A HIERARCHICAL METHODOLOGY FOR CHEMICAL PROCESS DESIGN BASED ON LIFE CYCLE ASSESSMENT

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Abstract

Considering environmental impacts in the design phase of chemical processes is one of the greatest challenges for the chemical industry. In this work, we propose a systematic process design procedure that incorporates Life Cycle Assessment (LCA) as an environmental metric in addition to the conventional economic optimization. Integration Definition Function Modeling (IDEF0) is used to represent the hierarchical methodology. IDEF0 defines each step of the activities, the information required, and the tools needed, and enables a systematic and at the same time transparent definition of the complex process design procedure. This leads to the systematic integration of tools that are conventionally available but separately existing in each field, such as the process simulator and LCA tools. A case study on the design of chemical recycling processes of beverage PET bottles is used to demonstrate the proposed approach.

Keywords

Environmentally benign process design, Life Cycle Assessment, IDEF0, PET bottle recycling

Introduction

Decisions made in the design phase of a chemical process determine most of the conditions during the operating phase, and finally affect the economic and environmental performance. However, in the conventional design approaches, economic benefits have been the main objective, while environmental issues have not received sufficient attention (Cano Ruiz and McRae 1998). First, the main aims of environmental considerations have been the reduction of energy consumption or waste directly from the process itself, although environmental impacts occur throughout the life cycle of chemicals such as raw material production, use phase and final disposal. Second, environmental concerns have been treated as constraints of the design. This results in the use of end-of-pipe technology, and limited flexibility for the frequently changing values in legislation.

Life Cycle Assessment (LCA) is a method to quantify environmental impacts of a product or a service in its entire life cycle. Environmentally benign processes with reduced end-of-pipe technologies can be realized by a novel design method that incorporates the result of LCA as an objective function. On the other hand, conventional process design is a well-defined activity in chemical engineering. In order to establish LCA in this field, it is still necessary to clarify in which design steps LCA is applicable and what kind of tools, data and model are required to conduct these design steps. In this work, we propose a systematic process design procedure that incorporates LCA as an environmental metric in addition to the conventional economic optimization. Integrated Function Definition Modeling (IDEF0 by Ross and Schoman 1977) is used to represent the hierarchical methodology. IDEF0 defines each step of the activities,

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the information required, and the tools needed, and enables a systematic and at the same time transparent definition of the complex process design procedure.

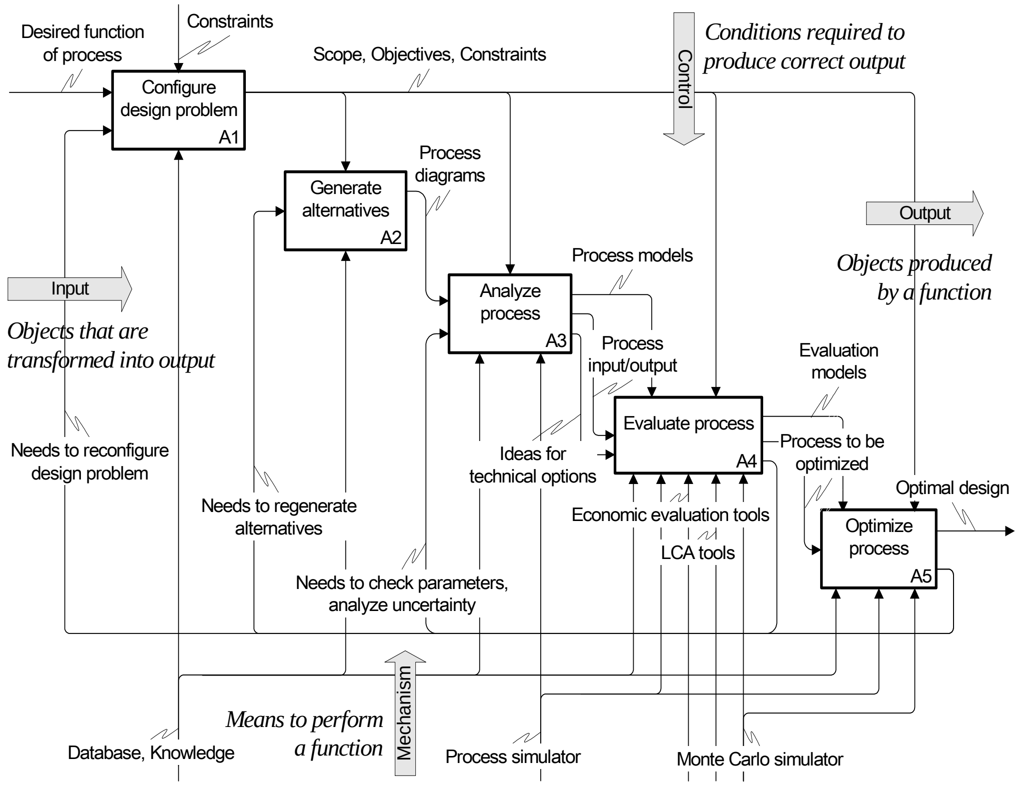

Figure 1. Overview of the whole process design activity: <u>Design chemical process</u>

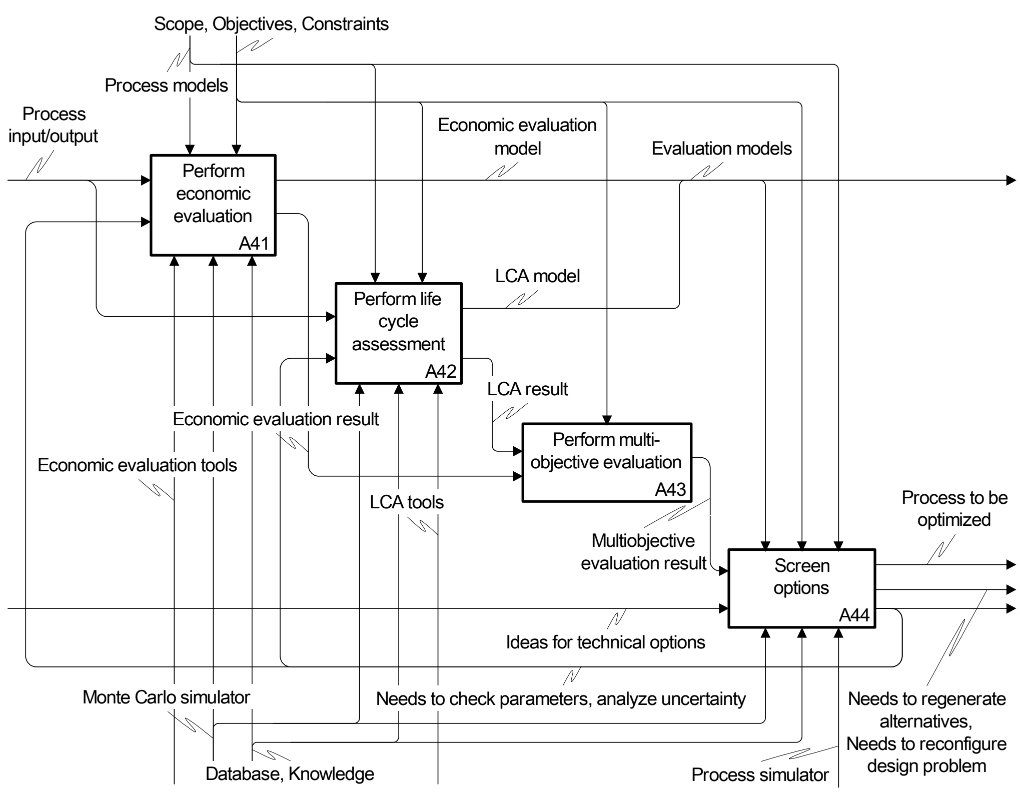

Figure 2. Sub activities in activity A4: <u>Evaluate process</u> (see Figure 1)

Description of Design Methodology

Overview of the whole design activity

Figure 1 shows the whole design activity: *Design chemical process* with syntax of IDEF0. IDEF0 is often used to represent business models. The initial input "*Desired function of the process*", i.e., a plan to design a process producing a certain chemical, is converted into the "*Optimal design*" from the economic and environmental perspectives by five steps of activities. In addition to the forward paths, several loops can be found reflecting the iterative nature of the process design. In activity A1: *Configure design problem*, general setting of the design problem such as the production target, objective functions and constraints are defined as "*Scope, Objectives, Constraints*" For environmental objectives, proper environmental impact models should be selected depending on the design situation. Process alternatives are generated in activity A2: *Generate alternatives*. Under the constraint of time and resources for survey, several conceptual structures of the process are produced as "*Process diagrams*". In activity A3: *Analyze process*, "*Process input/output*" for each process alternative is calculated using process simulator. In activity A4: *Evaluate process*, both economic evaluation and LCA are performed. The rigorous LCA can be performed here for the first time, because the system boundaries considered in the LCA are dependent on "*Process input/output*" which gives quantitative information on the substances entering and leaving the process. One promising alternative from the evaluation is further optimized in activity A5: *Optimize process*, and produced as a final outcome.

Decomposition of activity A4: Evaluate Process

Sub-activities of A4 are modeled as shown in Fig. 2. Activities related to LCA (A42) are defined parallel to the conventional economic evaluation (A41). As the start of the LCA study, the production target determined in activity A1 becomes the functional unit. The inventory analysis as a second step produces the life cycle inventory aggregated to the functional unit. In combination with "*Process input/output*" from activity A3, the total life cycle inventory is formed. The succeeding impact assessment converts the life cycle inventory to the specific environmental impact. Models and data required for the impact calculation (Eco indicator 99 by Goedkoop and Spriensma 1999, for example) are provided as the mechanism "*LCA tools*". Results from the process evaluation are transferred to "*Multiobjective evaluation result*" in activity A43 where both results are plotted in a two-dimensional plot. Activity A44 narrows the group of process alternatives down in order to find the most promising design. If "*Ideas for technical options*" arise during activity A3, which are not included in the current evaluation result, "*Needs to regenerate alternatives*" occurs. The outcome "*Needs to check parameters, analyze uncertainty*" is connected to the evaluation in activity A41 or A42 or the process analysis in activity A3 to check the sensitive parameters. When the uncertainty of the parameter can be classified as relevant to the result, uncertainty analysis is performed with "*Monte Carlo simulator*" obtaining the result as probability distribution. The set of promising options, or the Pareto surface, is found by comparing the probability distributions for each option. One design on the surface is selected as "*Process* [illegible] unctions.

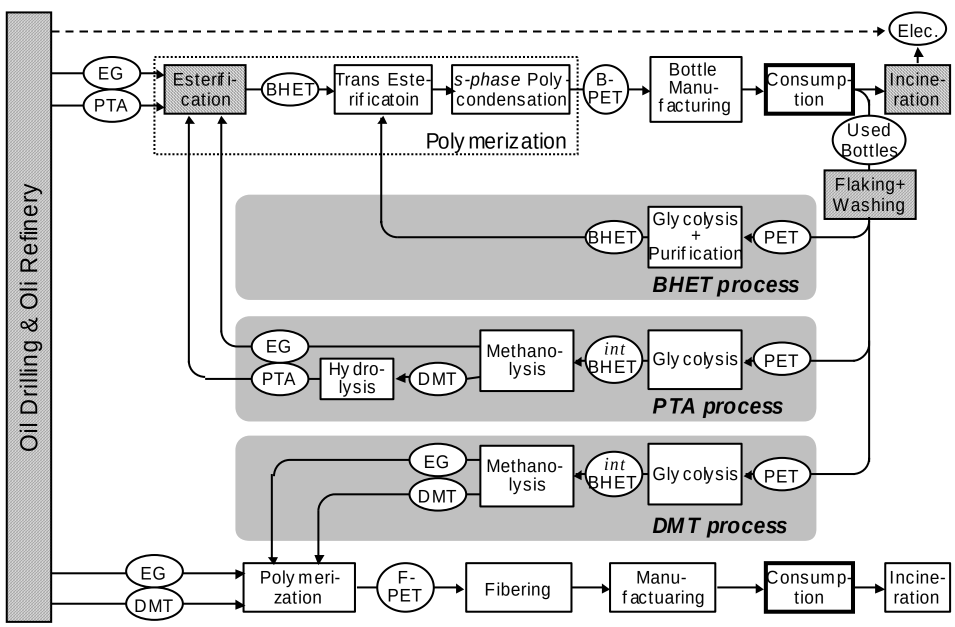

Figure 3. Life Cycle of PET products considering different chemical recycling processes. Int BHET represents intermediate state of BHET. Dark grey boxes indicate existing processes affected by the installation of process plants. Light grey boxes indicate chemical recycling processes.

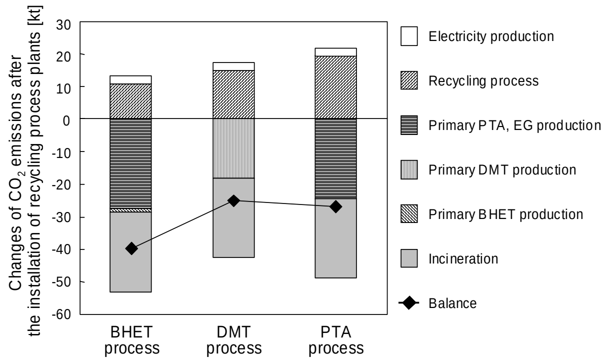

Figure 4. Change of CO_2 emissions

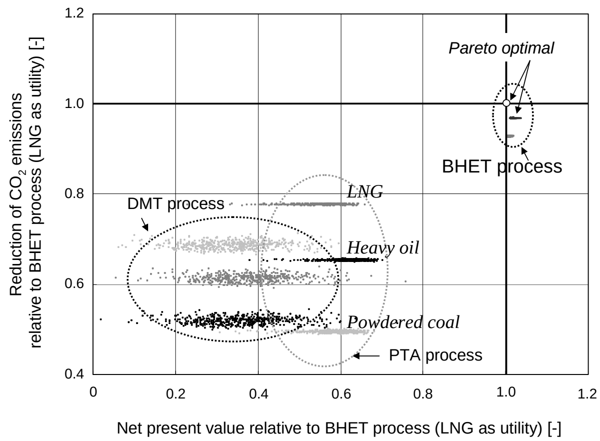

Figure 5. Pareto surface including uncertainty

CASE STUDY

A case study has been performed on the design of chemical recycling system for used PET bottles, which depolymerizes PET to monomers such as ethylene glycol (EG), purified terephthalic acid (PTA) or its derivatives: dimethyl terephthalate (DMT) and bis(hydroxyl)ethyl terephrhalate (BHET) as shown in Fig.3. Three different processes are simulated by using ASPEN PLUS®, producing the process input/output which corresponds to the input to activity A4.

Process evaluation by LCA (A42)

Here the objective of the LCA is to quantify the reduction of CO_2 emissions after the installation of these process plants and the processing at 10 kt/yr of used bottles that previously were incinerated or recycled as used resin. Under the assumption that the consumption rate is constant, the existing processes affected by the installation of process plants are detected as dark grey boxes in Fig. 3. Inventory data for these processes are surveyed, and changes of life cycle CO_2 emission are obtained as Fig. 4. An increase of CO_2 emissions can be observed in the recycling processes. On the other hand, substitutions by recycled monomers result in a decrease in primary monomer production. Substitution of BHET reduces CO_2 emissions in primary PTA and EG production as well as in the esterification process of PTA by EG producing primary BHET. Quitting the incineration of used PET bottles causes a decrease of CO_2 emission in the incineration process, which is independent of the recycling process. On the other hand, it causes an increase of CO_2 emission in the conventional electricity production to compensate the electricity that is recovered from the incineration process at 10% of thermal efficiency. The balance of these increases and decreases represents the reduction of CO_2 emissions after the installation of the recycling processes.

Multi-objective evaluation and selection of promising design (A43 and A44)

Concurrently with LCA, the net present value of each process was calculated. As a technical option, different types of utility supply are considered. Several sensitive parameters such as price or CO_2 emission factor (kg-CO_2 emitted to produce unit amount) of monomers are identified for uncertainty analysis. Probability distributions for sensitivity parameters are obtained in order to run Monte Carlo simulation. Evaluation result of each option are obtained as probability distribution, and compared in Fig. 5. BHET route using liquefied natural gas (LNG) is set as the reference of the comparison. Pareto surface is identified as BHET route using LNG or heavy oil. Depending on the weighting of objective functions, one of them is selected as promising design to be further optimized.

Conclusion

We have introduced a hierarchical design methodology of chemical process where LCA is incorporated as a design objective together with conventional economic metrics. IDEF0 defines each step of the activities, the information required, and the tools needed, and enables a systematic and at the same time transparent definition of the complex process design procedure. This leads to the systematic integration of tools that are conventionally available but separately existing in each field, such as the process simulator, LCA related tools, economic evaluation methods and the Monte Carlo simulator.

References

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