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Achieving Profitably, Operationally, and Environmentally Compromise Flow-Sheet Designs by a Single-Criterion Optimization

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Compromise designs that can be achieved to a certain extent in process flow-sheet optimization not only by multicriteria but also by single-criterion optimization are described. A well-balanced compromise between the profitability, operational, and environmental efficiencies can be achieved using a suitable economic criterion. From the financial point of view, the net present value (NPV) is the correct criterion for selection from among mutually exclusive solutions and, hence, for evaluating different designs in process optimization. Other criteria are also often used in engineering practice. It is shown that optimal designs obtained using different economic objectives vary not only in their investment and other financial indicators, but also in operational efficiencies and environmental indicators. Operationally more efficient and environmentally less harmful solutions can be obtained at lower profitability, by increasing the invested funds. The net present value generates the best compromise between these objectives, as illustrated by three flow-sheet synthesis problems.
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Introduction

Mathematical programming is being increasingly used for investment decision-making when designing and synthesizing the process flow-sheets of chemical, biochemical, and other processes. Mathematical models of process units and interconnection nodes at various levels of precision are used in process flow sheet optimization.[1,2] Early design models are formulated at the level of basic physical and chemical phenomena for the rough screening of alternatives. More-detailed equipment models are applied in the following stages to optimize smaller process subsystems more precisely.

Precise model representations of process flow-sheets can be very large, complex, and nonconvex. Over the last few decades, the process engineering community has put a great deal of effort into developing algorithms and strategies for the efficient solving of such optimization problems.[3] Less attention has been paid to the correctness of the economic criteria used in optimization-based flow-sheet synthesis and design. In process systems engineering, mathematical models with different economic objective functions are frequently used for process flow-sheet optimization, such as the total annual cost, annual profit before tax (P_B), the payback time, the net present value (NPV), and the internal rate of return (IRR). In financial theory, however, the NPV is regarded as the correct criterion for selecting from among mutually exclusive alternatives, while the other criteria are not totally correct.[4]

Several authors have observed that different economic criteria affect the optimal designs of processes. Buskies[5] established that those optimal values of process parameters obtained in the optimization of chemical processes depend on an objective function. Novak Pintarič and Kravanja[6] discussed the differences between those optimal process designs obtained by means of qualitative, quantitative, and compromised economic criteria. Faria and Bagajewicz[7] performed a mixed-integer nonlinear programming (MINLP) design for water utilization systems by maximizing the NPV and the IRR, and also observed different optimal solutions. Lee et al.[8] simultaneously optimized process plants for several economic objectives. Sandahl and Sjorgen[9] conducted a survey about the economic criteria used in Sweden's corporations for capital budgeting. They found that the payback method is the most commonly used method within all industries. The advantages and drawbacks of the payback method were discussed by Lefley.[10] Certain new criteria have also been developed, e.g., residual economic function[11] which can be used for expressing profitability under uncertainty, especially within the petrochemical industry. Bagajewicz[12] examined the validity of the NPV in investment capacity planning models, and suggested to utilize the capital at the maximum profitability possible.

In our recent work,[13] the origin of differences between optimal solutions obtained by different economic criteria was cleared up. It was shown that accuracy and precision of a flow-sheet optimization model is the key in explaining and exploring these differences. The simplification and

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aggregation of a process flow-sheet model may, in some cases, distort the major trade-offs between the investment and generated cash flow, and prevent the generating of a proper optimal solution with the correct economic criterion. On the contrary, more precise models establish proper trade-offs between investment and cash flows. Significant differences between optimal solutions generated by different economic criteria are observed only if precise and accurate modeling is used. Full advantage can be taken from using the correct optimization criterion in such models.

The process engineering community has also neglected the influences that different economic criteria have on the operating efficiencies and environmental performances of optimal flow-sheet designs, although the optimization is increasingly used for improving the operational and environmental efficiencies of various engineering systems. The great potential of the simultaneous optimization and heat integration of process flow sheets was discovered more than two decades ago. It was shown that a simultaneous approach leads to higher profit by producing substantial savings on raw materials and utility consumptions, while increasing the overall conversion.[14] Recently, the potential of process integration for improving the energy efficiencies of industrial processes, was described by Klemes et al.[15] Optimization was used for increasing the second-law efficiency in binary distillation.[16] The problem of optimal hydrogen storage design with maximum efficiency was addressed by Georgiadis et al.[17] The efficiency of the membrane process for upgrading synthetic natural gas produced from lignocellulosic biomass was studied by considering the costs and efficiency.[18] Brown et al.[19] studied a trade-off between total investment costs and the exergy efficiency of electricity production during wood gasification. Xu et al.[20] optimized a power generation system by maximizing its energy and system efficiencies, as well as its profit. The thermal efficiency of a combined cycle power plant was increased by minimizing the cost function.[21]

Besides the various types of operational efficiencies, many authors have also addressed the evaluation of environmental performance during optimization. The application of life cycle assessment to process optimization was discussed by Azapagic and Clift.[22] The WAR algorithm[23] was developed for assessing the generation of environmental impact within chemical processes. Mata et al.[24] used the WAR algorithm to analyze the environmental performance of gasoline blending components through their life cycles. Guillen-Gosalbez et al.[25] combined life cycle assessment and multiobjective MINLP techniques for the environmentally conscious design of sustainable chemical processes. The environmental impact of energy production from sunflower seeds was evaluated by Simone et al.[26] by applying life cycle assessment. Pistikopoulos et al.[27] combined economic and environmental criteria to optimize the energy systems of the future.

Some authors have addressed both, the operating efficiency and the environmental performance in multiobjective optimization of engineering systems. Emun et al.[28] applied simulation and optimization for improving the efficiency and environmental performance of an integrated gasification combined-cycle. Liu et al.[29] developed a mixed integer programming framework for the optimal design of energy systems with improved energy efficiency and environmental performance. Siitonen and Ahtila[30] investigated the relationship between energy efficiency improvement and CO_2 emission reduction in a pulp and paper mill, while maximizing the cost savings objective function.

The cited references show that operating efficiency and environmental impact have attracted great interest from the research community, whereas very little attention has been given to the types of economic objective functions used in optimization models. Therefore, the purpose of this article is to show how the economic decision criteria affect trade-offs between the profitability, and the operational and environmental efficiencies, in process flow-sheet optimization. The main goals of this work are to (1) discuss the correctness of the economic criteria often used in process flow-sheet optimization, (2) demonstrate that incorrect criteria affect not only the investment level and financial indicators of optimal flow-sheet designs but also their operational efficiencies and environmental indicators, and (3) demonstrate that a well-balanced compromise between the operational efficiency, profitability, and environmental impacts can be established to a certain extent, if a suitable economic function is applied to single-criterion flow-sheet optimization.

The above ideas are illustrated by three process synthesis examples which are handled in a nontrivial way: all case studies are modeled as rather large and complex MINLP problems with simultaneous topological and continuous decisions; detailed modeling of process units is used, like kinetic reactors and equilibrium-based separators. Heat integration is simultaneously considered in all case studies; environmental decision-making is included in some models, like waste water treatment and cogeneration.

Problem Statement for Single-Criterion Economic Flow-Sheet Optimization

The general mathematical model for single-criterion process synthesis and design is described by the following MINLP formulation

$$\begin{aligned} \text{min or max}\ \ & Z = c^{\mathrm{T}}\mathbf{y} + f(\mathbf{x}) \\ \text{s.t.}\ \ & \mathbf{h}(\mathbf{x}) = 0 \\ & \mathbf{g}(\mathbf{x}) + B\mathbf{y} \le 0 \\ & A\mathbf{y} \le a \\ & \mathbf{y} \in \{0,1\}^m, \ \ \mathbf{x} \in \Re^n \end{aligned} \qquad \text{(MINLP)}$$

where Z is the economic criterion which is either minimized, as the total cost, or maximized, as the profit. The objective function is composed of investment costs, c, and the term of continuous cash flows, f, which include the operating costs, revenues, depreciation, etc. $\mathbf{y}$ is the vector of binary variables for discrete decision making, and $\mathbf{x}$ is the vector of continuous variables, such as flow-rates, temperatures, and equipment sizes. The vector of design equalities $\mathbf{h}$ represents mass and heat balances, sizing constraints, etc., the vector of inequalities $\mathbf{g}$ represents the various production specifications, e.g., purity requirement, whereas a, c, A, and B are the constant vectors and matrices. The expression, $A\mathbf{y} \le a$, describes any logical constraints. The above model represents an efficient and advanced support tool for making discrete and continuous investment decisions, simultaneously. Discrete decisions relate to the selection of alternative equipment during the flow-sheet design, whereas continuous decisions relate to the selection of operating parameters and equipment sizes.

A general flow-sheet synthesis problem (MINLP) contains a single objective function. If several objectives, such as

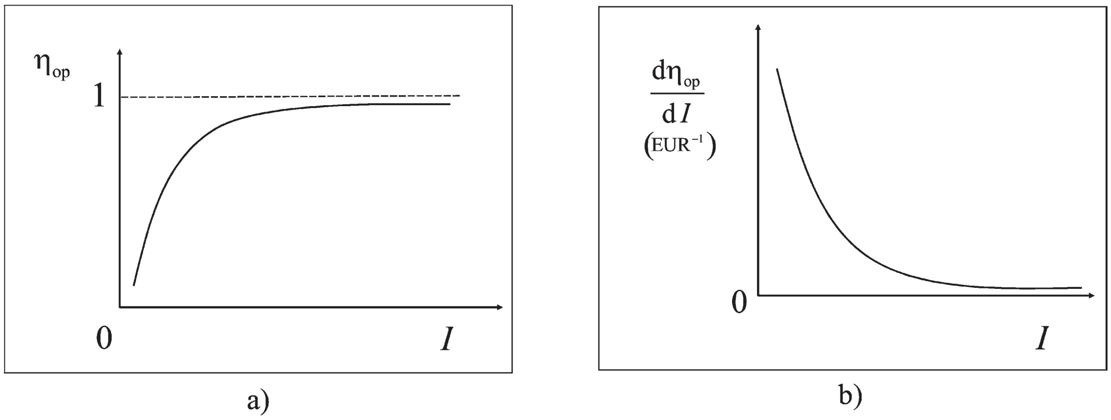

Figure 1. Efficiency curve (a) and its derivative (b) vs. investment.

economic, environmental, and technological, need to be considered simultaneously, a multicriteria optimization is applied to generate a set of Pareto optimal or efficient solutions that trade-off different (usually) conflicting criteria.[31,32] This can be achieved by the weighted sum method or different scalarization techniques, e.g., the ε-constrained method.[33] The problem with multiobjective optimization is that computational effort and difficulty of the results interpretation grow with the number of objectives. Systematic methods have been proposed to reduce the number of objectives.[34] Anyway, the final decision still should be done by the decision-makers, who must select a final, single flow-sheet design according to their goals and preferences.

Within economic-based single-criterion optimization, the ultimate decision criterion is a measure of economic performance, whereas the other criteria are not explicitly included in the decision process. In this work, the problem (MINLP) is solved as a single-criterion optimization problem for different economic criteria, either the profit, IRR, or the NPV. As these economic objectives produce different optimal solutions from the economic point of view, it is expected that the solutions are also different regarding their environmental end operational performances. The operational efficiencies and environmental indicators are, therefore, evaluated after optimization to compare the performances of those optimal flow-sheet designs obtained by different economic criteria. The subsequent chapters show, that more compromise solutions in terms of economic profitability, operational efficiency, and environmental performance can be achieved, not only by multicriteria but also by single-criterion optimization when applying a suitable economic criterion. However, let us first discuss the economic and operational efficiencies.2

Economic and Operational Efficiency

As already shown in the Introduction section, the efficiencies of engineering systems can be expressed in many different ways using economic and technological measures. Economic efficiency is defined as the ability of a company to produce and distribute its product at the lowest possible cost, whereas technological efficiency refers to the ability of producing maximum output at an acceptable quality, using minimum inputs.[35]

In the case of process flow-sheets, the overall technological efficiency of the process operation depends on several different efficiencies that cannot be directly expressed by a single technological indicator. For example, the efficiency of a reactor section can be measured by the per-pass conversion of the key reactant and/or by the overall conversion, the efficiency of the separation section by the main product's purity, the energetic efficiency by the level of heat integration between process streams, etc. In financial statement analysis, however, various ratios are used for analyzing a company's economic efficiency, e.g., (gross) profit margins or return on sales. Return on sales and the profit margin are computed as a ratio between the net income and sales.[36,37] A gross profit margin is defined as the difference between the sales and cost of goods sold, divided by the sales.[38]

An increase in technological efficiency results in increased economic efficiency, because it is reflected directly in higher revenue or lower operating costs. Assuming a constant efficiency of the business functions (accounting, finance, and marketing), the constant prices of raw materials, energy, labor, etc., and the constant production rate at nominal capacity, the economic efficiency ratio can be applied to express the overall technological efficiency by one single measure, i.e., operational efficiency, η_{op}

$$\eta_{op} = \frac{R - E}{R} \tag{1}$$

where R (€/year) represents the revenue from sales, and E (€/year) represents the expenses, e.g., cost of raw material, utilities, and labor.

The operational efficiency defined in this way can be used for comparing the overall technological efficiencies of those optimal solutions obtained by different economic criteria. Maximum efficiency ($\eta_{op} = 1$) could be theoretically obtained at zero expenses. By contrast, if the expenses were to approach or exceed the revenues, the efficiency would drop to zero or even lower. Within the industry, technological efficiency could be improved by investing money which results in increased benefit, e.g., higher conversion in the reactor, higher heat recovery in the heat exchanger network (HEN), higher purity of the products in the separator, and higher photovoltaic efficiency.[39] Such improvements increase the efficiency, as shown in Figure 1a. The more the money invested, the higher the efficiency achieved, but the growth rate slowly diminishes until the efficiency reaches a constant level. At a high investment levels, practically no additional increase in efficiency can be achieved by further investment. Because of the increasing shape of the efficiency curve, its derivative has a monotonically decreasing shape, which asymptotically approaches zero (Figure 1b).

Economic Optimization Criteria

Three economic criteria are considered in this work to analyze the relationships between the economic profitability, operational efficiencies, and environmental performances of those optimal solutions obtained in process flow-sheet optimization: annual P_B, the NPV, and the IRR. Several financial expressions need to be evaluated within the model (MINLP) to define these criteria. The cash flow and capital investment are the most important. Cash flow, F_C, is defined by the following equation

$$F_C = (1 - r_t)(R - E) + r_t \frac{I}{t_D} \quad (2)$$

where r_t represents the tax rate, I (€), the capital investment, and t_D (year), the depreciation period. The term ($R - E$) actually represents any gain resulting from the invested money. The second part is a tax credit of depreciation originating directly from the investment. In the case of a retrofit project, Eq. 2 can be transformed into the differential cash flow function, where the differences between the initial and retrofitted solutions are used, e.g., savings of the retrofitted solution and the differential investment needed for process retrofit. Revenues and expenses are calculated using the spot prices of products, raw materials, utilities, etc., whereas the investment cost can be assessed by various diagrams and correlations[40] or software programs.[41] Different economic criteria can be defined based on the evaluated cash flow and investment.

Quantitative criteria are expressed in monetary units. Typical examples are the cost and the profit. The P_B (€/year) is defined as follows

$$P_B = R - E - D \quad (3)$$

where D represents the annual investment charge, i.e., depreciation (€/year).

By combining Eqs. 2 and 3, and assuming a straight-line depreciation method with zero salvage value, the profit could be expressed in terms of the cash flow and investment

$$P_B = \frac{1}{1 - r_t}\left(F_C - \frac{I}{t_D}\right) \quad (4)$$

Qualitative criteria are expressed in nonmonetary terms, e.g., minimization of payback time or maximization of the IRR. The latter can be replaced by minimization of the present value annuity factor, which decreases monotonically with the IRR, r_{IRR}

$$f_{PA}(r_{IRR}) = \frac{I}{F_C} \quad (5)$$

where f_{PA} is a present value annuity factor at an IRR r_{IRR}, and the project's lifetime t_L

$$f_{PA}(r_{IRR}) = \frac{(1 + r_{IRR})^{t_L} - 1}{r_{IRR}(1 + r_{IRR})^{t_L}} \quad (6)$$

The IRR is calculated iteratively after optimization from Eq. 6. Equation 5 also presents the expression for payback time, assuming zero working capital.

Compromise criteria are based on discounted cash flow methodology. The most known representative is the NPV, V_{NP} (€)

$$V_{NP} = -I + f_{PA} \cdot F_C \quad (7)$$

where f_{PA} is a present value annuity factor at a given discount rate, r_d

$$f_{PA} = \frac{(1 + r_d)^{t_L} - 1}{r_d(1 + r_d)^{t_L}} \quad (8)$$

The optimality conditions for the above economic criteria are well-known. The maximum NPV is obtained at the investment level where the marginal (incremental) NPV is equal to zero and the marginal IRR is equal to the minimum acceptable rate of return (MARR).[6] In practice, this means that process units should only be enlarged as long as the incremental increase has a positive marginal NPV, and the incremental IRR is above MARR. The maximum P_B and the IRR are obtained at those investment levels where the marginal profit and the IRR, respectively, become equal to 0.

The above economic criteria produce different optimal results, as it should be expected from different stationary conditions. The financial consequences of using different criteria during process synthesis and design were discussed by Kasaš et al.[13] They showed that the investment levels of optimal solutions increase from the IRR, over the NPV to the P_B criterion. Maximization of IRR stimulates smaller process designs and fast (re)investment of capital. On the other hand, maximizing the profit results in large processes and higher cash flows, but also requires higher capital investments, thus achieving slower turnover. The NPV results in an intermediate size of the process. This is a compromise criterion, as it establishes a compromise between the investment costs, and the profitability of the invested money.

Each one of the optimal designs obtained by different criteria could be potentially interesting for particular investors, as investors seek various benefits in return for their investment. Nevertheless, some of the above-mentioned criteria are inappropriate for optimization-based investment decision-making, as discussed in the next section.

The Correct Criterion for Process Flow Sheet Optimization

The evaluation of different designs during process flow-sheet optimization represents a selection from among mutually exclusive alternatives. In financial theory, it is well-known that the NPV is the correct criterion for selection between competing projects, whereas IRR and profit are not. While the NPV increases the value of a firm over a long period, the IRR mistakenly favors projects with small investment cost, quick payback, and high profitability.[4] IRR apparently stimulates the fast reinvestment of capital, and ignores the amount of investment. Quantitative criteria, such as total annual costs and profit are accounting measures, which are not based on cash-flows and are, thus, inappropriate for investment decision-making. They do not take into account the time-value of money and favor late cash flows. These criteria stimulate large projects with lower profitabilities.

The flow-sheet optimization problem, as defined in the (MINLP) model, represents the selection of optimal design from the portfolio of alternatives included within the model.

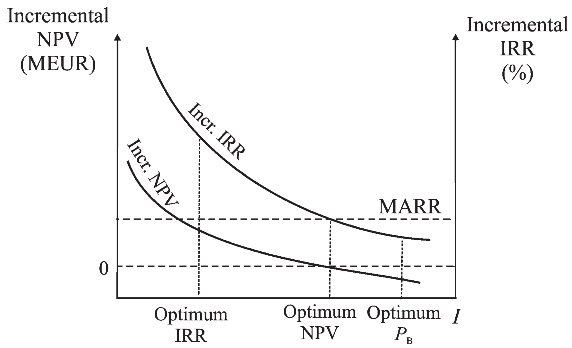

Figure 2. Incremental stationary conditions.

Capital investment is more often assumed to be the unconstrained variable, which means that funds are available for realization of the selected optimal solution. The mathematical model defines the boundaries of the investment project under consideration. Any investment option outside of the system's boundary is irrelevant for this study. According to finance and accounting textbooks, the NPV is the correct criterion for such types of investment projects.[42] The NPV uses all the cash flows of the project, and then discounts the cash flows properly. It can be used in its basic form for comparing exclusive process designs with different investment levels and equal lifetimes.[43] By contrast, mutually exclusive alternatives cannot be compared by their individual internal rates of return, and an incremental analysis of the IRR is needed. Figure 2 represents the incremental NPVs and IRRs of typical optimal solutions obtained by maximizing IRR, NPV and P_B criteria.

As seen in Figure 2, optimal NPV is obtained at the investment level where the incremental NPV drops to 0, and the incremental IRR drops to the MARR. Further increase of investment results in negative incremental NPV, and an incremental IRR below MARR. The optimum P_B solution occurs within this unfavorable region, because its investment level is always higher than the NPV solution.[13] The optimum IRR solution is achieved at a lower investment level than NPV. Within this region, the incremental NPV is higher than 0, and the incremental IRR is well-above the MARR. This indicates that investing the extra capital is completely justified up to the level of the optimum NPV solution, and confirms the economic superiority of the NPV solution for investors, over the remaining two results. IRR and P_B solutions, besides being financially less attractive, also have lower or falsely optimistic values regarding operational efficiency and environmental performance, as shown in the next sections.

Operational Efficiency and its Stationary Conditions

The relationships between the operational efficiencies of optimal solutions generated by different economic criteria can be derived through the expression of stationary conditions for economic criteria in terms of efficiency.

Stationary condition for P_B

The stationary condition for the operational efficiency of a maximum profit solution is obtained by the differentiation of Eq. 3

$$\frac{dP_B}{dI} = \frac{d(R-E)}{dI} - \frac{dI}{t_D dI} \tag{9}$$

Because at the stationary point of maximum profit, the derivative dP_B/dI is 0, it follows that

$$\left(\frac{d(R-E)}{dI}\right)_{\max\ P_B} = \frac{1}{t_D} \tag{10}$$

Assuming constant sales, Eq. 10 can be divided by the revenue R, which gives the stationary condition for the efficiency of the maximum profit solution

$$\left(\frac{d\eta_{op}}{dI}\right)_{\max\ P_B} = \frac{1}{R}\frac{1}{t_D} \tag{11}$$

It can be seen from the right-hand side of Eq. 11, that at the stationary point of maximum profit, the derivative of operational efficiency vs. investment has a constant positive value depending on the revenue and depreciation period.

Stationary condition for NPV

The stationary condition for operational efficiency of the maximum NPV solution is obtained by differentiating Eq. 7

$$\frac{dV_{NP}}{dI} = -1 + f_{PA} \cdot \frac{dF_C}{dI} \tag{12}$$

Considering Eq. 2 for F_C, we obtain

$$\frac{dV_{NP}}{dI} = -1 + f_{PA} \cdot \left[(1-r_t)\frac{d(R-E)}{dI} + \frac{r_t}{t_D}\frac{dI}{dI}\right] \tag{13}$$

Because the derivative dV_{NP}/dI is 0 at the stationary point of maximum NPV, it follows from Eq. 13

$$\left(\frac{d(R-E)}{dI}\right)_{\max\ NPV} = \frac{1}{1-r_t}\left(\frac{1}{f_{PA}} - \frac{r_t}{t_D}\right) \tag{14}$$

Stationary condition for the efficiency of the maximum NPV solution, is obtained by dividing both sides of Eq. 14 by R

$$\left(\frac{d\eta_{op}}{dI}\right)_{\max\ NPV} = \frac{1}{R} \cdot \frac{1}{1-r_t}\left(\frac{1}{f_{PA}} - \frac{r_t}{t_D}\right) \tag{15}$$

At the stationary point of maximum NPV, the operational efficiency again has a constant positive value which depends on the revenue, the predetermined values of the discount rate, the life and depreciation periods, and the tax rate.

The efficiency stationary conditions in Eqs. 11 and 15 are expressed in the inverse monetary unit, e.g., EUR^{-1}. To evaluate the relationships between stationary conditions independently of the revenue R, the expression $R(d\eta_{op}/dI)$ is graphically represented in Figure 3. This expression is shown for maximum P_B with respect to the length of the depreciation period, and for a family of NPV curves at two discount rates (r_d = 10 and 35%) and three tax rates (r_t = 15, 25, and 40%) with respect to the life and depreciation periods. Assuming, e.g., a 10-year lifetime, the value $R(d\eta_{op}/dI)$ at the point of maximum profit is 0.10 $year^{-1}$. Assuming a discount rate of 10%, life and depreciation periods of 10 years and a tax rate of 25%, the value $R(d\eta_{op}/dI)$ at the point of maximum NPV amounts to 0.18 $year^{-1}$.

It can be concluded from Figure 3 that the slope of the efficiency curve ($d\eta_{op}/dI$) at the stationary point of maximum NPV is always higher than at the stationary point of a maximum P_B. The difference between the optimal solutions is

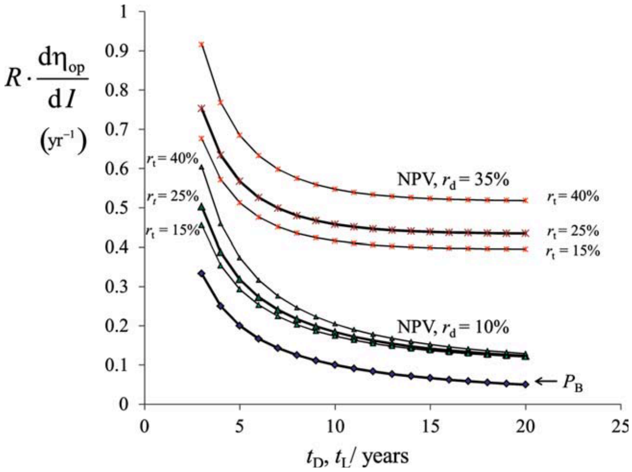

Figure 3. Efficiency derivative at maximum P_B and NPV.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

larger at higher discount rates, however, it is less-sensitive to the depreciation/lifetime period. When considering the higher efficiency derivative of the maximum NPV criterion and the decreasing shape of the efficiency derivative vs. investment, it can be concluded that the investment level of the optimal NPV solution is lower than the investment level of the optimal P_B solution (Figure 4a). Moreover, because of the increasing shape of the efficiency function vs. investment, the operational efficiency of the maximum NPV solution is always lower than the efficiency of the maximum P_B solution (Figure 4b).

Stationary condition for IRR

The stationary IRR condition for the minimum present value factor is obtained by the differentiation of Eq. 5

$$\frac{d[f_{PA}(r_{IRR})]}{dI} = \frac{1 \cdot F_C - I \cdot \frac{dF_C}{dI}}{(F_C)^2} = 0 \tag{16}$$

By inserting the Eq. 2 for F_C into Eq. 16 the following is obtained

$$\left(\frac{d(R-E)}{dI}\right)_{\text{max IRR}} = \frac{R-E}{I} \tag{17}$$

Dividing Eq. 17 by R, we obtain

$$\left(\frac{d\eta_{op}}{dI}\right)_{\text{max IRR}} = \frac{1}{R}\frac{R-E}{I} = \frac{\eta_{op}}{I} \tag{18}$$

At the stationary point of IRR, the value of the efficiency derivative is proportional to the ratio between $R - E$ and the investment I. As this ratio is maximized directly during the maximization of IRR, it could be expected that the stationary point of maximum IRR would occur at higher values of efficiency derivative, forcing the optimum IRR solution to lower investment levels than the NPV and P_B solutions (Figure 4a). The efficiency of the optimal IRR solution is thus lower than the efficiencies of the maximum NPV and P_B solutions (Figure 4b). The main conclusion that follows is that the operational efficiencies of those optimal solutions obtained using different economic criteria increase from the IRR, over the NPV, to the P_B solution.

Environmental performance

Although the relationships between operational efficiency and various economic criteria were derived analytically in the previous section, no such expressions can be derived for environmental performance. Nevertheless, various methods have been developed to assess environmental impacts of products and processes. Particularly, metrics based on life cycle assessment principles have gained wider interest in the recent past, as they assess environmental impacts from design to disposal i.e., across the entire lifecycle, a so-called cradle to grave approach, e.g., Ecoindicator 99 (http://www.pre.nl/content/eco-indicator-99), IMPACT 2002+ (http: //www.sph.umich.edu/riskcenter/jolliet/impact2002+.htm), CMLCA (http://www.cmlca.eu/), etc. The goal of our work is to measure and compare environmental impacts of optimal designs obtained by different economic criteria. These designs use the same chemicals and energy sources. The only things that vary are the amounts of input and output materials and energy consumptions. WAR algorithm is therefore preferred in this article for evaluating the environmental (un)friendliness of optimal process designs, by evaluating their potential environmental impacts (PEIs). The WAR algorithm was already employed as a sustainability assessment code in a software platform for computer aided design of sustainable processes.[44]

The PEI of any material and energy that enters and leaves a process flow-sheet is defined as the effect that this material and energy would have on the environment if they were to be emitted into it. If this release were to occur, it would have a quantifiable effect, i.e., a PEI. PEI is a conceptual quantity that cannot be measured directly, but can be estimated from measurable or estimable quantities.[23] The basis of PEI assessment is the following environmental impact balance

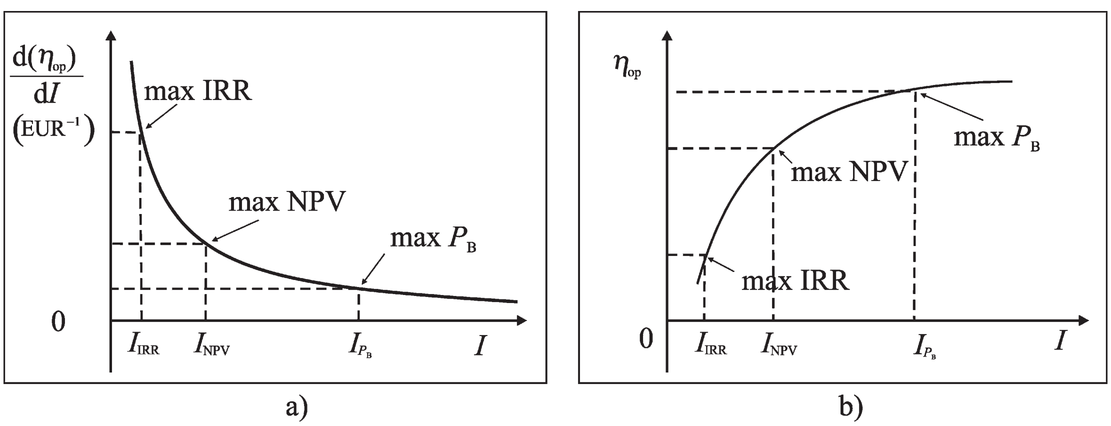

Figure 4. Efficiency derivative (a) and efficiency function (b) of optimal solutions.

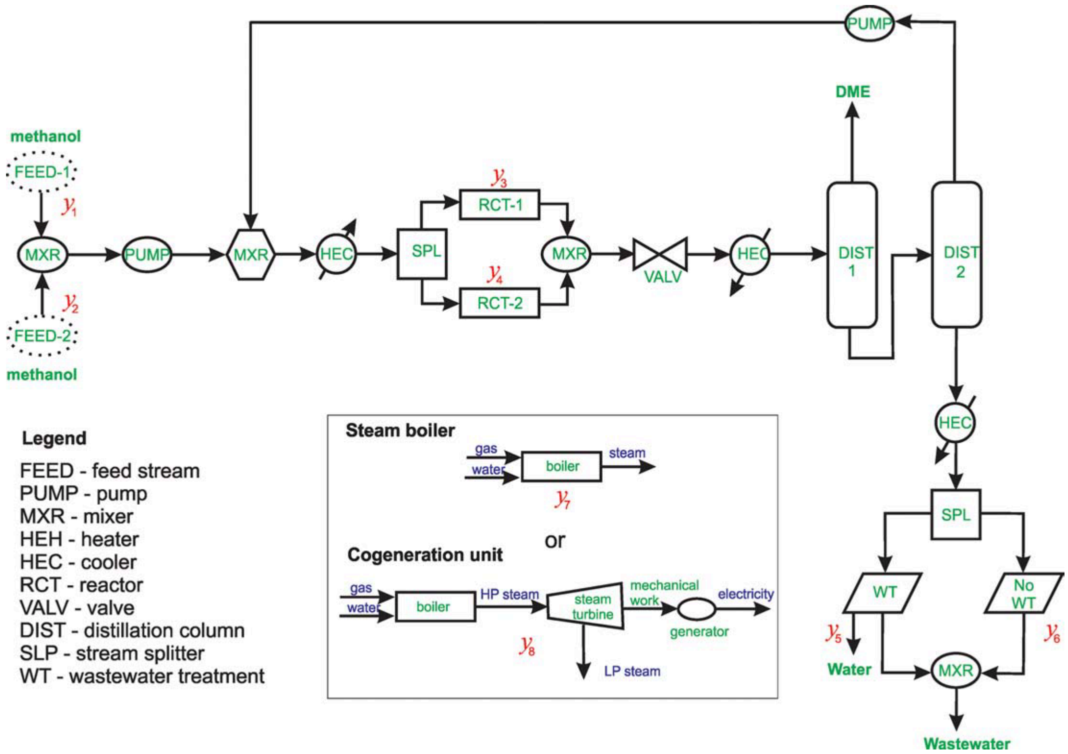

Figure 5. Superstructure of DME process.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

$$\frac{\partial I_t}{\partial t} = \dot{I}_{in}^{(cp)} + \dot{I}_{in}^{(ep)} - \dot{I}_{out}^{(cp)} - \dot{I}_{out}^{(ep)} - \dot{I}_{we}^{(cp)} - \dot{I}_{we}^{(ep)} + \dot{I}_{gen}^{(t)} \quad (19)$$

where I_t is the amount of PEI inside the system (chemical process plus energy generation process), $\dot{I}_{in}^{(cp)}$ and $\dot{I}_{out}^{(cp)}$ are the input and output rates of PEI to the chemical process, $\dot{I}_{in}^{(ep)}$ and $\dot{I}_{out}^{(ep)}$ are the input and output rates of PEI to the energy generation process, $\dot{I}_{we}^{(cp)}$ and $\dot{I}_{we}^{(ep)}$ are the outputs of PEI associated with waste energy lost from the chemical process and the energy generation process, and $\dot{I}_{gen}^{(t)}$ is the generation rate of PEI inside the system. The left-hand side of Eq. 15 becomes zero under the stationary conditions. The waste energy emission terms are usually neglected, while the inputs and outputs of chemical and energy processes are combined into total PEI input and output rate impacts $\dot{I}_{in}^{(t)}$ and $\dot{I}_{out}^{(t)}$, respectively, which results in the following expression

$$0 = \dot{I}_{in}^{(t)} - \dot{I}_{out}^{(t)} + \dot{I}_{gen}^{(t)} \quad (20)$$

The individual terms in Eq. 20 are evaluated based on the mass flow-rates of the input and output streams, their compositions, and the component-specific environmental impacts associated with different impact categories. The user has to define the component flow-rates for all inlet, outlet, waste streams, and total energy consumption in the processes. The WAR algorithm provides a database of eight impact categories for more than 1600 chemicals: (1) human toxicity potential by ingestion (HTPI), (2) human toxicity potential by exposure both dermal and inhalation, (3) terrestrial toxicity potential, (4) aquatic toxicity potential (ATP), (5) global warming potential (GWP), (6) ozone depletion potential, (7) photochemical oxidation potential (PCOP), and (8) acidification potential (AP).

The environmental friendliness of different flow-sheet designs can be compared based on the total PEI output expressed in the PEI per unit of time or production mass. In this work, the total output PEI includes the impacts of the nonproduct streams and the impacts of the energy generation/consumption processes. A design with lower PEI output rate is likely to have lower impact on the environment.

Case-Study Examples

In this section, MINLP syntheses of dimethyl ether (DME), methanol, and toluene hydrodealkylation (HDA) processes were performed, together with simultaneous heat integration. The syntheses were accomplished by single-criterion

Table 1. Economic, Technological, and Environmental Indicators of DME Process

	max IRR	max NPV	max PB
Economic indicators			
NPV (k€)	6111	6303	6207
P_B (k€/year)	1413	1477	1487
IRR (%)	33.01	31.91	30.22
Investment (k€)	3953	4300	4621
Cash flow (k€/year)	1323	1394	1423
Utility cost (k€/year)	568	540	526
CO_2 emission tax (k€/year)	73.8	33.5	32.6
Technological indicators			
Operational efficiency, η_{op}	0.1922	0.2000	0.2010
Recycle stream (kmol/s)	14.40	9.00	6.12
Reactor volume (m^3)	3.81	5.85	8.48
Reboiler power (MW)	2.19	–	–
Cogeneration power (MW)	–	0.28	0.27
Conversion per pass (%)	94.76	96.62	97.68
Environmental indicators			
CO_2 emission (tonnes per year)	4191	1904	1854
Total output PEI (h^{-1})	19.05	18.22	17.82
AP (h^{-1})	13.36	12.60	12.24
GWP (h^{-1})	1.29	1.22	1.18
ATP (h^{-1})	0.243	0.231	0.225

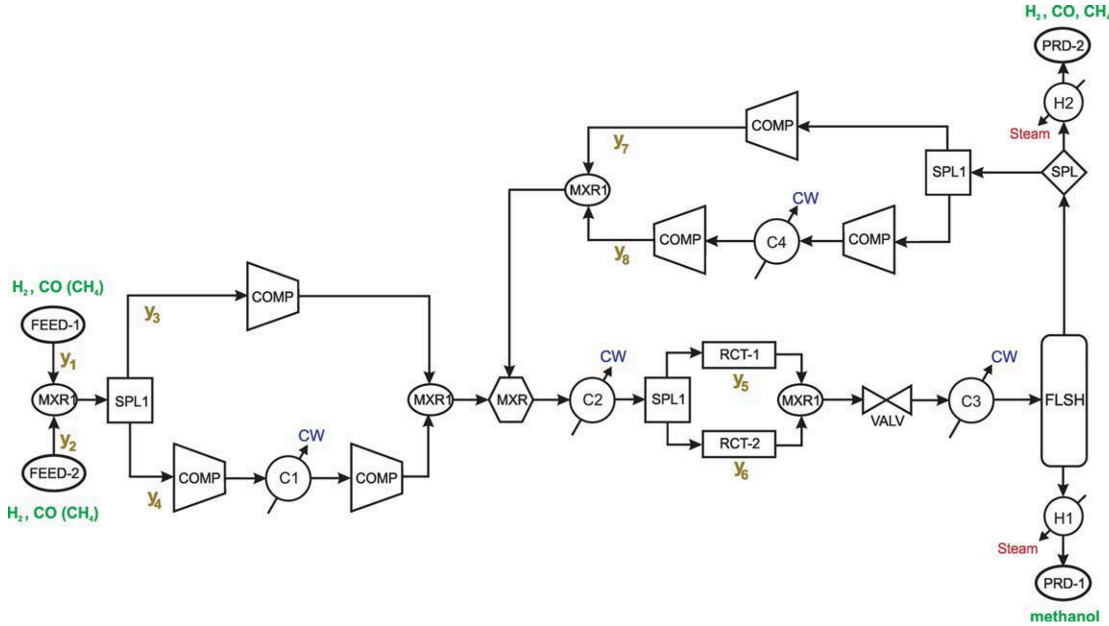

Figure 6. Superstructure of the methanol process.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

optimization using three economic criteria: the profit, the NPV, and the IRR. An MINLP Process Synthesizer MIPSYN was applied with an automated Outer Approximation/Equality Relaxation algorithm.[45] The PEIs of different optimal designs were evaluated after optimization, and the economic, operational, and environmental characteristics were compared.

Dimethyl ether process synthesis

A particular plant produces 50,000 tonnes of DME per year via the catalytic dehydration of methanol over an acid zeolite catalyst. Several impurities are present in the methanol input stream, e.g., acetone, acetic acid, and acetaldehyde. The superstructure of the process (Figure 5) involves topological selections between (1) two feed streams, one of them being more expensive as it contains less impurities, (2) two reactors from which more expensive allows for higher conversion, (3) discharging wastewater or implementing a wastewater treatment plant, and (4) a steam-boiler or cogeneration unit. The kinetic model is used for the reactors and the targeting model for the simultaneous heat integration.[46]

Three economic objective functions are optimized. The more expensive feed stream and reactor are selected in all three optimal solutions, while the wastewater treatment unit is ignored. A steam-boiler is selected for steam production when maximizing the IRR, and the cogeneration unit when using the profit and NPV criteria.

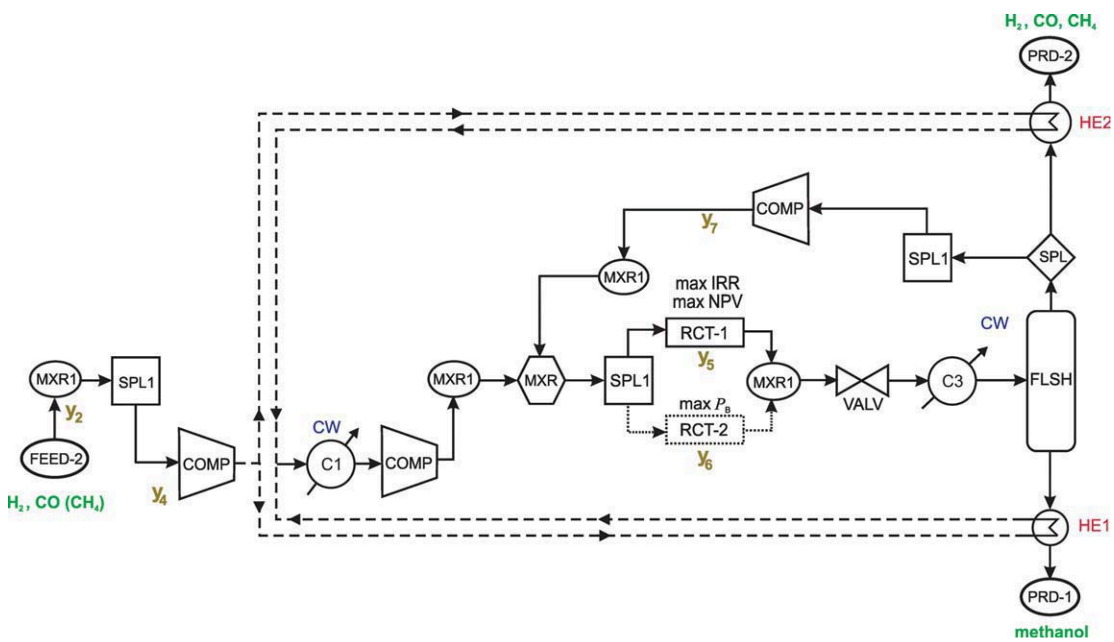

Figure 7. Optimal structure of the methanol process.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 2. Economic, Technological, and Environmental Indicators of Methanol Process

	max IRR	max NPV	max PB
Economic indicators			
NPV (M€)	180.80	181.98	180.92
P_B (M€/year)	38.83	39.26	39.41
IRR (%)	41.69	40.97	39.57
Investment (M€)	82.63	85.24	89.12
Cash flow (M€/year)	34.63	35.13	35.50
Utility cost (M€/year)	11.04	10.68	10.43
Technological indicators			
Operational efficiency, η_{op}	0.4111	0.4204	0.4266
Reactor volume (m^3)	24.60	31.70	29.37
Compressor power (MW)	40.30	38.78	37.87
HEN area (m^2)	2 769	3 285	3 783
Conversion per pass (%)	16.20	18.19	19.56
Environmental indicator			
CO_2 emission (tonnes per year)	76,046	73,177	71,460
Total output PEI (h^{-1})	1351	1067	900
PCOP (h^{-1})	677	504	403
AP (h^{-1})	272	270	164
HTPI (h^{-1})	124	73	45
GWP (h^{-1})	82	80	78

Table 3. Economic, Technological, and Environmental Indicators of HDA Process

	max IRR	max NPV	max PB
Economic indicators			
NPV (k€)	11,856	11,921	11,680
PB (k€/year)	4420	4455	4474
IRR (%)	17.14	17.10	16.80
Investment (k€)	27,097	27,383	28,090
Cash flow (k€/year)	5121	5167	5229
Operating expenses (k€/year)	18,868	18,762	18,704
Technological indicators			
Operational efficiency,η_{op}	0.2481	0.2508	0.2533
Reactor volume (m^3)	19.40	20.24	22.95
Total utility power (MW)	13.49	13.31	11.95
Conversion per pass (%)	42.30	43.18	47.77
Environmental indicators			
CO_2 emission (tonnes per year)	22,185	21,922	19,727
Total output PEI (h^{-1})	131.7	130.2	125.7
PCOP (h^{-1})	49.5	48.8	48.4
GWP (h^{-1})	16.7	16.6	16.1
AP (h^{-1})	48.2	47.5	42.7

The comparisons between different optimal solutions are given in Table 1. The optimal design obtained using the IRR criterion has the lowest operational efficiency with the lowest investment and cash flow, but the highest utility cost and CO_2 emission tax. The comparison of technological parameters shows that conversion per pass in the IRR solution is the lowest among the three solutions. The comparison of the environmental impacts shows that the total PEI output rate of the IRR solution is the highest. Significant differences are observed in the case of AP, GWP, and ATP.

Obviously, the IRR criterion leads to inefficient utilization of reactant and utilities, and high environmental impact. Moreover, the long-term use of IRR leads to suboptimal solutions with respect to NPV optimization. On the other hand, the solution with maximum P_B has the highest environmental and operational efficiencies, however, its economic profitability (expressed as IRR) is the lowest, as P_B does not take into account the time value of money, and thus, favors late cash flows. NPV produces an intermediate result which establishes a balance between a fast return on investment and long-term steady generation of cash flow with fair operational and environmental efficiencies.

Methanol process synthesis

This section discusses MINLP synthesis of a methanol process where methanol is produced from hydrogen and carbon monoxide. The mixture of reactants contains methane as an impurity. This example was taken from literature[47] with the capacity of 980,000 tonnes per year, while the prices were updated. The superstructure of the process (Figure 6)

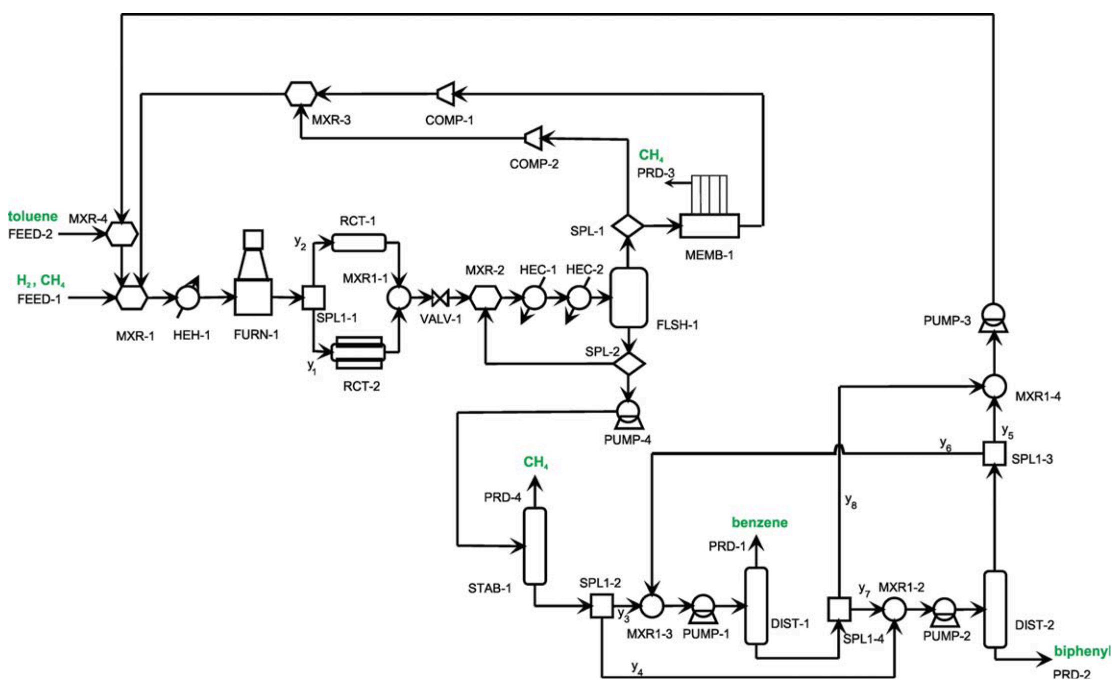

Figure 8. Superstructure of the HDA process.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

involves topological selections between (1) two feed streams, one of which contains less impurity and is more expensive than the other, (2) one-stage or two-stage compressions of the feed stream, (3) two reactors, one of which is more expensive and allows for higher conversion, and (4) one-stage or two-stage compressions of the recycle stream.

The MINLP model[48] is added to the mathematical model of the process superstructure for simultaneous heat integration and HEN synthesis. Three economic objective functions are optimized, as in the previous case. A more expensive feed stream is selected for all optimal solutions together with two-stage compression of the feed stream, and one-stage compression of the recycle stream (Figure 7). The cheaper reactor with lower conversion is selected by maximizing IRR and NPV, whereas a more expensive reactor with higher conversion is obtained by maximizing P_B.

Similarly, to the previous process, the lowest operational efficiency, investment, and cash flow are observed in the case of the IRR solution (Table 2). This solution has also significantly lower conversion per pass than the other two solutions. Heat recovery is low, and consequently, the utility cost is high and the area of HEN is small. Significant differences are obtained in the output PEI rates, in particular in the PCOP, AP, HTPI, and GWP. Apparently, the maximum IRR solution has the worst environmental performance. The P_B solution has good operational and environmental characteristics, but is less profitable, i.e., has a lower IRR value. The characteristics of optimal NPV solution are between the other two solutions.

HDA process synthesis

In this process, toluene and hydrogen are reacted to make 83,000 tonnes per year of benzene. By-products methane and biphenyl are also produced. Nonreacted hydrogen and toluene are separated from the products and recycled for another pass, whereas methane leaves the process within waste streams. The superstructure (Figure 8) involves topological selections between isothermal and adiabatic reactors, and between direct and indirect distillation sequences. The targeting model for minimum utility consumption is applied.

Optimal solutions are obtained by using three objective functions containing the adiabatic reactor and the direct distillation sequence, where benzene is removed as a distillate in the first column, followed by the separation of toluene and biphenyl in the second column. In this case study, the differences between the solutions are small, however, the same trends are observed as in the previous cases (Table 3).The lowest values of operational efficiency, reactor volume, and conversion are obtained by the IRR criterion, while the total operating expenses, including raw material and utility costs are the highest. This confirms the premise that designs with maximum IRR utilize resources less efficiently than other criteria. The IRR solution has the largest environmental impact and P_B solution has the smallest. The difference comes mostly from the differences in the PCOP, AP, and GWP. NPV criterion again establishes a compromise between the economic, operational, and environmental performances of the process flow-sheet.

Conclusion

From the financial point of view, the NPV is the correct criterion for investment projects when choosing from among mutually exclusive alternatives, whereas profit and IRR are not applicable decision criteria. Anyway, they are often used in process systems engineering.

This article presented the consequences of decision-making using different economic objectives within a single-criterion approach, in terms of the economic, operational, and environmental performances of optimal process flow-sheets. It has shown that the selection of economic criterion affects not only the investment level, cash flow, and other economic figures but also the overall operational efficiency and environmental performance of the obtained optimal solutions. Flow-sheet designs with low operational efficiency, ineffective resource utilization, and low sustainability performance are obtained when using the IRR. Maximization of profit produces the most efficient solutions with the lowest operating costs, which are achieved by e.g., the highest conversion, the best separation, and/or the highest level of heat integration. These solutions are, despite the highest investment level, the most environmentally conscious. However, profit is unsuitable for investment decision-making as it does not represent a cash flow, does not account for the time value of money, and favors late cash flows. Thus, IRR and profit are convenient from a practical but not from conceptual point of view. NPV establishes a balance between the profitability of investment and long-term steady generation of cash flow with fair environmental performance and operational efficiency. Such solutions represent correct compromise designs in the financial and environmental sense, as well as in the sense of efficient revenue generation and operating cost control.

The NPV optimization of process flow-sheets certainly cannot replace a multiobjective analysis which gives much deeper insights in the trade-offs between conflicting criteria. Anyway, multiobjective optimization still suffers from some disadvantages, e.g., a procedure is time consuming and sometimes gives small additional information, interpretation of the results can be difficult in case of many objectives, and selection of weights is often controversial, while decision makers still have to select one single design from a set of Pareto solutions according to their subjective preferences. In this perspective, the NPV optimization could be used as a simple alternative approach for quick screening of alternatives that provides a single solution as output, and establishes proper trade-offs between several objectives that could not be generated by other economic measures.

Future work will focus on the consequences of using different economic objectives within multicriteria optimization. It is expected that the selected economic criterion would also affect the set of the Pareto optimal solutions, and that some environmental indicators could not be improved if incorrect economic criteria were to be applied in process flow-sheet synthesis and design.

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