 runs) for the global warming impacts of both scenarios (a) and of the difference between scenarios (b). Results are presented as frequency distributions (bars, left axis) and cumulative frequency distributions (line, right axis). In figure b, a negative result means that the incineration scenario obtained more benefits than the AD scenario.