17th European Symposium on Computer Aided Process Engineering – ESCAPE17
V. Plesu and P.S. Agachi (Editors)

Application of life cycle assessment to the structural optimization of process flowsheets

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Abstract

This work proposes a novel framework for the optimal design of chemical processes whose main novelty lies on the incorporation of environmental concerns based on the Life Cycle Assessment (LCA) methodology. Our approach applies mixed integer modelling techniques to the superstructure optimisation of process flowsheets. As such, the resulting mathematical formulation incorporates the environmental impact as an additional objective that is appended to the objective function in which an economic performance indicator is also taken into account. The environmental impact is measured through the Eco-Indicator 99, which reflects the advances in the damaged oriented method recently developed for Life Cycle Impact Assessment. The main advantages of our approach are highlighted through a case study (hydrodealkylation of toluene), for which the set of non dominated solutions in terms of cost and environmental criteria is computed. The obtained results show that an inherent trade-off naturally exists between both objectives and suggest also that significant environmental improvements can be achieved if the decision-maker is willing to compromise the economic benefit of the process.

Keywords: optimization, sustainability, process synthesis

1. Introduction

Recently there has been a growing awareness of the importance of incorporating environmental concerns in the decision-making process associated with the design and operation of chemical processes. In this regard, the use of Life Cycle Assessment (LCA) (Consoli *et al.*, 1993) as a tool for assessing the environmental impacts of products, processes and activities is gaining wide acceptance. The application of LCA is motivated by its holistic approach, which includes the entire life cycle of the product, process or activity, encompassing extracting and processing of raw materials; manufacturing, transportation and distribution; re-use, maintenance; recycling and final disposal.

Although the potential benefits of applying LCA to process optimization have been often acknowledged in the literature (Azapagic and Clift, 1999), only a limited number of case studies have been reported to date. This work aims to extend the capabilities of the LCA methodology by applying it in conjunction with mixed integer modelling techniques. The combined use of such complementary methods allow us to explore a vast number of design alternatives at the same time, thus expanding the scope of the currently narrow approaches devised to date in this field.

2. Problem statement

Given is a superstructure which embeds a set of potential structural alternatives of a chemical process. Given are also the time horizon, the demand of the final products, the cost of the raw materials, utilities and equipment units as well as the prices of the final products. The problem then consists of selecting the optimal flowsheet structure as well as the parameters which describe the operation of a desired process such that both the total cost, which includes the investment and operation cost, and the environmental impact of the process are minimized over the entire time horizon.

3. Paper approach

The synthesis problem with environmental concerns can be formulated as a multi-objective mixed integer non linear problem (moMINLP):

$$
\begin{aligned}
& \min_{x,y}\{f_1(x,y);f_2(x)\} \\
st. \quad & h(x)=0, \\
& g(x)\le 0, \\
& Ax=a, \\
& By+Cx\le d \\
& x\in X=\{x\mid x\in R^n, x^L\le x\le x^U\}, \\
& y\in Y=\{y\mid y\in\{0,1\}^m, Ey\in e\}
\end{aligned}
$$

The continuous variables **x** represent the flows, operating conditions and design variables. The binary variables **y** denote the potential existence of process units. The non-linear performance and sizing equations correspond to $\mathbf{h(x) = 0}$ while the inequality constraints $\mathbf{g(x) \leq 0}$ include the design specifications, which are usually linear inequalities. With regard to the objective function, let us note that two different objectives are considered. The first one, which is denoted by $\mathbf{f_1(x,y)}$ is the total investment and operating cost of the process while the second one ($\mathbf{f_2(x)}$) is the environmental impact, which in our work is assessed through the Eco-Indicator 99. Thus, the solution of this problem consists of a set of Pareto optimal flowsheet configurations and their associated operating conditions.

3.1. Methodology: LCA and computation of Eco-Indicator 99

The LCA methodology (ISO 14040, 1997) that enables the computation of the environmental impact of the process is normally applied in four phases: 1) Goal and scope definition. In this phase, the system boundaries and the impact categories are identified. Since our approach focuses on decreasing the environmental impact of the manufacturing stage we restrict our analysis to this life cycle stage by considering a fixed production rate of the main desired product ("*cradle-to-gate*" analysis). The Eco-Indicator 99 proposes 11 impact categories than can be further classified into 3 specific damage categories, namely human health, ecosystem quality and resources. 2) Inventory analysis. This second phase provides the inputs and outputs of materials and energy associated with the process (Life Cycle Inventory). Based on these values, the set of environmental burdens of the process can be computed. In our problem the environmental burdens are expressed as a function of the continuous decision variables **x**, and specifically of the flows of raw materials and by-products and the energy consumed by the system. Such variables are regarded as free variables by the optimization algorithm. Furthermore, all the burdens must be expressed per unit of reference flow of the main product.

3) Impact assessment. In this stage the process data are translated into environmental information. Specifically, for each impact category, the damage caused by all the environmental burdens ($damage_d$) is computed from the emissions associated with them (β_b) and the corresponding set of damage factors (α_{bd}). Next, the damages are normalised and aggregated into a single impact factor. For this purpose, normalisation (δ_d) and weighting (ω_d) factors are required. Notice that the damage factors and the normalisation and weighing parameters will depend on the LCA version being applied in each case (*i.e.*, Hierarchist model with average weighting, Egalitarian model with Egalitarian weigthing, etc.). Thus the Eco-Indicator 99 is computed through Eq. (1).

$$f_2(x) = Eco - Indicator\ 99 = \sum_d damage_d \cdot \delta_d \cdot \omega_d = \sum_d \sum_b \alpha_{bd} \cdot \beta_b \cdot \delta_d \cdot \omega_d \qquad (1)$$

4) Interpretation. Finally, the results are analysed and a set of conclusions or recommendations for the system are formulated.

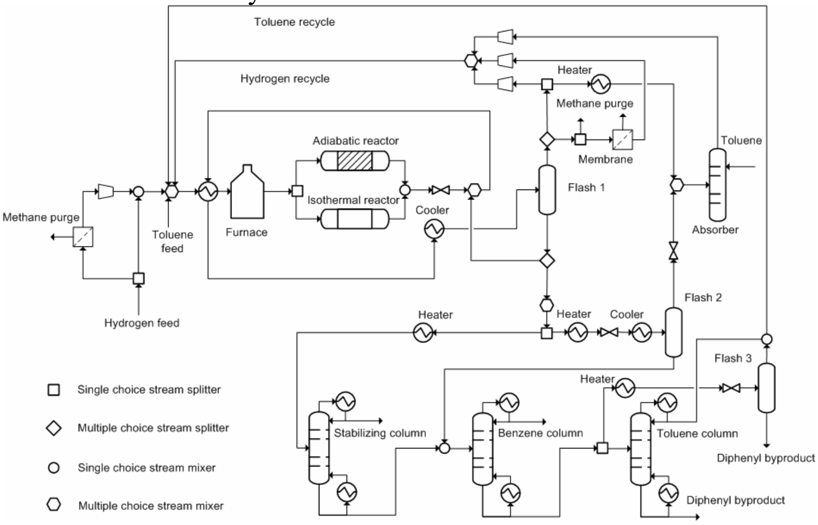

Figure 1. Superstructure for the hydrodealkylation of toluene.

3.2. Case study

The methodology previously described is applied to the hydrodealkylation of toluene. The superstructure selected for this problem and all the associated data have been taken from the work of Kocis and Grossmann (1989) (see Figure 1). Specifically, we consider the production of 1060 tons of benzene per year during a time horizon of 10 years. The desired reaction in the HDA process is the following: *toluene* + *hydrogen* → *benzene* + *methane*. An undesired reversible reaction also occurs: *2benzene* ↔ *diphenyl* + *hydrogen*. A hydrogen raw material stream is available at a purity of 95 % (the rest is methane). A membrane separator can be used to yield a higher purity feed stream by removing methane. A toluene fresh feed is also available. Both feed streams are combined with recycled hydrogen and toluene and heated before being fed to the reactor. The exothermic reactor can be carried out in a plug flow reactor operating either adiabatically or isothermally. The reactor product stream must be quenched immediately and cooled further in order to condense the aromatics that are removed from the non-condensable hydrogen and methane in a flash separator. Part of the vapour stream from the flash separator has to be purged to avoid accumulation of methane. Alternative a membrane separator can be used to decrease the hydrogen loss in the purge stream. Another alternative is to treat the flash separator vapour stream in an absorber with toluene feed to recover the benzene lost in the flash separator. A portion of the flash separation liquid stream is used to quench the reactor product stream and the remainder is sent to the liquid separation system. Hydrogen and methane are removed by using either a stabilizing column or a second flash separator operating at a lower pressure than the first one. Then, a distillation column is used to yield a benzene stream with the desired purity. The split of the bottom stream, which contains primarily toluene, can be accomplished in a flash separator or a column. With regard to the environmental issues, let us note that the environmental loads of the raw materials are retrieved from the Ecoinvent database from SimaPro^{TM} whereas the ones associated with the electricity and steam generation are taken from the TEAM^{TM} database. Furthermore, the Hierarchist damage model and normalisation with the average weighting are considered.

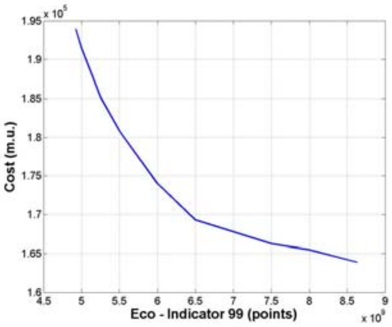

Figure 2. Trade-off solutions of the case study.

3.3. Results and discussions

The resulting moMINLP optimization problem contains 724 constraints, 710 continuous variables and 13 binary variables and it is solved by applying the ε-constraint method. Each single-objective problem is implemented in GAMS and solved with DICOPT. Notice that since we are using the ε-constraint method we cannot guarantee the Pareto optimality of the solutions. Furthermore, the optimality of each constrained single-objective problem cannot be guaranteed either as the outer approximation method is being used to solve them.

As shown in Figure 2, there is a clear trade-off between both objectives, as a reduction in the Eco-Indicator 99 can only be achieved at the expense of an increase in the cost. Notice that each point of the curve corresponds to a chemical process flowsheet operating at specific conditions (this information is not shown here due to space limitations). The first point of the curve represents the most profitable design (*i.e.*, the one that yields the minimum cost), whereas the last one is the less environmentally harmful (*i.e.*, the one with the lowest Eco-Indicator 99).

By analysing the specific configurations and operating conditions associated with the trade-off solutions, one can see how the model is forced to seek structural alternatives that are less energy demanding to gradually satisfy the increasing environmental requirements imposed by the ε-constraint method. Certainly, the minimum cost and the minimum Eco-Indicator 99 solutions exhibit different configurations. Specifically, both of them avoid the use of the membrane in the input stream and also the absorber. Furthermore, both use the isothermal reactor, the stabilizing column and the second flash. However, the former solution uses the membrane in the purge to reduce the amount of hydrogen lost while the latter does not. By doing so, the less environmentally harmful design reduces the hydrogen recycle stream at the expense of requiring more hydrogen in the fed stream. From the environmental point of view, the former positive effect dominates the latter negative impact, as the Eco-Indicator 99 is very sensitive to the burdens associated with the electricity generation. Thus, the Eco-Indicator 99 is finally greatly reduced by decreasing the energy consumed in the compressors. At the same time, the increase in the cost of the raw materials is not compensated by the decrease in the energy consumption and thus the total cost of the process increases accordingly.

4. Conclusions

This work has proposed a novel framework for the design of sustainable chemical processes. The design process with environmental concerns has been formulated as a multi-objective mixed integer non-linear problem (moMINLP) accounting for the minimisation of cost and the Eco-Indicator 99. The proposed approach has been applied to a case study (hydrodealkylation of toluene) for which the set of trade-off solutions has been computed. The obtained results have shown that there is a clear trade-off between economic an environmental criteria and that significant environmental improvements can be achieved through structural modifications in the process flowsheet.

Acknowledgements: Gonzalo Guillén-Gosálbez expresses his gratitude for the financial support received from the Fulbright/Spanish Ministry of Education and Science Postdoctoral Visiting Scholar Program.

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