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Mathematical Programming Approach to Sustainable System Synthesis

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This contribution presents some basic ideas, challenges, and advantages when performing the mathematical programming approach to sustainable system synthesis. A two-step multi-objective mixed-integer nonlinear programming (MINLP) synthesis is described, where a single-criterion MINLP-1 is performed during the first step in order to obtain economically-efficient solutions, and then multi-criteria MINLP-2 during the second step in order to achieve sustainable solutions. A special normalized LCA index is defined, suitable for ε-constrained multi-objective synthesis. Several examples of problems in the areas of process synthesis, bio-process network synthesis, the synthesis of municipal solid waste networks, and the synthesis of regional renewable supply and demand networks indicate that more profitable and yet less environmentally-harmful systems can be obtained.

1. Introduction

Process (Problem) Systems Engineering (PSE) is a relatively new area which emerged in 1960s due to the breakthrough in computer science. The main contribution of PSE is that it enables the shifting of scientific minds from the analytical approach where the objectives were to understand individual operations and phenomena, to the synthesis approach where individual operations and phenomena are designed more towards overall process performance. Since system synthesis can be understood as an activity for the automatic generation of design alternatives and the selection of better ones (Westerberg, 1991), two main questions arise (i) which approach is the most suitable and effective for the automatic generation of numerous alternatives and (ii) under which criteria selection of better ones has to be carried out?

In respect to the former question approaches can be, in principle, classified as heuristic, the one relying on physical insights, and the optimization approach based on mathematical programming and stochastic methods. Whilst driving algorithms for stochastic methods were usually taken from nature, e.g. genetic algorithms, simulated annealing, etc., the mathematical programming approach is a product of pure mind based on powerful mathematical principles: optimality, feasibility and integrality of solutions. It is therefore apparent that the heuristical approach has become more and more redundant and that the mathematical programming approach, together with

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available computerized solution tools, can be regarded as one of the more important technologies at the beginning of 21st century which enables, not only the gaining of significant competitive advantages, but even more importantly, obtaining fundamentally new design solutions that are integral with respect to different objectives. Thus, with respect to the latter question it is then evident that the use of a single economic or technological criterion is inefficient for obtaining an integrated solution. Due to the increasing importance of sustainability regarding economics, our environment and our society, the activities in process design/synthesis (Stefanis et al., 1997; Kravanja et al., 2005; Azapagic et al., 2006), product process design (Gani, 2004) and PSE in general (Guillén-Gosálbez and Grossmann, 2009) should be improved by considering the sustainability principle in the design and synthesis. Additional criteria constraints and alternatives based on these principles have to be incorporated into mathematical models which give rise to the multi-objective sustainable mixed-integer nonlinear programming (MINLP) approach to system synthesis, in general, or process synthesis in particular. Given the fact that great accomplishments in PSE (Grossmann and Westerberg, 2000) were achieved over the last two or three decades, we are still confronted with some very important challenges: i) expanding the scopes of synthesis problems to their whole supply-chains, ii) the definition of sustainability measures suitable for integrated-system optimization and synthesis and iii) performing efficient multi-objective optimization and synthesis.

2. Expanding the scope of the synthesis

Traditionally, systems syntheses have so far been concerned with processes isolated from the rest of their supply-chains. Supply-chains can be represented by several layers either by temporal vs. spatial representation or supply-demand oriented superstructures. Typical examples of the former are (bio)chemical supply-chain (Marquardt et al., 2000) which in a simplified form can be represented by molecular, reaction-path and process network layers (Kravanja, 2010; Figure 1), and energy supply-chain comprised of reactions, production and transmission layers where, in the first layer, energy is released from interactions with electromagnetic waves or atomic or chemical reactions. In the second layer energy is produced during the production processes, and finally, it is distributed to consumers at local or even global levels (Kravanja, 2009; Figure 2). An example of the latter representation of supply-chains is a supply-demand superstructure for a regional municipal solid waste (MSW) network which typically comprises alternatives for minimal or zero waste emissions, minimal use of land, minimal transportation and operation, and maximal amounts of recycled material and energy at waste collection, recycling, treatment, selling of secondary material and energy, and final disposal (Iršič Bedenik and Kravanja, 2007; Figure 3). Another example is a superstructure for a regional renewable supply and demand networks, consisting of supply, pre-processing, processing, and consumption layers (Čuček et al., 2010a; Figure 4).

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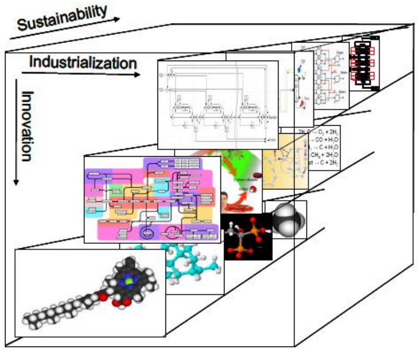

Figure 1: Simplified (bio)chemical supply-chain

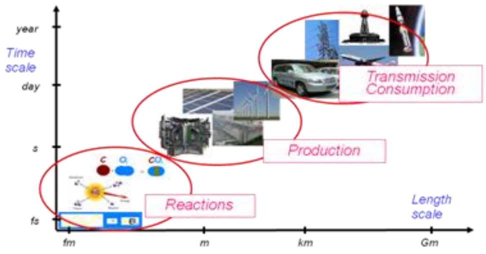

Figure 2: Simplified energy supply-chain

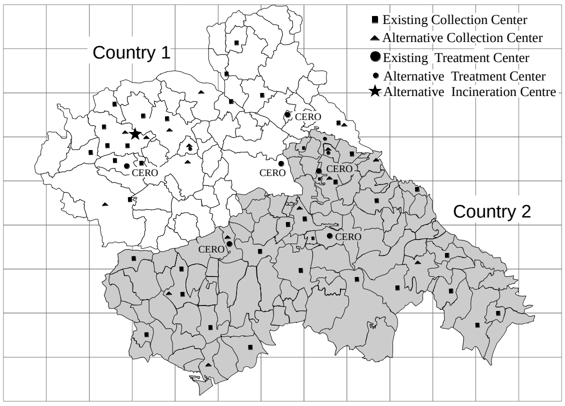

Figure 3: The regional municipal solid waste network

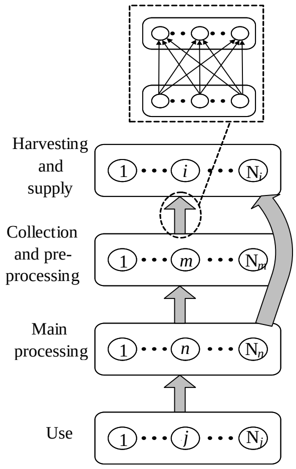

Figure 4: The regional renewable supply and demand network

3. Definitions of sustainability criteria

Economic indicators: In order to establish an appropriate trade-off between continuous cash-flows and investment, either yearly profit (P) or the net present worth (NPW) can be used as economic indicators. If the P or NPW of a studied alternative is compared to a given base case P^0 or NPW^0, relative profit (RP) and relative NPW ($RNPW$) are obtained:

$$RP = P / P^0; \qquad RNPW = NPW / NPW^0 \tag{1}$$

Environmental and social indicators: Environmental indicators are typically grouped into resource usage indicators (material, energy, and water) and pollution indicators (global warming, atmospheric acidification, photochemical smog formation, human health effect, etc.). Social indicators relating to housing and environment, employment, education, safety and health are usually overlooked since their assessment is not a straightforward task.

Different indicators are expressed in different units, e.g. environmental indicators are usually expressed as a burden per some functional unit. Since their units are different, they cannot be composed unless they are normalized. When the indicators (I) of a

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studied alternative represent cradle-to-grave impacts and are compared to those of the selected base case (I^0), relative indicators are obtained, which can then be composed into a life cycle assessment index (*LCAI*), by suitable weighting factors:

$$LCAI = \sum_{i=1}^{N} w_i \cdot \frac{I_i}{I_i^0} \tag{2}$$

4. Multi-objective optimization and synthesis

It should be noted that not all indicators can be easily expressed as eco-costs, and included directly in the objective function, e.g. social indicators. It is usually easier to assign weighting factors to indicators according to our judgement about their importance, and to define *LCAI* (Eq. 2) as a single LCA indicator. Then a multi-objective synthesis can be performed, e.g. by applying ε-constraint method:

$$\begin{array}{ll}
\max PR = (c^{\mathrm{T}} y + f(x)) / P^0 & \\
\text{s.t.} \quad \left.\begin{array}{l} h_l(x, y_l) = 0 \\ g_l(x, y_l) \le 0 \\ LCAI(x, y_l) \le \varepsilon_k \end{array}\right\} \ \forall l \in L & \\
\qquad x \in X = \left\{ x \mid x \in \mathrm{R}^n;\ x^{LO} \le x \le x^{UP} \right\} & \qquad \text{(MO-I-MINLP)}_k \\
\qquad y_l = Y_l,\ \forall l \in L;\ Y_1 \cup Y_2 ... \cup Y_L = Y = \{0,1\}^m & \\
\qquad \varepsilon_k = \varepsilon_{k-1} - \Delta\varepsilon &
\end{array}$$

where profit or relative profit is maximized subject to *LCAI* which decreases sequentially by a suitable step size $\Delta\varepsilon$ until there is no feasible solution. Pareto inferior solutions are obtained in this way. In cases when *P* does not decreases monotonically with *LCAI*, ε-equality constraint can be used rather than the inequality constraint.

The two-step multi-objective MINLP system synthesis

The basic idea is to perform MINLP-1 synthesis of the base case first in order to obtain a reference solution for the sustainable multi-objective MINLP-2 at the second step.

MINLP-1: Problem (I-MINLP) is employed in the first step using a single economic optimization criterion for the selected base case superstructure. The superstructure is composed of economically and technologically-efficient alternatives. The life cycle inventory of the economically-efficient solution obtained provides different base-case indicators, which are used in the next step to normalize the LCA index.

MINLP-2: A sequence of problems $(\text{MO-I-MINLP})_k$ are carried-out in order to perform the multi-objective sustainable synthesis using the ε-constraint or weigthed objective function methods. The superstructure is augmented for additional sustainable alternatives. Pareto solutions are obtained in this way, which are normalized and compared to the solution obtained at MINLP-1.

5. Examples of problems

Several examples taken from literature and solved by the advanced system synthesizer MIPSYN (Kravanja, 2010) serve to illustrate the sustainable MINLP system synthesis:

i) Sustainable process flowsheet synthesis (Kravanja et al., 2005): The well-known hydrodealkylation (HDA) process was studied in the first example. The optimal solution of MINLP-1 yielded a profit of 5.579 M$/a. When the superstructure was extended with alternatives for better conservation of energy, exergy and materials in the process, a set of Pareto optimal solutions was generated in the multi-objective MINLP-2 (Figure 5). It is interesting to note that some economically better solutions were obtained with smaller LCA indexes than in MINLP-1.

ii) Sustainable bioethanol process network synthesis (Čuček et al., 2010b): The MINLP-1 resembles an economically-effective corn-based production process. The solution yielded a profit of 22.786 M$/a for 2 kg/s of ethanol production. In the second step the superstructure is extended to a process network comprising diluted acid pre-treatment, alkaline pre-treatment, and thermochemical conversion routes capable of producing bioethanol from different raw materials which are competing for the same agricultural area of 50,000 ha. A special social indicator for the conversion of food into energy was introduced in order to minimize competition between the food and energy sectors. Figure 6 again shows that significantly higher profit can be obtained with less harmful solutions.

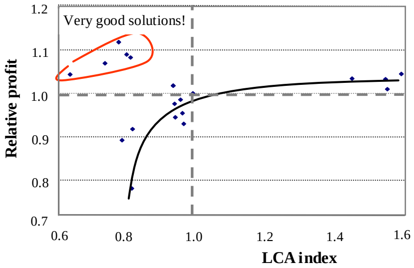

Figure 5: Pareto multi-objective solutions of the HDA example

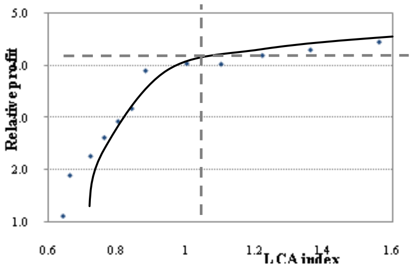

Figure 6: Pareto optimal solutions for a bioethanol process network problem

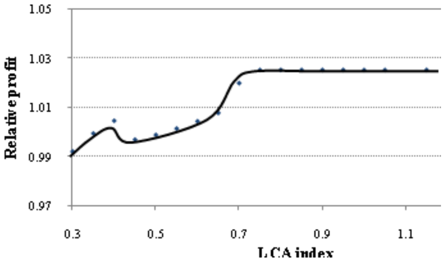

Figure 7: Pareto solutions for the regional renewable network problem

iii) Sustainable synthesis of regional renewable supply and demand networks : The objective was to maximize the profit while satisfying regional demand. A profit of 160 M$/ (a·m^2), carbon footprint of 27.9 kg/m^2 of net production of CO_2 and a food-energy indicator of 4.1 kg/m^2 were achieved and presented for the base-case regional super-structure without pre-treatment. When additional alternatives for densification and the drying of intermediate products were added to the superstructure, somewhat higher profits were obtained, at again significantly smaller LCA indexes (Figure 7).

6. Conclusions

The exampled problems from different applications clearly indicate that, regardless of the general opposition between economics on the one side and environmental sustainability on the other side, significantly more profit and yet less harmful solutions could be obtained if sustainably effective alternatives were embedded into the superstructures. The two-step MINLP approach to sustainable system synthesis proved to be capable of solving simpler supply-chain problems. However, solving of the whole sustainable (bio)chemical and energy supply-chains still remains one of the greatest challenges of the PSE community.

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