Integration of LCA in a thermo-economic model for multi-objective process optimization of SNG production from woody biomass

Léda Gerber, Martin Gassner, François Maréchal

Abstract

This paper presents a methodology to integrate life cycle assessment (LCA) in models used to design energy conversion systems. It is illustrated by an application to a thermo-economic model for the multi-objective optimization of synthetic natural gas (SNG) production from woody biomass. The life cycle inventory (LCI) is written as a function of the parameters of the thermo-economic model. The obtained environmental indicators from the Life Cycle Impact Assessment (LCIA) are thus adapted to process design and scale. The conceived thermo-environomic model allows for taking into account the environmental impacts as a criterion in addition to economic and thermodynamic criteria in the process design and optimization.

Keywords: Process design, Biofuels, Synthetic Natural Gas, Life Cycle Assessment, Optimization

1. Introduction

Environmental impacts of emerging technologies such as the production of biofuels have become an important concern. To assess these impacts, life cycle assessment (LCA) is a widely used and well-established method [1]. However, for these processes, conventional LCAs are generally based on an average technology at lab- or pilot-scale that are extrapolated at large scale typically using linear models and based on data that are not necessarily consistent since
these are collected from different sources [2]. Therefore, changes in process design and integration, future installation size and technology evolution are not considered. At the most a few scenarios based on average technologies are made, but do not consider process integration aspects. It is therefore difficult for engineers to integrate LCA at design stage to target not only economic performances but also simultaneously minimal environmental impacts. This paper presents a methodology developed to link process design and scale-up with the LCA. It is illustrated by an application to a thermo-economic model used for the multi-objective optimization of thermochemical production of synthetic natural gas (SNG) from woody biomass [3,4].

2. Methodology

The thermo-economic design platform is used to create an interface between different models that represent the energy system design [5]. Like the economic layer, an environmental layer, the LCA model, has been added to the thermo-economic model for SNG production from woody biomass. As depicted in figure 1, it takes the simulation results, like flows and equipment sizes, to perform a LCIA based on reference data in EcoSpold format [6] from the ecoinvent® [7] life cycle inventories database.

The developed general methodology for the integration of LCA within a thermo-economic model is displayed in figure 2. In black are displayed the parts that are of particular importance to link the LCA model with process design. It is crucial while listing LCI flows to identify at which step of the process the flows are occurring and what is their function. This is necessary because they are then mathematically expressed as functions of the decision variables of the thermo-economic model. The scaling of impacts due to changes in operating conditions and sizes of process equipment is as well taken into account. Eventually, a LCA function including all the mathematical expressions for LCI flows and impact due to process equipment allows calculating the whole LCI for a given process configuration. ecoinvent® life cycle inventories database is used for the processes of the life cycle inventories and for the impact assessment methods. This allows to account for induced off-site emissions.
2.1. Goal and Scope definition

The goal and scope of the study is defined as the quantification of the environmental impacts associated with the production of SNG from woody biomass, related to the changes in process design and scale that are occurring during a multi-objective optimization. Since the interest of the study is to focus on the influence of the design of the conversion process, the different possible allocations of produced SNG are not considered. Therefore, a cradle-to-gate LCA approach is applied, and the chosen functional unit (FU) is 1 [MJ] of SNG, meeting the swiss quality standards to be injected in the gas grid. SNG production from woody biomass is divided in two phases: the wood chips production and the wood-to-SNG conversion. The wood-to-SNG conversion is of particular interest, since it is at this step that engineering decisions that can have effects on environmental impacts have to be taken. The relation between the biomass logistic and the plant size has also to be studied.

2.2. Identification of LCI flows

The defined system is taken as a basis to identify the different material and energy flows of the LCI. Substitution for electricity production, if produced, and fossil natural gas production, are also included. Though this is a cradle-to-gate approach, avoided fossil CO₂ emissions are as well included, since they are assumed to be a consequence of any allocation of the produced SNG. For each flow, an equivalence is found in the processes of the ecoinvent® life cycle inventories database. At this step, the stage of the wood-to-SNG conversion process at which the flows are entering or leaving the system is already identified, and linked to the parameters of the thermo-economic model. Figure 3 displays the LCI flows within the system limits, identified from [2,8], and at which step of the SNG production they occur.
Infrastructure is also included in the LCI. For the wood-to-SNG conversion part, it consists in the necessary process equipment of different types such as reactors, heat exchangers, pumps or compressors. A list of all the different process equipment is made, based on the costs calculation, and a specific type is assigned to each unit. For each type, ecoinvent® equivalences are found.

2.3. Quantification of LCI flows

2.3.1. Flows related to operation
Once the different flows of the LCI are identified, they are quantified by being linked to the design and the scale of the process. This involves expressing each LCI flow as a function of design and scale parameters. A list of the necessary parameters to calculate the LCI flows is done, and compared with the available parameters from the thermo-economic model. If some of these parameters are not available from the model, the latter is extended with the necessary ones.

2.3.2. Infrastructure
Impact functions are written to perform the scaling of the impacts for the different types of process equipment. From the basis dataset of ecoinvent®, they return scaled emissions and impact as output. The scale-up law is based on the similitude assumption between costing methods [9,10] and emissions. This can be justified by the fact that both cost and emissions are proportional to the size and therefore to the material used to build the equipment. The scale-up formulation (Eqn. 1) has the same form as the cost estimation correlation, considering as well a correcting factor related to operating conditions, equipment type and materials:

\[ \frac{E_{A,i}}{E_{ref,i}} = \left( \frac{A}{A_{ref}} \right)^k * c(P, M, type) \]  

(Eqn. 1)

Where \( E_{A,i} \) is the scaled emission of substance \( i \), \( E_{ref,i} \) is the reference emission of the ecoinvent® dataset, \( A \) is the functional parameter related to the size of the type of process equipment, \( A_{ref} \) is the value of this functional parameter for the reference dataset, \( k \) is an exponent calculated for different values of \( A_{ref} \), and \( c(P, M, type) \) is a correction factor depending on operating conditions, equipment type, and materials.
and \( c \) is the correction factor. When information available in ecoinvent® database allows it, the parameters of the equation are identified from it, otherwise the cost estimation values are used. Emissions due to maintenance, assembly, transports and end-of-life of process equipment are also calculated.

### 2.4. Impact assessment (LCIA)

The impact assessment computes the environmental impact by aggregating the emissions of the different substances emitted. For the impact assessment, 4 different impact assessment methods are chosen in ecoinvent® and are implemented in the model: Ecoindicator99-(H,A), Ecoscarcity06, some categories of the CML2001-West Europe, and Cumulative Energy Demand-fossil, non-renewable. Their impact categories are used as indicators to quantify the variations in environmental impacts due to SNG production.

### 2.5. Optimization strategy

To investigate the effect of process design and scale variations on environmental impacts, an economic optimization of the SNG production at multiple scale is performed, and the associated impacts with each one of the optimal solutions are calculated. To take into account the different possible technological choices and technology evolution, optimization is performed for 6 different scenarios, considering different stages of maturity for the process (1st, 2nd generation), different scales (small, medium, large), different technologies (indirect gasification using \( \text{H}_2\text{O} \), direct gasification using \( \text{O}_2 \), pressurized gasification or methanation, use of a steam cycle for electricity generation).

![Graph 1](image1.png)

**Figure 4:** Optimization of SNG production costs with respect to installation scale, and associated environmental impact.

![Graph 2](image2.png)

**Figure 5:** Variation in global warming potential with respect to SNG production costs.

Results are used to identify the trade-offs between costs and environmental impacts. They can also be used to perform preliminary design selection among different possible process configurations, by taking into account economic, thermodynamic and environmental aspects. Figure 4 shows the obtained Pareto
curve for economic optimization, with decreasing costs over size for all scenarios, and one associated environmental impact, the global warming potential. Figure 5 shows the variation of one environmental impact, the global warming potential, as a function of SNG production costs in the corresponding Pareto set. The analysis shows a trade-off between impacts and costs, since impacts increase with respect to the size, while specific cost is decreasing, except for scenario D. If scenario comparison is made, technology evolution reduces both costs and impacts, except for scenario D. Regarding scaling effects on environmental impacts, results are discussed more in details in [11].

3. Conclusions

A LCA model linked with process design and scale has been implemented as an extension of a thermo-economic model for the production of SNG from woody biomass. The methodology developed to link LCI with process design and scale can be potentially applied to other technologies for energy conversion or biofuels production. Such thermo-environmental models might be useful to orientate technological choices at an early development stage and to select appropriate process configurations, by considering economic, thermodynamic and environmental aspects.

4. References