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The importance of proper economic criteria and process modeling for single- and multi-objective optimizations

Zorka Novak Pintarič*, Zdravko Kravanja

University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova 17, SI-2000 Maribor, Slovenia

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ABSTRACT

This paper provides an overview of the influences that different economic objectives have on the efficiencies of those optimal process designs obtained by using single- and multi-objective optimizations. Optimizations of monetary criteria, like the profit, lead to operationally and environmentally more efficient but economically less attractive designs than optimization of non-monetary economic objectives, like the internal rate of return. The net present value produces compromise designs with intermediate efficiencies and environmental impacts. These differences are significant only if the processes' mathematical models are sufficiently accurate for establishing appropriate trade-offs between investment and cash flow. The Pareto curves obtained by different economic objectives vary regarding the maximum environmental impacts and in the intervals of the environmental indicators. The composed criteria that combine the economic and environmental indicators into one single objective produce smaller differences between optimum designs that are closer to those designs with minimum possible environmental impacts.

1. Introduction

Nowadays, process optimization is an important tool for reducing resource consumption and operating costs as well as increasing the values of the companies (Mohr et al., 2012). Process flow sheets could be optimized either for one or more objectives leading to single- and multi-objective optimizations, respectively (Lee et al., 2008). The advantages of a single-objective optimization (SOO) are clear definitions of the objective functions, straightforward solution approaches, single best optimum result generated, and a rather clearer interpretation of this result. However, when optimizing one criterion (usually the economic one) other important objectives remain ignored (Savić, 2002) which may lead to environmentally and operationally less efficient process designs. This shortcoming can be overcome by using multi-objective optimization (MOO) where several objectives are taken into account, and the trade-offs between them are established (Rangaiah and Bonilla-Petriciolet, 2013), thus providing more realistic solutions. The drawbacks of this approach are that the definitions of multi-criteria objective functions are not straightforward and often include subjective assessments. Besides, there are many different solution approaches and very large sets of non-dominated optimum results can be generated, from which it can be difficult to choose a single final process design.

In the past, the Process Systems Engineering community has devoted special attention to developing modeling approaches and solution strategies for more and more complex problems in terms of the number of optimization variables and model equations (Hartwich and Marquardt, 2010), as well as the complexities in the models like the nonconvexities and bilinearities (Ruiz and Grossmann, 2013). The influences of process modeling and the types of objective functions on the optimum designs have received less attention. The characteristics of optimal process designs obtained by different economic optimization criteria within single-objective optimization were described by Novak Pintarič and Kravanja (2006). Kasaš et al. (2010) have classified specific consequences of using different economic objectives into three groups: the economic, operational and environmental consequences. It was shown by Kasaš et al. (2011) that the appropriate modeling of process flow sheets in connection with proper optimization criteria are crucial for generating good trade-offs between invested funds and generated cash flows.

The most common economic objectives for process optimization are profit and cost. These criteria have been applied to various problems, for example, a gross annual profit was optimized during reactive distillation optimal design (Domingues et al., 2014), and the total annualized cost within wastewater network synthesis

* Corresponding author. Tel.: +386 2 2294 482; fax: +386 2 252 7774.
E-mail addresses: zorka.novak@um.si (Z.N. Pintarič), zdravko.kravanja@um.si (Z. Kravanja).

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(Graciano and Le Roux, 2013). Net present value is used less frequently, for example, Nemet et al. (2015) maximized the expected net present value during Total Site synthesis by considering variations in utility prices. Less than usual economic objectives were also observed, for example, the incremental cumulative net present value for the optimal control of polymer flooding (Zhou et al., 2013), and the total cumulative incremental cost for the online optimization and control of HEN with bypasses (Luo et al., 2013). A few novel economic metrics have also been developed, for example, the normalized and annualized net present value (Mellichamp, 2013).

Specific studies into the influences of economic objectives on optimal process designs were performed by Faria and Bagajewicz (2009) for maximum net present value and return on investment of continuous water networks. The authors demonstrated that both criteria generated substantially different water systems. Typical characteristics of batch and continuous water networks obtained by the more widespread economic criteria were classified by Novak Pintarič et al. (2014).

It was shown recently that single-objective optimization with proper economic objectives, like the net present value, produce specific process designs that represent good compromises between several objectives, like the economic, environmental and operational efficiencies (Kasaš et al., 2012). Anyway, multi-objective optimization has become an important tool for decision-making over the last decade as it explicitly takes into account several conflicting objectives. Multi-objective optimization exploits interactions between these objectives and generates a set of non-dominated (Pareto) solutions from which a compromise process design can be selected (Burger et al., 2014).

A lot of work has been done on solving practical industrial problems for multiple objectives in order to introduce environmental aspects into process design; for example, Liu et al. (2010) optimized a polygeneration system for the net present value as the economic objective and greenhouse gas emissions as the environmental objective. Tokos et al. (2013) performed a bi-objective optimization of a water network within a brewery by considering the total costs and fresh water consumption. The supply network of a large poultry company was optimized for profit and carbon-, nitrogen- and water footprints (Kiraly et al., 2013). The CO_2 removal process was optimized with respect to CO_2 capture rate and minimization of the investment (Tock and Marechal, 2014). Vadenbo et al. (2014) assessed and optimized the thermal treatment of sewage sludge according to six environmental objectives. In order to support decision-making in the conflicting design problems, a simulation-based computer tool for multi-objective optimization and visualization of the Pareto frontiers was presented by Burger et al. (2014).

As the number of the objectives can be very high in practical applications, several methods have been developed for reducing the dimensionalities of multi-objective problems based on, for example, Principal Component Analysis (Pozo et al., 2012), the Mixed Integer Linear Programming method for eliminating the non-conflicting objectives (Kostin et al., 2012) or the Representative Objectives Method (Čuček et al., 2014). Another approach for considering several objectives is to convert multi-objective problems to single-objective ones by using the aggregation of several objectives. This can be done by the monetization of environmental impacts by using LCA-based methods, for example, Environmental Priority Strategies (Lim et al., 2013b) or the eco-costs method (Vogtländer et al., 2001a). Economic measures are then combined with the monetized environmental impacts into a single-objective function producing a single optimal solution based on direct trade-offs between several criteria (Kravanja and Čuček, 2013).

The literature review revealed that many efficient solution methods and strategies for both single- and multi-objective optimizations have been developed in the past, applying various economic objective functions. However, the types of economic objectives, their proper mathematical expressions, and the influences on the optimum results has not attracted a lot of attention. The intention of this paper is to fill this gap by demonstrating the effects of optimum process flow sheet designs over varying economic objectives during both single- and multi-objective optimizations, and to present novel definitions of the composite objective functions that would generate suitable compromises between the conflicting goals during single-objective optimizations. Overall, this paper should guide process engineers toward using: (i) proper economic objectives for optimizations of their processes, (ii) precise and accurate models, and (iii) different approaches to multi-objective optimization that most nearly meet the requirements of decision-making process.

This paper is organized as follows: Section 2 highlights the more important characteristics of using different economic objective functions for single-objective optimization, and presents a summary of our previous work. In Section 3, these concepts are extended to multi-objective optimization in order to show the impacts of different economic objectives on the Pareto curves, and the composed objective functions defined by merging pure economic measures with the eco-economic criteria based on the LCA eco-costs. Two case studies are presented in Sections 4 and 5 in order to illustrate the influences of process modeling, economic objectives, and multi-objective optimization methods on the obtained optimum designs.

2. Single-objective optimization using different economic criteria

The well-known general Mixed-Integer Nonlinear Programming (MINLP) optimization problem in which a single economic objective function is optimized is given by Eq. (1).

$$\begin{aligned} &\max \text{ or } \min f_{\text{econ}}(x, y) \\ &\text{s.t.} \\ &h(x, y) = 0 \\ &g(x, y) \leq 0 \\ &x \in \Re,\ y \in \{0, 1\} \end{aligned} \tag{1}$$

where f_{econ} is a selected economic criterion, h and g are the vectors of the equality and inequality constraints, and x and y are the vectors of the continuous and binary variables.

The most common economic criteria used within the objective functions of process optimization models can be classified into three groups regarding the characteristics of their measurement units: quantitative, qualitative, and compromise criteria (Novak Pintarič and Kravanja, 2006). Quantitative criteria are expressed in monetary units, like profit before or after tax, and total annual cost. Qualitative criteria are expressed in various non-monetary units, like return on investment, payback time, and internal rate of return. These two groups can produce completely different optimal results regarding the economic, operational, and environmental efficiencies. The third group, the compromise criteria produce those optimum solutions that are between the solutions of the other two groups, hence the name *compromise* criteria. A typical representative of this group is the net present value. The more typical economic variables and objectives are the cash flow, net present value (NPV), profit before tax (PR), total annual cost (TAC), and the internal rate of return (IRR). Their definitions are summarized in Appendix A.

It should be noted that many uncertain and varying input parameters appear in these expressions, for example, the tax rate, the discount rate, the depreciation period etc. Sensitivity analyses could reveal the impacts of the fluctuations in various input