Selection of the Economic Objective Function for the Optimization of Process Flow Sheets

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This paper highlights the problem of selecting the most suitable economic optimization criteria for mathematical programming approaches to the synthesis, design, and optimization of chemical process flow sheets or their subsystems. Minimization of costs and maximization of profit are the most frequently used economic criteria in technical papers. However, there are many other financial measures which can lead to different optimal solutions if applied in the objective function. This paper describes the characteristics of the optimal solutions obtained with various optimization criteria like the total annual cost, the profit, the payback time, the equivalent annual cost, the net present worth, and the internal rate of return. It was concluded that the maximization of the net present worth (NPW) with a discount rate equal to the minimum acceptable rate of return (MARR) is probably the most appropriate method for the optimization of process flow sheets or their subsystems. Similar or equal solutions can be obtained by simpler criteria of minimum equivalent annual cost or maximum profit if the annual investment cost is calculated by using the MARR instead of the straight-line depreciation method. These criteria represent a thorough compromise between quantitative and qualitative measures, because they consider the absolute terms of future cash flows of investments equally important as profitability through the life cycle of the project. The uncertainty related to the value of the MARR was considered by the generation of Pareto optimal solutions for the NPW and by the stochastic analyses of two design example problems.

1. Introduction

Engineers in chemical, biochemical, and other process industries are often faced with the problem of selecting the best solution from a set of alternative projects with respect to selected decision criteria. These criteria are often economical in nature, e.g., minimal cost or maximal profit, and comprise the evaluation of alternatives economics. The latter refers to the evaluation of capital costs, revenues, operating costs, etc. Various approaches, methods, and techniques exist to accomplish the task, and many textbooks treat these topics.[1−4]

Presently, techniques of mathematical programming provide an excellent systematic tool for selecting the optimal alternative if the mathematical description of the problem is available. The optimization process then represents the generation of the best solution, i.e., the selection of the process units in the flow sheet, the sizes of units, the operating parameters, etc. The development of a mathematical model is the crucial step in implementing mathematical programming in the decision-making process. The general model has the following form:

$$\max_{y,x,d} \text{ or } \min_{y,x,d} f(\mathbf{y},\mathbf{x},\mathbf{d})$$
$$\text{s.t.}$$
$$\mathbf{h}(\mathbf{y},\mathbf{x},\mathbf{d}) = 0$$
$$\mathbf{g}(\mathbf{y},\mathbf{x},\mathbf{d}) \leq 0$$
$$\mathbf{x},\, \mathbf{d} \in R,\ \mathbf{y} \in \{0,1\}^m \qquad \text{(P1)}$$

In the model (P1), the vector of binary (0, 1) variables, **y**, is used to denote the rejection or the acceptance of a particular alternative solution (e.g., alternative process structures). The vector of the continuous variables, **x**, represents the operating and control variables, e.g., flow rates, temperatures, pressures, etc. **d** is the vector of the design variables, representing the sizes of the process units, e.g., area, diameter, height, power, etc. **h** and **g** represent various equality and inequality constraints such as mass and energy balances. Problem (P1) in general corresponds to a mixed-integer nonlinear programming (MINLP) problem. In special cases, when the structure of the process is given and when the binary variables are not presented and only the continuous variables are optimized, the problem is reduced to a nonlinear programming (NLP) optimization problem.

The alternative solutions are compared on the basis of the selected decision criterion represented by the objective function *f* in (P1). Frequently, the decision criteria in the mathematical programming problems have an economic character.[5] Indeed, noneconomic, e.g., technical, operating, ecological, and social, criteria can also be considered in the objective function, giving rise to the multiobjective optimization problems that are beyond the scope of this paper.

A brief survey of the economic objective functions used for the synthesis and design of process flow sheets or their parts was performed over the year 2004 in five journals: (1) *Computers and Chemical Engineering*, (2) *Industrial and Engineering Chemistry Research*, (3) *Chemical Engineering and Processing*, (4) *Chemical Engineering Research and Design*, and (5) *AIChE Journal*. The present survey identified 64 papers with economic objective functions used for the optimization of process flow sheets. The objective functions in 36 papers were expressed as the minimization of different types of cost, e.g., the total cost, the operating cost, the logistic and investment cost, etc.[6−41] A maximization of the profit or economic potential was observed in 17 papers, most often expressed as a difference between the incomes and the costs.[42−58] The latter usually comprised different types of operating costs and sometimes also the annualized capital cost. The net present worth (NPW) criterion appeared only in 7 papers.[59−65] Other interesting but less-common criteria were maximization of the cumulative cash

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10.1021/ie050496z CCC: $33.50
Published on Web 05/06/2006

flow,[66] maximization of the monetary value added,[67] the minimization of the investment and inventory opportunity costs reduced for the benefit to the stockholders,[68] and real-options-based valuation to incorporate uncertainty.[69] It is interesting to note that the most common objective functions in the flow sheet optimization problems are expressed as simple cost or profit functions. The maximization of the net present worth was applied in 10% of the papers.

The selection of the optimization criterion strongly influences the generation of the optimal solution, as observed also by Buskies,[70] who applied different economic criteria in the objective function and investigated the differences in the optimal values of the process parameters obtained. The question then arises as to whether engineers use the most suitable criteria for the flow sheet optimization problems.

The aim of this paper is to highlight the problem of selecting the most suitable criteria for the design and synthesis of process flow sheets or their parts by means of mathematical programming, which would consider the future cash flows of investments equally important as their profitability. The main conclusion of the paper is that the compromise criteria, like maximization of the NPW, minimization of the equivalent annual cost, and maximization of the modified profit with the discount rate equal to the minimum acceptable rate of return (MARR), are the most appropriate criteria for the optimization of process flow sheets, since an appropriate tradeoff is established, resulting in a substantial cash flow and high profitability.

2. Profitability Measures for Economic Evaluations of Investment Projects in the Chemical Industry

The goal of the economic evaluation of projects in the preliminary stage is to determine whether they are economically acceptable and to select the best ones for further studies. This evaluation comprises three major steps, the last of which will be discussed in greater depth: (a) estimation of capital costs, (b) estimation of incomes and expenditures, and (c) evaluation of the profitability criteria.

(a) **Capital costs** represent discrete (one-time) expenditures comprising a fixed capital and a working capital. Fixed capital costs are usually estimated by means of fast assessment methods such as factored methods.[71−73] Software for speedy capital cost estimation[74,75] is also available. The working capital (inventories, cash, and accounts receivable) can represent a significant part of the investment in the chemical industry (10−20% of the fixed capital).

The capital costs, also called investment costs, are discrete cash flows and are, therefore, expressed in specific monetary units, e.g., USD, EUR, YEN, etc., whose values are defined in a specified period of time. The estimated capital costs need to be adjusted from one period to another by applying cost indices.[76]

(b) **Estimation of the surplus of the incomes over the expenditures** comprises the determination of all continuous, i.e., positive and negative, cash flows generated by the project such as the revenues, operating costs, etc. On the basis of these figures, the difference between the positive and the negative cash flows can be evaluated. The estimation of the revenues is a relatively simple task since the market (spot) prices of chemicals are usually available, e.g., in the *Chemical Market Reporter*. On the other hand, the estimation of the operating (production) costs of the finished products in a large chemical plant can prove to be quite a difficult task.[77,78] Continuous cash flows are expressed in monetary units per unit of time, e.g., EUR/yr, USD/month, USD/day, etc.

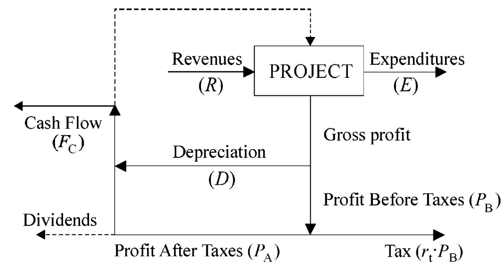

Figure 1. Cash and (non)cash flows in the project.

(c) **Evaluation of the profitability criteria** represents a certain combination of discrete and continuous cash flows, which serves as a measure of the project's profitability and, thus, represents the decision criteria for the selection from among alternatives. The basic financial categories that have to be determined before evaluating profitability criteria, e.g., cash flow, profit, etc., are graphically presented in Figure 1, while the mathematical definitions are given in Appendix I. The economic criteria most frequently used in engineering economics are described in the continuation.

Total Annual Cost, c_t. The total annual cost is a simple criterion which is often used in chemical engineering. It comprises the annual operating costs, c_{op}, and the annual depreciation, D, estimated by the straight-line method,

$$c_t = c_{op} + D = c_{op} + \frac{I_F}{t_D} \tag{1}$$

where I_F is the fixed capital cost and t_D is the depreciation period. The criterion of the total annual cost (TAC) is simple but not based on a real cash flow: it does not consider the time value of money nor taxes.

Profit Before Taxes, P_B. The profit before taxes is calculated as a difference between the revenues, R, and the annual costs including depreciation:

$$P_B = R - c_{op} - D \tag{2}$$

Payback Time, t_{PB}. The payback time measures the period of time required to pay off the initial investment in the fixed capital, I_F, from the annual cash flows, F_C. For a series of equal cash flows, the payback time can be expressed as

$$t_{PB} = \frac{I_F}{F_C} \tag{3}$$

The working capital is usually not considered in the numerator of eq 3 since it is recovered, at least in principle, at the end of the project's lifetime.

Return on Investment, R_{OIB}. The return on investment is usually defined on the basis of profit before taxes, P_B, rather than on the basis of cash flow, which is the case in the majority of other criteria. For this reason, it is more suitable for the economic evaluation of projects in countries with planned economies. It represents a fraction of the total capital investment realized as the profit before taxes each year,

$$R_{OIB} = \frac{P_B}{I} = \frac{P_B}{I_F + I_W} \tag{4}$$

where I represents the total capital investment composed of the fixed capital, I_F, and the working capital, I_W. The return on investment after taxes can be defined by replacing the profit before taxes, P_B, in the numerator of eq 4 with the profit after taxes, P_A. It should be noted that the four profitability measures mentioned above do not take into account the time value of money, i.e., discounting, and can thus be considered static economic criteria.

Net Present Worth, W_{NP}. The net present worth is the arithmetic sum of all cash flows' present worths. It combines the discrete and continuous cash flows for each year into the net cash flow of the project. In a simple case, when the investment is carried out at year 0 and yearly cash flows follow regularly at the end of each year, the net present worth can be expressed as

$$W_{NP} = -I + \sum_{k=1}^{t_\ell} \frac{F_{C,k}}{(1 + r_d)^k} \tag{5}$$

where r_d is the selected discount rate and t_ℓ is the given project's lifetime. Note that the sum of the cash flows incorporates the regular yearly cash flows arising from the production process as well as the positive discrete cash flows arising from the recovered invested capital at the end of the project's lifetime, e.g., the salvage value and the working capital. The selection of the applied discount rate, r_d, is not a straightforward task. The cost of the borrowed capital or the average effectiveness of the realized projects can serve as the reference values for choosing the appropriate discount rate. A higher rate represents more restrictive profitability criteria and, thus, a lower NPW of alternatives. In the early evaluation of projects, constant cash flows can be assumed, which enables eq 5 to be reformulated as follows:

$$W_{NP} = -I + F_C \frac{(1 + r_d)^{t_\ell} - 1}{r_d (1 + r_d)^{t_\ell}} = -I + F_C f_{PA}(r_d) \tag{6}$$

Factor $f_{PA}(r_d)$ is the annuity present worth factor corresponding to the discount rate r_d:

$$f_{PA}(r_d) = \frac{(1 + r_d)^{t_\ell} - 1}{r_d (1 + r_d)^{t_\ell}} \tag{7}$$

Internal Rate of Return, r_{IRR}. The internal rate of return is very often called the *discounted cash flow rate of return*. It is defined as the discount rate at which the net present worth of a project equals zero,

$$W_{NP} = -I + F_C f_{PA}(r_{IRR}) = 0 \tag{8}$$

and

$$f_{PA}(r_{IRR}) = \frac{I}{F_C} \tag{9}$$

With eq 9, the annuity present worth factor can be calculated, and with eq 7, the corresponding discount rate, r_d, which in this case represents the internal rate of return, r_{IRR}, can also be iteratively calculated.

The annuity present worth factor decreases monotonically as the internal rate of return (IRR) increases. Therefore, the programming problem with the maximization of the IRR can be transformed into the minimization of the present worth factor, f_{PA}, from which the corresponding IRR is calculated after the optimization. Note that, in the case of zero working capital, eq 9 for the annuity present worth factor is equal to eq 3 for payback time.

The lowest value of IRR which is acceptable for the investors is usually determined by the MARR, which is selected by the management of the company. The selected MARR value depends on the given economic, political, and social environment into which the investors intend to put their money. The important roles have the risks associated with the project, the market of capital, e.g., cost of debts, and the opportunity costs of the firm's capital. Typically, MARR is set compared to a nonrisk investment, e.g., in the bank. Investors in well-developed and politically stable economy markets will accept the MARR value of, for example, 6%, whereas they will increase this value by up to 5% in the newer markets and even by 20% for any investment in the riskier markets.

Equivalent Annual Cost, c_{eq}. The equivalent annual cost is the sum of the annual investment cost and the total annual outcomes after taxes. The annual investment cost is estimated as the annuity required for the capital to be returned over the lifetime. The total annual outcomes after taxes are the negative values of the cash flow after taxes. In the case of a zero salvage value, the equivalent annual costs, EAC, are estimated by the following expression:

$$c_{eq} = \frac{I}{f_{PA}(r_d)} - F_C \tag{10}$$

The first term in the equation above represents the annualized investment cost calculated with a specified discount rate, which could be chosen as the IRR of previous successful projects or as the MARR.

3. Project Selection by Optimization of Profitability Measures

Engineers are usually faced with several alternative projects rather than one single project. Recently the use of optimization techniques for selecting the best process alternative by means of mathematical programming methods has increased. As the decision space in mathematical formulations of these problems has a positive degree of freedom, solving such optimization problems defacto represents the analysis of an infinite number of alternatives.

Various profitability measures as defined in Section 2 can be applied to the objective function of optimization problems. The solution of such problems is actually equivalent to the incremental economic analysis in which the alternatives are compared on the basis of incremental profitability measures calculated from the differences in costs, cash flows, investments, etc. For example, by the maximization of the NPW, a necessary stationary condition is that the first derivative with respect to the vector of decision variables, **d**, is zero,

$$\frac{dW_{NP}}{d\mathbf{d}} = 0 \tag{11}$$

from which it then follows that the optimal solution with maximum NPW is identical to the solution with the incremental NPW equal to zero.

Another example is maximization of the IRR, which is a qualitative criterion. However, for the optimization, it is important that the incremental IRR of the solution is greater than or equal to the MARR. Applying eq 6 for NPW in the stationary condition (eq 11) gives the following equation:

$$\frac{dW_{NP}}{d\mathbf{d}} = -\frac{dI}{d\mathbf{d}} + \frac{dF_C}{d\mathbf{d}} f_{PA}(r_d) = 0 \tag{12}$$

If the above equation is multiplied by d**d** and the discount rate r_d is selected to be MARR, an expression is obtained which is actually the definition of the incremental IRR:

$$-\mathrm{d}I + \mathrm{d}F_C\, f_{PA}(r_{MARR}) = 0$$
$$f_{PA}(r_{MARR}) = \frac{\mathrm{d}I}{\mathrm{d}F_C} \approx \frac{\Delta I}{\Delta F_C} \tag{13}$$

From the above expressions, it follows that the solution with the maximum absolute NPW is identical to the solution with an incremental IRR equal to the MARR if the latter is applied as the discount rate in the maximization of the NPW. If **d** in eq 12 represents the dimensions of process units, these should be increased as long as the incremental IRR of a small increase remains above the MARR.

The stationary conditions for minimum EAC and maximum profit lead to similar conclusions:

$$\frac{\mathrm{d}c_{eq}}{\mathrm{d}d} = \frac{1}{f_{PA}(r_d)}\frac{\mathrm{d}I}{\mathrm{d}d} - \frac{\mathrm{d}F_C}{\mathrm{d}d} = 0$$
$$\mathrm{d}I - \mathrm{d}F_C\, f_{PA}(r_d) = 0 \tag{14}$$

Profit before taxes can be expressed by the following equation when applying eqs A4 and A5 from Appendix I,

$$P_B = \frac{1}{1 - r_t}(F_C - D) \tag{15}$$

where r_t represents the tax rate. The first derivative of this expression is then

$$\frac{\mathrm{d}P_B}{\mathrm{d}d} = \frac{1}{1 - r_t}\left(\frac{\mathrm{d}F_C}{\mathrm{d}d} - \frac{1}{t_D}\frac{\mathrm{d}I}{\mathrm{d}d}\right) = 0$$
$$-\mathrm{d}I + \mathrm{d}F_C\, t_D = 0 \tag{16}$$

From eq 16, it follows that maximization of the profit would lead to the same result as the maximization of the NPW if the annuity present worth factor, f_{PA}, with the discount rate equal to the MARR, is applied instead of the straight-line depreciation period, t_D:

$$\max P_B' = R - c_{op} - \frac{I}{f_{PA}(r_{MARR})} = \frac{1}{1 - r_t}\left(F_C - \frac{I}{f_{PA}(r_{MARR})}\right) \tag{17}$$

This conclusion is very important for engineers who usually prefer annual profitability measures over the NPW criterion.

Optimal solutions obtained by optimization of the NPW, the EAC, and the modified profit, P_B', exhibit high cash flows on one hand and substantial profitability on the other. These solutions can be considered compromise results, as they simultaneously take into account qualitative as well as quantitative criteria.

4. Influence of the Profitability Measure on the Optimal Solution

In mathematical programming, the solutions obtained by optimizing different economic criteria in the objective function will usually be different. Let us consider a simple heat exchanger network (HEN) consisting of one hot and one cold stream, as shown in Figure 2. The data of the example are shown in Table 1. The goal of the HEN design problem is to find an optimal size of process heat exchanger (HE) in order for an appropriate tradeoff between the operating cost and the investment one to be achieved at the highest possible benefit. The latter is expressed in the objective function as one of the previously defined profitability criteria.

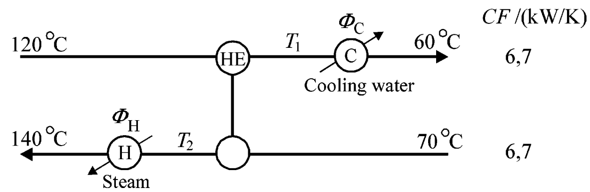

Figure 2. Illustrative heat exchanger network.

Table 1. HEN Example Model Parameters

price of hot utility	$p_H = 80$ \$/(kW·yr)
price of cold utility	$p_C = 20$ \$/(kW·yr)
overall heat transfer coefficients	$U_{HE} = U_C = 0.5$ kW/(m^2·K) $U_H = 0.778$ kW/(m^2·K)
fixed capital cost of heat transfer units (\$)	$I_F = 6\,110A^{0.65}$
tax rate	$r_t = 0.25$
discount rate	$r_d = 0.12$ yr^{-1}
depreciation period	$t_D = 10$ yr
capital cost of nonintegrated solution	$I_F^0 = 58\,162$ \$
utility cost of nonintegrated solution	$c_{op}^0 = 45\,560$ \$/yr
cooling water supply temperature	20 °C
cooling water target temperature	35 °C
steam supply temperature	180 °C
steam target temperature	179 °C

Table 2. Optimal Solutions of the HEN Example

	profitability measure in the objective function of (NLP1), f_{OBJ}		
	qualitative criteria	quantitative criteria	compromise criteria
	min t_{PB}, max R_{OIB}, max r_{IRR}	min c_t, max P_B	maxW_{NP}, min c_{eq} max P_B'
A_{HE} (m^2)	8.4	59.3	35.1
$I_{F,ret}$ (USD)	16 276	65 362	43 767
c_{op} (USD/yr)	32 671	18 232	21 311
$F_{C,ret}$ (USD/yr)	10 074	22 130	19 280
W_{NP} (USD)	40 635	59 677	65 170
r_{IRR} (yr^{-1})	0.614	0.317	0.428

As there is no income in this example, the problem was modeled as a retrofit model in which the alternative with no heat integration between the streams was selected as the base case. To ensure the desired target temperatures in the base case, the consumption of the hot utility amounted to (140 − 70) × 6.7 = 469 kW and the consumption of the cold utility amounted to (120 − 60) × 6.7 = 402 kW. Considering the prices of the utilities given in Table 1, the operating cost of the utilities in a nonintegrated solution amounted to $c_{op}^0 = 45\,560$ \$/yr. The fixed capital cost of the heater and the cooler was estimated to be $I_F^0 = 58\,162$ \$, while the working capital was neglected. These two figures served as the reference points to which the retrofitted solutions were matched. The mathematical model of the problem was then written as the following nonlinear programming problem (NLP1).

The HEN design problem (NLP1) was solved for seven profitability criteria defined in Section 2, which were applied to the objective function, f_{OBJ}. The solutions obtained with GAMS/CONOPT are presented in Table 2.

Table 2 shows that the optimization of frequently used criteria, i.e., the total annual cost (c_t) and the profit (P_B), increases the size of the process and cash flows but minimizes the profitability. These measures can be classified as quantitative ones, as they are expressed in purely financial terms. On the other hand, qualitative criteria such as the payback time (t_{PB}), the return on investment (R_{OIB}), and the IRR (r_{IRR}) minimize the process equipment and cash flows but maximize profitability. Optimizations of the NPW (W_{NP}), the EAC (c_{eq}), and the modified profit (P_B') are somewhere between the quantitative and qualitative criteria.

$$\min \text{ or } \max f_{OBJ}$$

$$\text{s.t.}$$

$$120 - T_1 = T_2 - 70$$

$$\Phi_C = CF_H(T_1 - 60)$$

$$\Phi_H = CF_C(140 - T_2)$$

$$c_{op} = p_C\Phi_C + p_H\Phi_H$$

$$A_{HE} = \frac{CF_H(120 - T_1)}{U_{HE}(120 - T_2)}$$

$$A_C = \frac{\Phi_C}{U_C\Delta_{ln}T_C} \quad \Delta_{ln}T_C = \frac{T_1 - 35 - 40}{\ln((T_1 - 35)/40)}$$

$$A_H = \frac{\Phi_H}{U_H\Delta_{ln}T_H} \quad \Delta_{ln}T_H = \frac{179 - T_2 - 40}{\ln((179 - T_2)/40)}$$

$$I_{F,ret} = 6110(A_{HE}{}^{0.65} + A_C{}^{0.65} + A_H{}^{0.65}) - I_F^0$$

$$F_{C,ret} = (1 - r_t)(c_{op}^0 - c_{op}) + r_t\frac{I_{F,\,ret}}{t_D}$$

$$P_{B,ret} = (c_{op}^0 - c_{op}) - \frac{I_{F,ret}}{t_D}$$

$$P'_{B,ret} = (c_{op}^0 - c_{op}) - \frac{I_{F,ret}}{f_{PA}(r_d)}$$

$$T_1, T_2, \Phi_C, \Phi_H, c_{op}, A_{HE}, A_C, A_H, \Delta_{ln}T_C, \Delta_{ln}T_H, I_{F,ret}, F_{C,ret}, P_{B,ret} \in R$$

$$c_{op}^0 = 45\,560 \text{ \$/yr}, \quad I_F^0 = 58\,162 \text{ \$}$$

$$U_{HE} = U_C = 0.5 \text{ kW/(m}^2\cdot\text{K)}, \quad U_H = 0.778 \text{ kW/(m}^2\cdot\text{K)} \qquad \text{(NLP1)}$$

It should be mentioned that, in this simple example, the revenues and working capital have been ignored in the evaluation, which resulted in the same optimal value obtained by many profitability measures. For example, the expressions for minimization of the payback time and maximization of the IRR, or minimization of the TAC and maximization of the profit, are identical or different only in constant terms. Some measures differ in certain categories that influence the optimization in the same direction, like minimization of the payback time and maximization of the return on investment, where the cash flow appears in the first measure and the profit in the second one. As the cash flow is derived from the profit, both criteria result in the same optimal solution.

4.1. Sensitivity Analysis of Design Problem. From the above results, we can conclude that optimizations of compromise criteria result in solutions with moderate capital investment, cash flows, and profitability. However, this compromise relies on the definition of various tunable parameters, such as project lifetime and the minimum acceptable rate of return that is used as a discount rate for optimization.

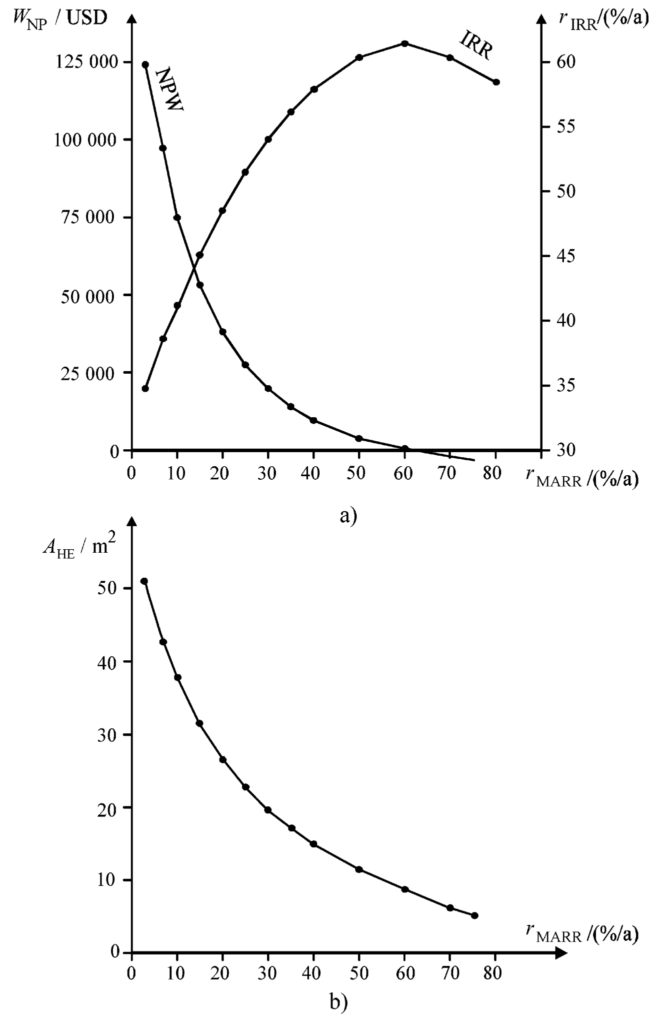

Figure 3. Sensitivity analysis of HEN example: (a) NPW and IRR vs MARR, (b) area vs MARR.

By performing a sensitivity analysis of the HEN problem with respect to the MARR, different Pareto curves were obtained (Figure 3). The curves in Figure 3a illustrate that, at low values of the MARR, solutions with a high NPW and a low IRR are obtained, yielding a large exchanger area (Figure 3b) and a high investment. These solutions tend toward those obtained by means of the quantitative criteria, i.e., total cost or profit. By increasing the MARR, the heat exchanger area and the NPW decrease, but the IRR increases, which is similar to the results obtained with the optimizations of the qualitative measures, e.g., the payback time or the IRR. This may be explained with the premise that, if the value of the MARR is low, the investors are willing to accept projects with moderate profitability and wait for the return of their money for a longer time period, since this will be compensated with future higher cash flows. On the other hand, if the value of the MARR is high, the money should return in a shorter period of time, and this requires higher profitability. Similar conclusions can be derived for other compromise criteria, namely, the EAC and the modified profit.

4.2. Stochastic Design Problem. The generation of the Pareto curves with respect to the MARR corresponds to biobjective optimization, since it produces a series of optimal solutions from which decision makers select the best one according to their subjective perceptions of risk and opportunity costs. An alterna-

Table 3. Gauss−Legendre Points for Stochastic Solution of HEN Example

MARR (yr^{-1})	0.0425	0.0531	0.0709	0.094	0.12	0.1459	0.1691	0.1869	0.1974
probability	0.0014	0.0093	0.0575	0.2335	0.3963	0.2335	0.0575	0.0093	0.0014

tive and advanced approach would be the stochastic analysis of the design problem. This problem can be approached, assuming that the probability distribution of the MARR is available, by selecting the discrete values of the MARR and then maximizing the NPW for each MARR, yielding the distribution of the NPW as output. Sampling of the MARR values can be performed, for example, by means of the Monte Carlo method with random selection, but this will usually require a huge number of points. In this example, the quadrature method was applied as described below.

It was assumed that the normal distribution function for the MARR is given with a mean value $\mu = 12\%$ and a standard deviation $\sigma = 2.66\%$. The 6-sigma rule was used for defining the interval of MARR values as $\mu \pm 3\sigma$, i.e., from 4% to 20%. Then the abscissas and weights of the ninth-order Gauss−Legendre polynomial were used to sample the discrete values of the MARR and to determine the corresponding probabilities (Table 3). The problem (NLP1) was solved for each MARR, yielding the distribution of the NPW as shown in Figure 4a. From these results, a cumulative probability diagram of the NPW was obtained (Figure 4b), from which one can estimate the probability of the NPW being less or equal to the specified value. For example, it is unlikely that the NPW of the HEN design project will be lower than 40 000 USD, and on the other hand, it will certainly not exceed 113 000 USD.

5. Flow Sheet Example

The following section considers a flow sheet example of the Williams−Otto process.[79] Reactants A and B and the recycle

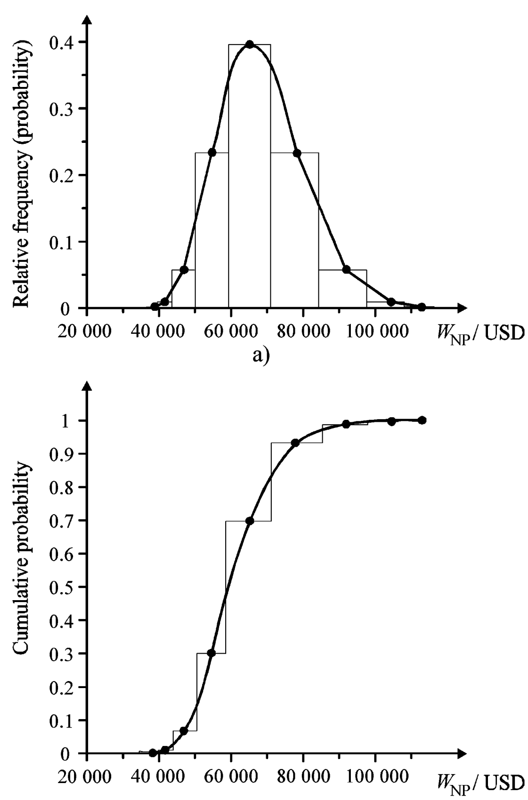

Figure 4. Distribution of NPW−HEN example: (a) relative frequency, (b) cumulative probability.

Table 4. Optimal Solutions of the Flow Sheet Example

	profitability measure in the objective function of (WO-1), f_{OBJ}			
	qualitative criteria	quantitative criteria		compromise criteria
	max r_{IRR}, min t_{PB}	max P_B	min c_t	max W_{NP}, min c_{eq}, max P_B'
V (m^3)	0.873	6.82	7.90	3.75
T (K)	374	342	342	351
η	0.100	0.113	0.102	0.109
$q_{m,1}^{A}$ (kg/h)	6123	4957	4808	5239
$q_{m,2}^{B}$ (kg/h)	13 956	11 113	10 880	11 792
I_F (MUSD)	0.925	7.22	8.37	3.97
F_C (MUSD/yr)	0.876	2.42	2.52	2.00
W_{NP} (MUSD)	4.02	6.44	5.86	7.30
r_{IRR} (yr^{-1})	0.945	0.313	0.274	0.493

stream enter the continuous-flow stirred-tank reactor (Figure 5), where the main product P is produced together with the byproduct E and the waste product G, while C is an intermediate:

$$A + B \rightarrow C$$

$$C + B \rightarrow P + E$$

$$P + C \rightarrow G$$

In the decanter, component G is entirely removed from the other components. Product P is removed from the overhead of the distillation column, but some of the product is retained in the bottom due to the formation of an azeotrope. Part of the bottom stream is purged in order to avoid accumulation of the byproduct, while most of it is recycled to the reactor. The purge stream has a substantial fuel value and can be sold on the market.

5.1. Optimization of Flow Sheet Example with Different Profitability Measures. The mathematical model of the above process (WO-1) consists of 86 variables and 81 equality constraints and is given in Appendix II. The cash flow, F_C, is composed of the sale of product P ($q_{m,7}$) and the purge stream ($q_{m,9}$) minus the cost of the raw materials ($q_{m,1}$ and $q_{m,2}$), the utility cost ($q_{m,10}$, $q_{m,1}$, and $q_{m,2}$), the waste-removal cost ($q_{m,6}$), and the fixed cost. The last term represents the tax credit generated by the depreciation charges. The problem (WO-1) has 5 degrees of freedom and is optimized with various objective functions, as shown in Table 4.

Similar to that observed in the HEN example, the largest reactors with the highest capital costs and cash flows were also selected in this flow sheet by applying quantitative criteria of

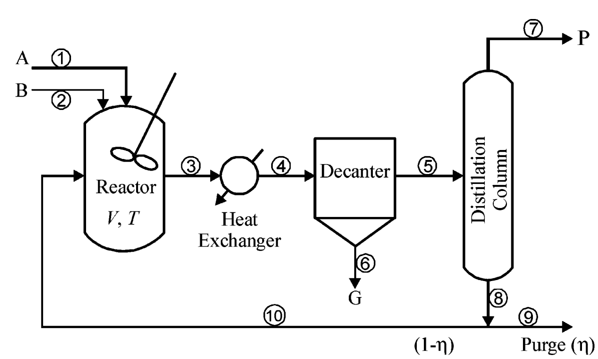

Figure 5. Williams and Otto flow sheet.

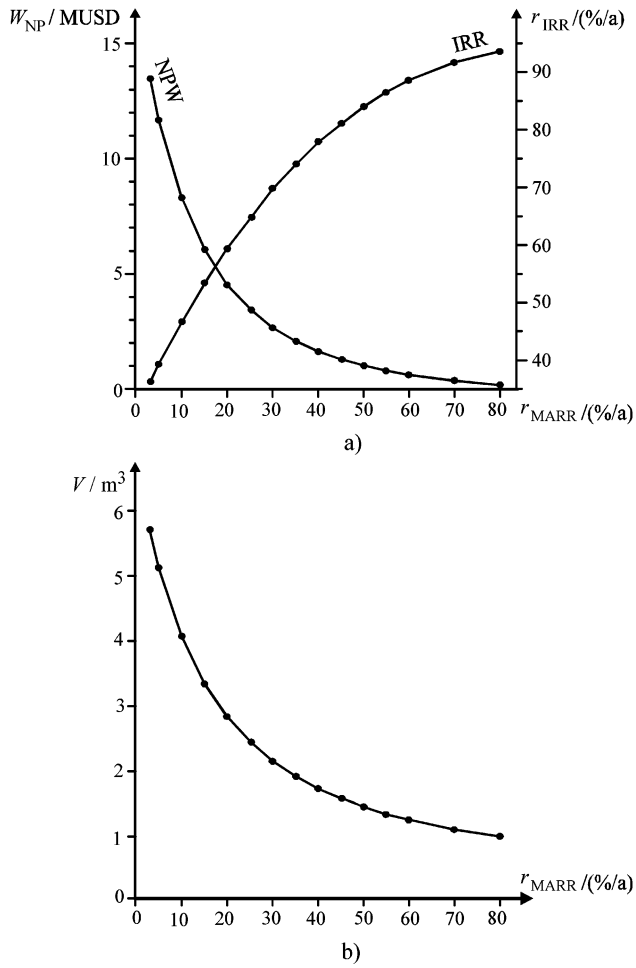

Figure 6. Sensitivity analysis of flow sheet example: (a) NPW and IRR vs MARR, (b) volume vs MARR.

total annual cost and profit. On the other hand, the smallest reactor with the lowest capital cost and the highest profitability is obtained by optimizing the qualitative criteria, namely, the payback time and the IRR. An intermediate solution is obtained by optimizing the compromise criteria of the NPW, the equivalent annual cost, and the modified profit.

5.2. Design of Flow Sheet Example Considering the Uncertainty in the MARR. The uncertainty involved in the MARR value was considered similarly as in the HEN example, namely, by means of a sensitivity analysis and with the stochastic approach. The NPW of the solution decreases with increasing the value of the MARR, while the profitability expressed as the IRR is maximized (Figure 6a). This is accompanied by a decrease in the reactor's volume (Figure 6b).

The stochastic analysis was performed assuming the same distribution function for the MARR as in the HEN example, N[12, 2.66]%, and nine Gauss−Legendre points. The relative frequency and the cumulative probability for the NPW are presented in Figure 7.

6. Conclusion

This paper highlights a problem which appears in mathematical programming, namely, that different profitability measures do not give unique optimal solutions when they are applied in the objective functions of process flow sheet optimization problems. Some qualitative profitability measures, such as the internal rate of return and the payback time, favor less expensive solutions with small cash flows and high profitability. Quantitative criteria, however, like the total annual cost and the profit, produce solutions with the highest capital cost and cash flows, but with low profitability. The optimization of compromise measures, such as the NPW, the EAC, and the modified profit, yields a reasonable compromise between both types of criteria, resulting in a solution with relatively large cash flows and a promising IRR. Here, an appropriate tradeoff is established between the absolute terms of the future cash flows and the profitability of the investment.

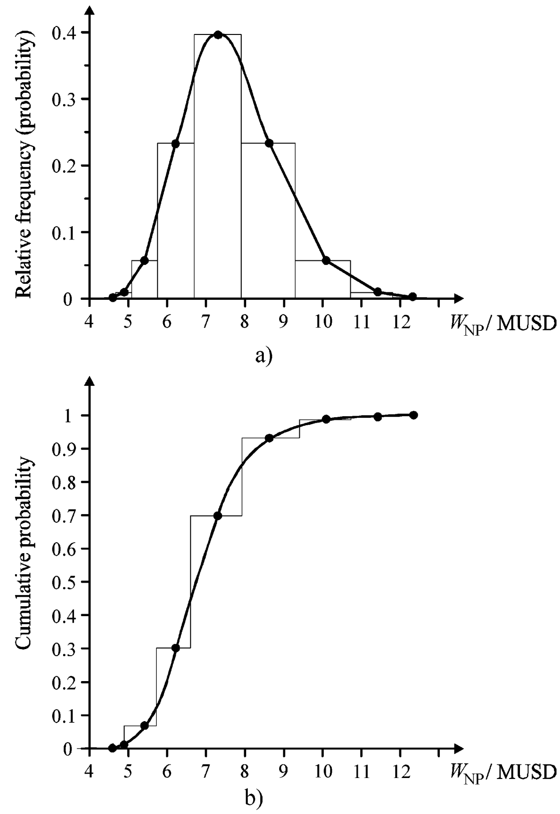

Figure 7. Distribution of NPW—flow sheet example: (a) relative frequency, (b) cumulative probability.

The net present worth is a measure which properly takes into account the complete economics of the project throughout the project's life cycle, i.e., from the initial investment expenditures to the annual cash flows and, finally, to the investment capital recovered at the end of the project's lifetime. The maximization of the net present worth with the discount rate equal to the MARR is, therefore, the recommended criterion for the synthesis and design of process flow sheets, instead of simple cost or profit objective functions. Similar or identical results may be obtained by applying more obvious and, by engineers, more favored annual criteria, such as the equivalent annual cost and the profit, if the annual investment charge is calculated by using the MARR. However, any uncertainty in the tunable parameters must be taken into account before arriving at the final decision.

Acknowledgment

The authors are grateful to the Slovenian Ministry of Higher Education, Science and Technology for its financial support (Program P2-0032 and Project J2-6637).

Appendix I

This appendix describes the expressions for the major financial categories used in the preliminary evaluations of the projects.

Revenue, R, is a positive cash flow, which in the chemical industry arises mainly from the sale of products, byproducts, and surplus utilities. The company may also have other incomes, e.g., dividends and interests, but these are usually neglected in the preliminary evaluations.

Expenditures, E, represent all the negative cash flows, e.g., costs of the raw material, the energy, the salaries, the maintenance, the insurance, etc., which are often called operating costs or costs of manufacture. In addition, E also comprises general expenses such as selling costs, research costs, etc. Many case studies indicate that raw materials and utilities represent, by far, the largest part of the operating costs in the chemical industry.

Depreciation, D, does not belong to the cash-flow items. It represents an annualized investment cost which serves to define the reduction of the value of the fixed capital, I_F, and influences the amount of taxes that the company is obliged to pay. For the early stages of the project evaluations, a straight-line depreciation is recommended to be taken over a 10-year depreciation period, t_D, with a zero salvage value:

$$D = \frac{I_F}{t_D} \qquad \text{(A1)}$$

The total investment, I, is a discrete cash flow composed of the fixed, I_F, and working capital, I_W:

$$I = I_F + I_W \qquad \text{(A2)}$$

Profit before taxes, P_B, is calculated as the difference between the revenues, R, and all the cash expenditures, E, minus the depreciation, D.

$$P_B = R - E - D \qquad \text{(A3)}$$

Profit after taxes, P_A, is determined on the basis of a given tax rate, r_t, which determines the amount of the taxes paid. The tax rates may vary from low 10% to around 45%, depending on the financial policies of the governments.

$$P_A = (1 - r_t)P_B \qquad \text{(A4)}$$

The net cash flow, F_C, is finally estimated by eq A5. Note that depreciation is the only term by which the net cash flow should be differentiated from the profit:

$$F_C = P_A + D = (1 - r_t)(R - E) + r_t D \qquad \text{(A5)}$$

The upper relation is reasonable for early evaluations where paying dividends to the shareholders and other incomes (outcomes) are often neglected (dashed line in Figure 1). Cash flow actually represents the money from depreciation and the remaining profit that flows back to the company and can be spent for research, expansions, improvements, etc.

Appendix II

$$\min \text{ or } \max f_{OBJ}$$

$$\text{s.t.}$$

$$q^A_{m,3} = (q^A_{m,1} + q^A_{m,10}) - k_1 w_A w_B V\rho$$

$$q^B_{m,3} = (q^B_{m,2} + q^B_{m,10}) - (k_1 w_A + k_2 w_C) w_B V\rho$$

$$q^C_{m,3} = q^C_{m,10} + (2k_1 w_A w_B - 2k_2 w_B w_C - k_3 w_P w_C)V\rho$$

$$q^E_{m,3} = q^E_{m,10} + (2k_2 w_B w_C)V\rho$$

$$q^P_{m,3} = q^P_{m,10} + (k_2 w_B w_C - 0.5k_3 w_P w_C)V\rho$$

$$q^G_{m,3} = q^G_{m,10} + (1.5k_3 w_P w_C)V\rho$$

$$w_j = q^j_{m,3}/\sum_j q^j_{m,3} \quad j = \text{A,B,C,E,P,G}$$

$$k_1 = (5.9755 \times 10^9) \exp\left(\frac{-12\,000}{1.8T}\right)$$

$$k_2 = (2.5962 \times 10^{12}) \exp\left(\frac{-15\,000}{1.8T}\right) \qquad \text{(WO-1)}$$

$$k_3 = (9.6283 \times 10^{15}) \exp\left(\frac{-20\,000}{1.8T}\right)$$

$$q^j_{m,1} = 0 \quad j = \text{B,C,E,P,G}$$

$$q^j_{m,2} = 0 \quad j = \text{A,C,E,P,G}$$

$$q^j_{m,4} = q^j_{m,3} \quad j = \text{A,B,C,E,P,G}$$

$$q^j_{m,5} = q^j_{m,4} \quad j = \text{A,B,C,E,P}$$

$$q^G_{m,5} = 0$$

$$q^j_{m,6} = 0 \quad j = \text{A,B,C,E,P}$$

$$q^G_{m,6} = q^G_{m,4}$$

$$q^j_{m,7} = 0 \quad j = \text{A,B,C,E,G}$$

$$q^P_{m,7} = q^P_{m,5} - 0.1\, q^E_{m,5}$$

$$q^j_{m,8} = q^j_{m,5} \quad j = \text{A,B,C,E}$$

$$q^P_{m,8} = 0.1\, q^E_{m,5}$$

$$q^G_{m,8} = 0$$

$$q^j_{m,9} = \eta q^j_{m,8} \quad j = \text{A,B,C,E,P}$$

$$q^G_{m,9} = 0$$

$$q^j_{m,10} = (1 - \eta) q^j_{m,8} \quad j = \text{A,B,C,E,P}$$

$$q^G_{m,10} = 0$$

$$q_{m,i} = \sum_j q^j_{m,i} \quad i = 1,2,...,10 \quad j = \text{A,B,C,E,P,G}$$

$$I_F = (1/0.453) \times 600 V\rho$$

$$c_{op} = \frac{1}{0.453}(168 q_{m,1} + 252 q_{m,2} + 2.22(q_{m,10} + q_{m,1} + q_{m,2}) + 84 q_{m,6}) + 1041.6$$

$$F_C = (1 - r_t)[(1/0.453)(2\,207 q_{m,7} + 50 q_{m,9} - 168 q_{m,1} - 252 q_{m,2} - 2.22(q_{m,10} + q_{m,1} + q_{m,2}) - 84 q_{m,6}) - 1041.6] + r_t \frac{I_F}{t_D}$$

$$322 \text{ K} \le T \le 378 \text{ K}$$

$$0 \le \eta \le 0.99$$

$$V \ge 0.85 \text{ m}^3$$

$$q_{m,7} = 2\,160 \text{ kg/h} \qquad \text{(WO-1)}_{\text{contin}}$$

$$q_{m,i}, q_{m,i}^{j}, w_j \in R \quad i = 1,2,...,10 \quad j = A,B,C,E,P,G$$

$$V, T, k_1, k_2, k_3, I_F, F_C, \eta, c_{op} \in R$$

Data: $r_d = 0.12\ yr^{-1}$, $r_t = 0.3$, $t_D = t_l = 10$ yr, $\rho = 801$ kg/m^3

Nomenclature

A = heat transfer area, m^2
c_{eq} = equivalent annual cost, USD/yr
c_{op} = operating cost, USD/yr
c_t = total annual cost, USD/yr
CF = heat capacity flow rate, kW/K
d = vector of design variables
D = depreciation, USD/yr
E = expenditures, USD/yr
f = objective function
F_C = cash flow after taxes, USD/yr
f_{PA} = present worth annuity factor, yr
g = vector of inequality constraints
h = vector of equality constraints
I = total capital investment, USD
I_F = fixed capital investment, USD
I_W = working capital investment, USD
k = reaction rate constant, h^{-1} (mass fraction)$^{-1}$
p = price of utility, \$/(kW·yr)
P_A = profit after taxes, USD/yr
P_B = profit before taxes, USD/yr
P_B' = modified profit before taxes, USD/yr
q_m = mass flow rate, kg/h
R = revenues, USD/ yr
R_{OIB} = return on investment before taxes, yr^{-1}
r_d = discount rate, yr^{-1}
r_{IRR} = internal rate of return, yr^{-1}
r_{MARR} = minimum acceptable rate of return, yr^{-1}
r_t = tax rate
T = temperature, K
t_D = depreciation period, yr
t_l = project's lifetime, yr
t_{PB} = payback time, yr
U = overall heat transfer coefficient, kW/(m^2·K)
V = volume, m^3
w = mass fraction
W_{NP} = net present worth, USD
x = vector of continuous variables
y = vector of discrete variables

Subscripts and superscripts

0 = base case
C = cold, cooler
H = hot, heater
HE = heat exchanger
i = number of process stream in Williams and Otto flow sheet
j = components in Williams and Otto flow sheet (A, B, C, E, P, G)
ret = retrofitted solution

Greek

Δ = differential
Φ = heat flow rate, kW
η = fraction of purged stream
μ = mean value
ρ = density, kg/m^3
σ = standard deviation

Abbreviations

EAC = equivalent annual cost
IRR = internal rate of return
MARR = minimum acceptable rate of return
MINLP = mixed-integer nonlinear programming
NLP = nonlinear programming
NPW = net present worth
TAC = total annual cost

Literature Cited

(1) Valle-Riestra, J. F. *Project evaluation in the chemical process industries*; McGraw-Hill: New York, 1983.

(2) Allen, D. *Economic Evaluation of Projects*; Inst Chem Eng: Rugby, U.K., 1991.

(3) Petters, M. S.; Timmerhaus, K. D. *Plant Design and Economics for Chemical Engineers*; McGraw-Hill: New York, 1991.

(4) Chauvel, A.; Fournier, G.; Raimbault, C. *Manual of Process Economic Evaluation*; Editions Technip: Paris, 2003.

(5) Edgar, T. F.; Himmelblau, D. M. *Optimization of Chemical Processes*, 2nd ed.; McGraw-Hill: New York, 2001; pp 83−110.

(6) Hirata, K.; Sakamoto, H.; O'Young, L.; Cheung, K.-Y.; Hui, C.-W. Multisite utility integration-an industrial case study. *Comput. Chem. Eng.* **2004**, *28* (1/2), 139.

(7) Soršak, A.; Kravanja, Z. MINLP retrofit of heat exchanger networks comprising different exchanger types. *Comput. Chem. Eng.* **2004**, *28* (1/2), 235.

(8) Cisternas, L.; Cueto, J.; Swaney, R. Flowsheet synthesis of fractional crystallization processes with cake washing. *Comput. Chem. Eng*. **2004**, *28* (5), 613.

(9) Oliveira Francisco, A. P.; Matos, H. A. Multiperiod synthesis and operational planning of utility systems with environmental concerns. *Comput. Chem. Eng*. **2004**, *28* (5), 745.

(10) Pintarič, Z. N.; Kravanja, Z. A strategy for MINLP synthesis of flexible and operable processes. *Comput. Chem. Eng*. **2004**, *28* (6/7), 1105.

(11) Leboreiro, J.; Acevedo, J. Processes synthesis and design of distillation sequences using modular simulators: A genetic algorithm framework. *Comput. Chem. Eng*. **2004**, *28* (8), 1223.

(12) Lin, B.; Miller, D. C. Solving heat exchanger network synthesis problems with Tabu Search. *Comput. Chem. Eng.* **2004**, *28* (8), 1451.

(13) Goyal, V.; Ierapetritou, M. G. Computational studies using a novel simplicial-approximation based algorithm for MINLP optimization. *Comput. Chem. Eng.* **2004**, *28* (9), 1771.

(14) Almeida-Rivera, C. P.; Swinkels, P. L. J.; Grievink, J. Designing reactive distillation processes: Present and future. *Comput. Chem. Eng*. **2004**, *28* (10), 1997.

(15) Sakizlis, V.; Perkins, J. D.; Pistikopoulos, E. N. Recent advances in optimization-based simultaneous process and control design. *Comput. Chem. Eng*. **2004**, *28* (10), 2069.

(16) Barttfeld, M.; Aguirre, P. A.; Grossmann, I. E. A decomposition method for synthesizing complex column configurations using tray-by-tray GDP models. *Comput. Chem. Eng.* **2004**, *28* (11), 2165.

(17) Lin, B.; Miller, D. C. Tabu search algorithm for chemical process optimization. *Comput. Chem. Eng*. **2004**, *28* (11), 2287.

(18) Papadopoulos, A. I.; Linke, P. On the synthesis and optimization of liquid−liquid extraction processes using stochastic search methods. *Comput. Chem. Eng*. **2004**, *28* (11), 2391.

(19) Yan, L.; Shen, K.; Hu, S. Solving mixed integer nonlinear programming problems with line-up competition algorithm. *Comput. Chem. Eng.* **2004**, *28* (12), 2647.

(20) Hernández-Suárez, R.; Castellanos-Fernández, J.; Zamora, J. M. Superstructure Decomposition and Parametric Optimization Approach for the Synthesis of Distributed Wastewater Treatment Networks. *Ind. Eng. Chem. Res.* **2004**, *43* (9), 2175.

(21) Kaymak, D. B.; Luyben, W. L. Quantitative Comparison of Reactive Distillation with Conventional Multiunit Reactor/Column/Recycle Systems for Different Chemical Equilibrium Constants. *Ind. Eng. Chem. Res.* **2004**, *43* (10), 2493.

(22) Kaymak, D. B.; Luyben, W. L.; Smith, O. J., IV. Effect of Relative Volatility on the Quantitative Comparison of Reactive Distillation and Conventional Multi-unit Systems. *Ind. Eng. Chem. Res.* **2004**, *43* (12), 3151.

(23) Zhang, L.; Linninger, A. A. Temperature Collocation Algorithm for Fast and Robust Distillation Design. *Ind. Eng. Chem. Res.* **2004**, *43* (12), 3163.

(24) Daviou, M. C.; Hoch, P. M.; Eliceche, A. M. Design of Membrane Modules Used in Hybrid Distillation/Pervaporation Systems. *Ind. Eng. Chem. Res.* **2004**, *43* (13), 3403.

(25) Kaymak, D. B.; Luyben, W. L. Effect of the Chemical Equilibrium Constant on the Design of Reactive Distillation Columns. *Ind. Eng. Chem. Res.* **2004**, *43* (14), 3666.

(26) Qin, X.; Gabriel, F.; Harell, D.; El-Halwagi, M. M. Algebraic Techniques for Property Integration via Componentless Design. *Ind. Eng. Chem. Res.* **2004**, *43* (14), 3792.

(27) Ward, J. D.; Mellichamp, D. A.; Doherty, M. F. Importance of Process Chemistry in Selecting the Operating Policy for Plants with Recycle. *Ind. Eng. Chem. Res.* **2004**, *43* (14), 3957.

(28) Corsano, G.; Aguirre, P. A.; Iribarren, O. A.; Montagna, J. M. Batch Fermentation Networks Model for Optimal Synthesis, Design, and Operation. *Ind. Eng. Chem. Res.* **2004**, *43* (15), 4211.

(29) Montagna, J. M.; Iribarren, O. A.; Vecchietti, A. R. Synthesis of Biotechnological Processes Using Generalized Disjunctive Programming. *Ind. Eng. Chem. Res.* **2004**, *43* (15), 4220.

(30) Uppaluri, R. V. S.; Linke, P.; Kokossis, A. C. Synthesis and Optimization of Gas Permeation Membrane Networks. *Ind. Eng. Chem. Res.* **2004**, *43* (15), 4305.

(31) Baker, R.; Swartz, C. L. E. Rigorous Handling of Input Saturation in the Design of Dynamically Operable Plants. *Ind. Eng. Chem. Res.* **2004**, *43* (18), 5880.

(32) Serna-González, M.; Ponce-Ortega, J. M.; Jiménez-Gutiérrez, A. Two-Level Optimization Algorithm for Heat Exchanger Networks Including Pressure Drop Considerations. *Ind. Eng. Chem. Res.* **2004**, *43* (21), 6766.

(33) Goyal, V.; Ierapetritou, M. G. Deterministic Framework for Robust Modular Design with Integrated-Demand Data Analysis. *Ind. Eng. Chem. Res.* **2004**, *43* (21), 6813.

(34) Cauley, F. G.; Xie, Y.; Wang, N.-H. L. Optimization of SMB Systems with Linear Adsorption Isotherms by the Standing Wave Annealing Technique. *Ind. Eng. Chem. Res.* **2004**, *43* (23), 7588.

(35) Holiastos, K.; Manousiouthakis, V. Infinite-Dimensional State-Space (IDEAS) Approach to Globally Optimal Design of Distillation Networks Featuring Heat and Power Integration. *Ind. Eng. Chem. Res.* **2004**, *43* (24), 7826.

(36) Kaymak, D. B.; Luyben, W. L. Design of Distillation Columns with External Side Reactors. *Ind. Eng. Chem. Res.* **2004**, *43* (25), 8049.

(37) Varbanov, P. S.; Doyle, S.; Smith, R. Modelling and Optimization of Utility Systems. *Chem. Eng. Res. Des.* **2004**, *82* (A5), 561.

(38) Patsiatzis, D. I.; Knight, G.; Papageorgiou, L. G. An MILP Approach to Safe Process Plant Layout. *Chem. Eng. Res. Des.* **2004**, *82* (A5), 579.

(39) Varbanov, P.; Perry, S.; Makwana, Y.; Zhu, X. X.; Smith, R. Top-level Analysis of Site Utility Systems. *Chem. Eng. Res. Des.* **2004**, *82* (A6), 784.

(40) Hamad, A.; Fayed, M. E. Simulation-aided Optimization of Volatile Organic Compounds Recovery Using Condensation. *Chem. Eng. Res. Des.* **2004**, *82* (A7), 895.

(41) Bagajewicz, M.; Fuxman, A.; Uribe, A. Instrumentation network design and upgrade for process monitoring and fault detection. *AIChE J.* **2004**, *50* (8), 1870.

(42) Iršič Bedenik, N.; Kravanja, Z. An integrated strategy for the hierarchical multilevel MINLP synthesis of overall process flowsheets using the combined synthesis/analysis approach. *Comput. Chem. Eng*. **2004**, *28* (5), 693.

(43) Sarkar, D.; Modak, J. M. Optimization of fed-batch bioreactors using genetic algorithm: Multiple control variables. *Comput. Chem. Eng*. **2004**, *28* (5), 789.

(44) Kheawhom, S.; Hirao, M. Decision support tools for environmentally benign process design under uncertainty. *Comput. Chem. Eng.* **2004**, *28* (9), 1715.

(45) Suman, B. Study of simulated annealing based algorithms for multiobjective optimization of a constrained problem. *Comput. Chem. Eng.* **2004**, *28* (9), 1849.

(46) Miladi, M. M.; Mujtaba, I. M. Optimisation of design and operation policies of binary batch distillation with fixed product demand. *Comput. Chem. Eng.* **2004**, *28* (11), 2377.

(47) Cheng, L.; Subrahmanian, E.; Westerberg, A. W. Multi-objective Decisions on Capacity Planning and Production—Inventory Control under Uncertainty. *Ind. Eng. Chem. Res*. **2004**, *43* (9), 2192.

(48) Kim, K.-J.; Smith, R. L. Parallel Multiobjective Evolutionary Algorithms for Waste Solvent Recycling. *Ind. Eng. Chem. Res*. **2004**, *43* (11), 2669.

(49) Aseeri, A.; Gorman, P.; Bagajewicz, M. J. Financial Risk Management in Offshore Oil Infrastructure Planning and Scheduling. *Ind. Eng. Chem. Res*. **2004**, *43* (12), 3063.

(50) Goel, H. D.; Weijnen, M. P. C.; Grievink, J. Optimal Reliable Retrofit Design of Multiproduct Batch Plants. *Ind. Eng. Chem. Res*. **2004**, *43* (14), 3799.

(51) Hoffmann, V. H.; McRae, G. J.; Hungerbühler, K. Methodology for Early-Stage Technology Assessment and Decision Making under Uncertainty: Application to the Selection of Chemical Processes. *Ind. Eng. Chem. Res*. **2004**, *43* (15), 4337.

(52) Lim, H.; Kang, M.-G.; Park, S.; Lee, J. Modeling and Optimization of a Styrene Monomer Reactor System Using a Hybrid Neural Network Model. *Ind. Eng. Chem. Res*. **2004**, *43* (20), 6441.

(53) Low, K. H.; Sorensen, E. Simultaneous optimal design and operation of multipurpose batch distillation. *Chem. Eng. Process*. **2004**, *43* (3), 273.

(54) Chakraborty, A.; Purkarthofer, K. A.; Linninger, A. A. Conceptual design of metallurgical processes based on thermodynamic and economic insights. *Chem. Eng. Process*. **2004**, *43* (5), 625.

(55) Wang, K.; Salhi, A.; Fraga, E. S. Process design optimisation using embedded hybrid visualisation and data analysis techniques within a genetic algorithm optimisation framework. *Chem. Eng. Process*. **2004**, *43* (5), 663.

(56) Han, I.-S.; Riggs, J. B.; Chung, C.-B. Modeling and optimization of a fluidized catalytic cracking process under full and partial combustion modes. *Chem. Eng. Process*. **2004**, *43* (8), 1063.

(57) Inamdar, S. V.; Gupta, S. K.; Saraf, D. N. Multi-Objective Optimization of an Industrial Crude Distillation Unit Using the Elitist Non-Dominated Sorting Genetic Algorithm. *Chem. Eng. Res. Des*. **2004**, *82* (A5), 611.

(58) Bollas, G. M.; Papadokonstantakis, S.; Michalopoulos, J.; Arampatzis, G.; Lappas, A. A.; Vasalos, I. A.; Lygeros, A. A Computer-Aided Tool For the Simulation And Optimization of the Combined HDS−FCC Processes. *Chem. Eng. Res. Des*. **2004**, *82* (A7), 881.

(59) Levis, A. A.; Papageorgiou, L. G. A hierarchical solution approach for multisite capacity planning under uncertainty in the pharmaceutical industry. *Comput. Chem. Eng.* **2004**, *28* (5), 707.

(60) Maravelias, C. T.; Grossmann, I. E. Optimal resource investment and scheduling of tests for new product development. *Comput. Chem. Eng.* **2004**, *28* (6/7), 1021.

(61) Aseeri, A.; Bagajewicz, M. J. New measures and procedures to manage financial risk with applications to the planning of gas commercialization in Asia. *Comput. Chem. Eng.* **2004**, *28* (12), 2791.

(62) Chen, H.; Shonnard, D. R. Systematic Framework for Environmentally Conscious Chemical Process Design: Early and Detailed Design Stages. *Ind. Eng. Chem. Res.* **2004**, *43* (2), 535.

(63) Oh, H.-C.; Karimi, I. A. Regulatory Factors and Capacity-Expansion Planning in Global Chemical Supply Chains. *Ind. Eng. Chem. Res.* **2004**, *43* (13), 3364.

(64) Barbaro, A.; Bagajewicz, M. J. Managing financial risk in planning under uncertainty. *AIChE J.* **2004**, *50* (5), 963.

(65) Barbaro, A.; Bagajewicz, M. J. Use of inventory and option contracts to hedge financial risk in planning under uncertainty. *AIChE J.* **2004**, *50* (5), 990.

(66) Santos, J. C.; Portugal, A. F.; Magalhães, F. D.; Mendes, A. Simulation and Optimization of Small Oxygen Pressure Swing Adsorption Units. *Ind. Eng. Chem. Res.* **2004**, *43* (26), 8328.

(67) Umeda, T. A Conceptual Framework for the Process System Synthesis and Design Congruent with Corporate Strategy. *Ind. Eng. Chem. Res.* **2004**, *43* (14), 3827.

(68) Yi, G.; Reklaitis, G. V. Optimal design of batch-storage network with financial transactions and cash flows. *AIChE J.* **2004**, *50* (11), 2849.

(69) Gupta, A.; Maranas, C. D. Real-Options-Based Planning Strategies under Uncertainty. *Ind. Eng. Chem. Res.* **2004**, *43* (14), 3870.

(70) Buskies, U. Economic process optimization strategies. *Chem. Eng. Technol*. **1997**, *20* (1), 63.

(71) Guthrie, K. M. Capital Cost Estimating. *Chem. Eng. (N. Y.)* **1969**, *76*, 114.

(72) Dysert, L. Sharpen your capital-cost-estimation skills. *Chem. Eng. (N. Y.)* **2001**, *108* (11), 70.

(73) Seider, W. D.; Seader, J. D.; Lewin, D. R. *Product and process design principles: Synthesis, analysis, and evaluation*, 2nd ed.; Wiley: New York, 2004.

(74) Vasudevan, P. T.; Agrawal, D. A software package for capital cost estimation. *Chem. Eng. Educ.* **1999**, *33* (3), 254.

(75) *Aspen Icarus Process Evaluator 12.1, User*'s *Guide*; Aspen Technology, Inc.: Cambridge, MA, 2003.

(76) Vatavuk, W. M. Updating the CE plant cost index. *Chem. Eng. (N. Y.)* **2002**, *109* (1), 62.

(77) Brown, T. R. Estimating product cost. *Chem. Eng. (N. Y.)* **2000**, *107* (8), 86.

(78) Lal, D. P. Accurately estimate production costs. *Chem. Eng. Prog.* **2002**, *98* (4), 72.

(79) Biegler, L. T.; Grossmann, I. E.; Westerberg, A. W. *Systematic methods of chemical process design*; Prentice Hall: Upper Saddle River, NJ, 1997; Chapters 8 and 9.

Received for review April 26, 2005
Revised manuscript received March 7, 2006
Accepted March 28, 2006

IE050496Z