Combining Technology Modelling with Life Cycle Assessment Modelling for Eco-Innovation in the Chemical Process Industry

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Abstract

Contemporary environmental policy demands a life cycle perspective. This presents a challenge to the chemical industry, where process simulation software traditionally focuses on optimizing facility design and operating conditions for a small subset of the full life cycle. This papers discusses an *ad hoc* solution for the case of a biorefinery, and presents a vision for generalizing and facilitating the combined use of process simulation software and life cycle assessment software.

Keywords: LCA, process simulation, technology modelling, biorefinery

Introduction

It is nowadays a well-accepted point of departure that environmental policy should adopt a life cycle perspective. For instance, the EU has developed around the concept of life cycle thinking (LCT) a series of communications [1-4]. The EU has also developed a set of activities related to life cycle assessment (LCA), such as the European Platform on Life Cycle Assessment, Life Cycle-based Indicators, Waste Management Guidance, Land Use Assessment, Carbon Footprint, and the European Food Sustainable Consumption and Production Round Table [5].
These European perspectives are an important example, but they are by no means an exceptional example. The US EPA is carrying out similar activities [6], and UNEP and SETAC have a Life Cycle Initiative [7]. Similar activities have been and are being undertaken by business associations, such as the Japan Environmental Management Association for Industry (JEMAI) [8] and the Association of Plastics Manufacturers in Europe (APME) [9].
In short, the life cycle perspective is an unavoidable and apparently promising way to go, both for governments and for industry. LCA is now applied to an incredibly large number of products. Just to mention a few: fruit, waste incineration, electronic equipment, biofuels, floor covering, and ammunition.

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At the same time, one should recognize the limitations of LCA. LCA is basically a tool to analyse a given situation, typically representing the present production technology, but equally applicable to future technology specifications. An LCA-practitioner is supposed to possess data on the production of materials and products, in terms of the required inputs and the generated products and released pollutants. Such data can be collected from production facilities (in which case one often speaks of foreground data), or they can be taken from literature surveys or general purpose databases (the background data). Data demands have always formed a major bottleneck for LCA. With the advent of large generic online databases [10-12] data availability is no longer the main issue. Rather, it is the fixed nature of such data that restricts the usefulness of LCA to an analysis of a status quo (either past, present or future), and that exclude its use in a more flexible, dynamic context.

In particular, the use of life cycle assessment in the context of process optimisation presents a situation where the dynamics of adapting the process conditions is at variance with the fixed coefficients requirements of the LCA-process. This situation occurs in a number of cases:

- output-driven requirements, e.g., in electric power mixes, where the optimal share of different modes of electricity production depends on the demand for electricity, with economic and environmental criteria as optimization goals;
- input-driven requirements, e.g. for waste treatment processes, where the instantaneous composition of the waste streams in terms of calorific value, water, and other characteristics determines the optimal process conditions;
- product design, e.g. where a product's performance depends on its shape and mass, but where the choice of materials and design influences the upstream and downstream requirements;
- process design, e.g. of a installation that can produce different chemicals in different proportions depending on temperature, pressure, catalysts, and other circumstances.

In this paper, we concentrate on this latter situation with an emphasis on biotechnological processes.

Process simulation is a generic term for the use of mathematical simulation techniques to analyze or predict the performance of a physical, chemical, or biological operation, or of a network of such operations. Examples of such operations and systems include (bio)refineries, chemicals production, and biochemical synthesis. In general, software for process simulation consists of a graphical interface where flow diagrams can be manipulated, and where data on the characteristics of the process steps can be loaded or defined. Typical building blocks are reactors, heaters, coolers, valves, etc. They are connected by flows of chemicals (pure components or mixtures), water, heat, etc. The relation between the sizes of these flows depend on a lot of parameters, mainly the properties of the

chemicals (surface tension, viscosity, etc.), and the conditions of the process (temperature, pressure, etc.). The designer adds an objective (a goal function) to be maximised or minimised. Examples of such objectives are production volume, economic profit, energy use, and emission of polluting chemicals. A constrained solving algorithm then computes the optimal design in terms of the tuning of the parameters.
Process simulation is an important tool for process engineers. Wikipedia [13] has a list of several dozens of software packages to support process design. However, most if not all have limited information on the environmental side, and they certainly do not reflect the life cycle perspective in an environmental way. As a consequence, process simulation in a life cycle perspective is far from easy. It requires a three-step sequence:

- model the processes system with certain conditions using a certain objective function;
- translate the obtained process specification (in terms of the apparent inputs and outputs (chemicals, energy, emissions)) into an LCA process format and feed it into an LCA program;
- connect this process to the other LCA processes and calculate the upstream and downstream environmental repercussions.

The results of this sequence should then be evaluated in terms of unforeseen side-effects within the life cycle. Alternatively, a model can be constructed that runs the optimization principles and includes upstream activities and their environmental impacts.
In literature, we can find a number of interesting exercises where process simulation has been combined with a life cycle perspective [15-21], or where some other form of optimization has taken a life cycle perspective [22-26]. However, by inspecting an comparing these contributions, it becomes clear that a generic application is cumbersome. Most models are really custom-made, and they are the result of long and tedious work. A more streamlined approach seems to be required for more daily use.

Experimental Part

The raw material of the work reported here is the following:

- a process simulation of a biorefinery, modelled in the process simulation software SuperPro Designer [27];
- an LCA using the data for the biorefinery and upstream and downstream data, modelled in the LCA software CMLCA [28].

From a contents perspective, the work has been reported in [21]. In this paper, we concentrate on the procedural perspective, with a view on generalizing the idea of connecting process simulation to LCA in a more generic set-up. This section is, however, restricted to a discussion of the biorefinery.

The SuperPro Designer process simulation software has been used to model a biorefinery, producing ethanol, succinic acid, acetic acid, and electricity. Figure 1 gives a screenshot from SuperPro Designer, showing the conventional way process simulation software models such a system.

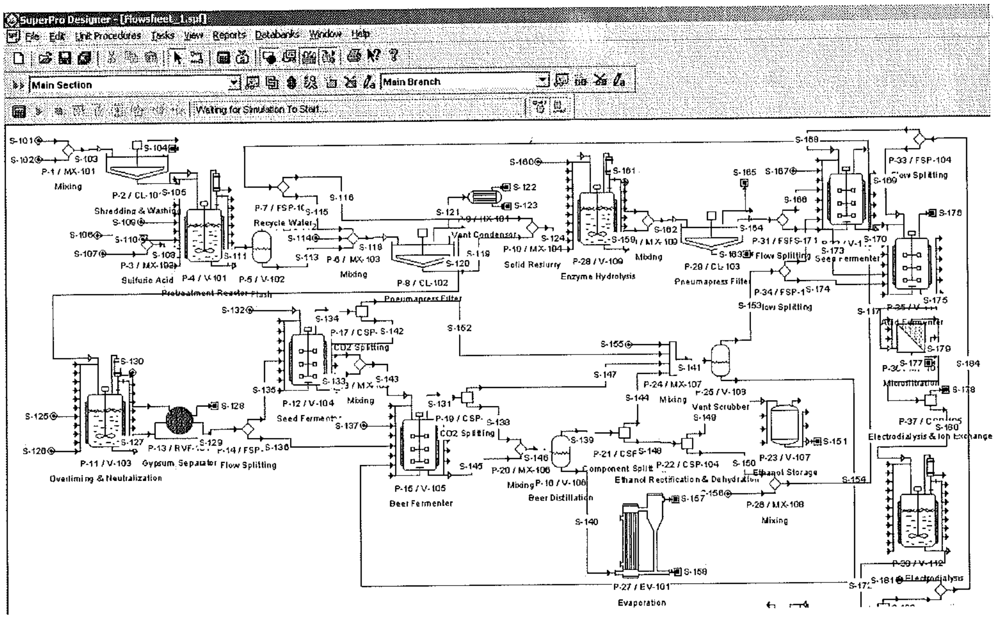

Fig. 1. Screenshot from SuperPro Designer, showing the modelled biorefinery

SuperPro Designer has been used to optimize the system according to the objective function, solving all mass and energy balances. The resulting description of the process, in terms of their inputs and outputs of chemicals, energy, pollutants, etc., have been exported and fed into the CMLCA software. The processes are now considered all alike: just as a black-box with inputs and outputs in fixed proportion.

A graphical summary of this is shown in Figure 2, where we see the flow diagram of the different steps within the refinery (shaded big rectangle) as well as a number of supplying processes that are not part of the refinery itself. Figure 2 also shows the magnitudes of the flows in tons/year as calculated by SuperPro Designer.

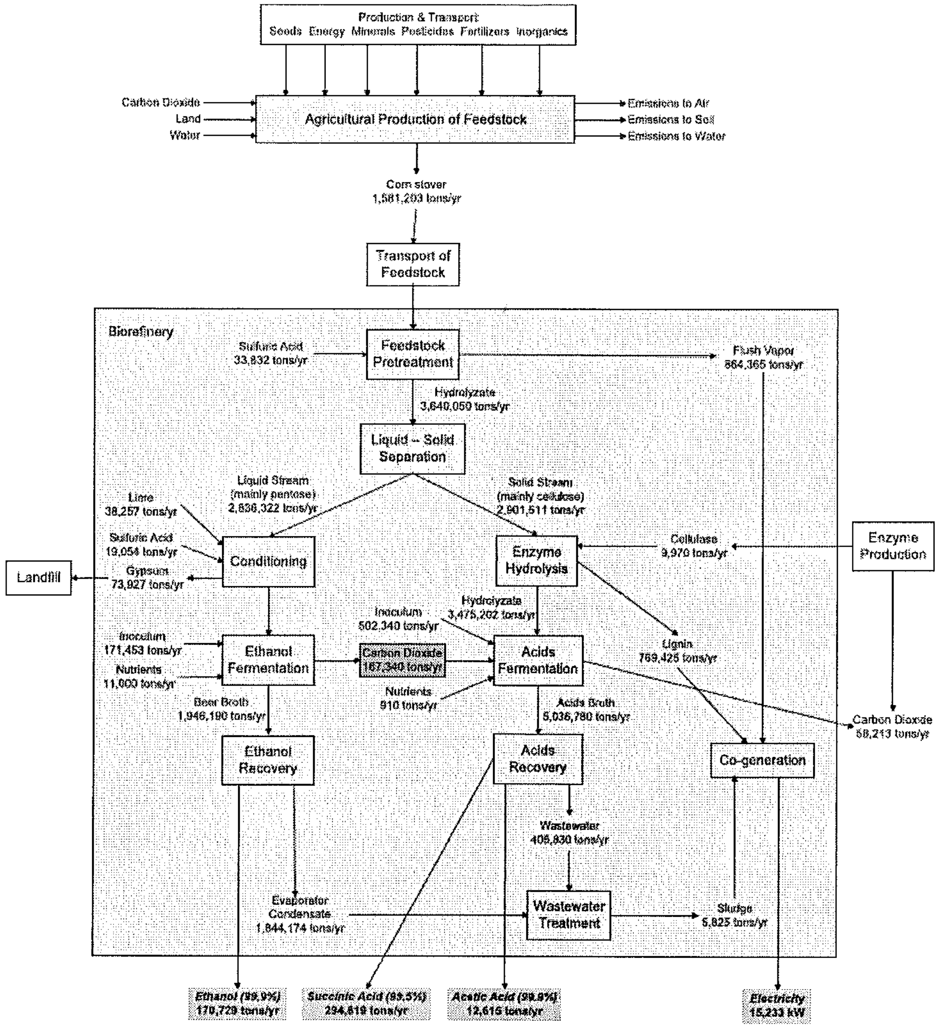

Fig. 2. Flow diagram of the lignocellulosic feedstock biorefinery, including the flows obtained from SuperPro Designer, source: [28]

The CMLCA software for LCA has been used together with the ecoinvent database [10] for modelling the cradle-to-gate supply chain of the inputs of the refinery or its feedstock, such as electricity, transport, and pesticides. In total, the full set of 3949 processes from ecoinvent has been used as an interconnected system of goods and services.

The optimal design of the refinery system resulted in an output of SuperPro Designer in terms of process specifications for 12 processes. These have been introduced into CMLCA on top of the 3949 process specifications from ecoinvent.

Altogether, a system of 3960 processes resulted. The system-wide emissions and resource requirements were calculated using the matrix balancing method [29] of CMLCA.

CMLCA also comprises the algorithms to calculate the impacts on a number of impact categories on the basis of the system-wide emissions and resource requirements. For this, the CML-IA method has been used [30]. This produced a list of environmental impact scores, such as global warming, photochemical ozone creation, and abiotic resource depletion. Detailed results, again, are given in [21].

Results and Discussion

The exercise described above, and in more detail in [21] shows that it is possible to use process simulation software and LCA software in a sequential way. The importance of this is not to be underestimated:

- Standard LCA databases, like ecoinvent, contain generic process data for established technologies, often in a country-averaged way. Modern developments, such as biorefineries for second generation crops, are not part of such databases, and have to be added whenever they become the object of study. The process simulation software is able to provide such data in a way that can be made compatible with the LCA data.
- Process simulation software can suggest clever designs for modern installations, but they have the danger of optimizing the design with a too narrow scope, as they miss all sorts of upstream and downstream processes, including their impacts.

How is one supposed to use this combination of tools? The optimal design from the process simulation software is embedded into an LCA system. The results of the LCA may give rise to a change in design, or to a revised objective function. The changes need then to be inserted in the first step, and the entire sequence of process simulation, translating its result in the LCA format, the LCA simulation, and translating its results in the process simulation format, takes off again. Figure 3 illustrates the four steps described.

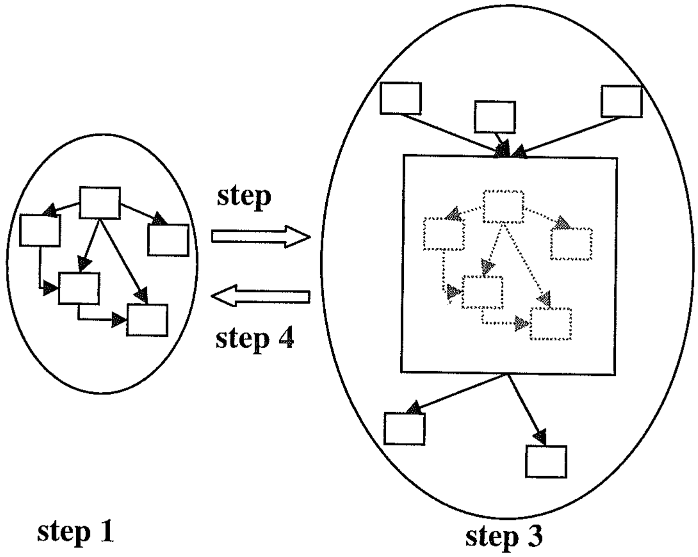

Fig. 3. Illustration of the integration of sequential use of process simulation software (step 1) and LCA software (step 3). Step 2 indicates feeding the results of step 1 into step 3, and step 4 indicates the converse route. Boxes indicate process steps, arrows flows of materials, energy and products. Solid boxes and arrows refer to processes and flows that are modelled, while the dotted boxes and arrows represent internal details that are not modelled, although they are known to exist. The oval represents the system boundary of the model.

The work reported here should be seen as a first demonstration of the feasibility of integrating process simulation and LCA. Several questions come up:

- Can this procedure be used for other cases than a biorefiery?
- Can we use other software tools than SuperPro designer and CMLCA?
- Can we somehow skip the steps 2 and 4 of converting the process simulation results in LCA-compatible terms and the other way around?
- Shouldn't one integrate process simulation and LCA in one software tool?

Although we so far applied this principle to a biorefinery, there is no reason that it cannot be done for many other types of processing facilities. Concerning the question of the choice of software, the use of SuperPro Designer and CMLCA is a bit coincidental. But we, as owners and developers of CMLCA, are in a position to adapt the import of CMLCA to the output format of process simulation software. We will soon do this for SuperPro Designer, as a first test case of a more narrow integration of the two types of software.

Concerning the last two questions, whether a real integration should be achieved in the end, we advise negatively. An extension of CMLCA by integrating the principles of process simulation, however attractive it sounds, may be a problematic thing. It might face the danger of the Swiss army knife, which can do anything, but which is not optimal for any of its tasks, and which moreover may be difficult to operate as well. Therefore, we continue to proceed along a different strategy. This strategy employs a fast exchange of data between the process simulation software and the LCA software, and the other way around. As such, it represents a compromise between a fully integrated life cycle-process simulation tool and a cumbersome retyping of the results of one program into the input screen of another program. This basically answers the third question as well: Yes, it must be possible to design ways to rapidly exchange data between process simulation software and LCA software. Two directions in that respect should be mentioned: the use of a uniform nomenclature (like the CAS-numbers for chemicals) and the use of XML as a vehicle for cross-program data exchange. In a more distant future, the use of UML [31] for defining the ontologies of the models is an appealing perspective.

Conclusions

While a preliminary study [21] has shown that process simulation can be combined with life cycle assessment modelling for a biotechnological system, a more easy and generic way of doing so can be developed. Such a combination will be implemented soon for SuperPro Designer and CMLCA, using XML interfaces. It will be applicable to chemical industry in a broader way.

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