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The Effect of Economic Objective Function on Economic, Operational and Environmental Performance of Optimal Chemical Processes

Mihael Kasaš, Zdravko Kravanja, Zorka Novak Pintarič*
University of Maribor, Faculty of Chemistry and Chemical Engineering
Smetanova 17, 2000 Maribor, Slovenia
zorka.novak@uni-mb.si

In this work, three of the more used economic criteria were applied in the economic objective function when synthesizing chemical processes using mathematical programming approach: the profit before taxes (PB), the net present value (NPV), and the internal rate of return (IRR). The effects on the economic, operational, and environmental performances of optimal process flow sheets were studied since different criteria, in general, produce different optimal solutions.
Mixed integer nonlinear programming (MINLP) syntheses of three processes, methanol, dimethyl ether and HDA were performed as case-studies together with simultaneous heat integration. It was observed that optimal process flow sheets obtained by three distinct criteria differ not only in process topology and capacities but also in operating and economic figures, efficiency of feed and utility utilization, as well as the sustainability measurements, e.g. toxicological and ecological indices, and total potential environmental impact of the process. In particular, it was shown that the main cause of these differences is the shape of the cash flow function vs. investment level, which is strongly dependent on the level of details incorporated in the mathematical model. Only those models with sufficient trade-offs between investment and cash flow generate proper optimal solutions with the correct economic criterion. The consequences of decision-making based on wrong optimization criteria are discussed.

1. Introduction

In the financial theory, the net present value is the correct criterion for selection among mutually exclusive alternatives, while the other criteria, e.g. the profit and internal rate of return, are not totally correct. In process systems engineering, however, mathematical models with different economic objective functions and at different levels of complexity are frequently used for process flow sheet optimization. Several authors have observed that different economic criteria affect the optimal design of processes. Buskies (1997) established that optimal values of process parameters obtained during the optimization of chemical processes depend on the objective function. Novak Pintarič and Kravanja (2006) discussed the differences between optimal process designs obtained by means of qualitative, quantitative and, compromise economic criteria. Faria and Bagajewicz

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(2009) performed a MINLP design of water utilization systems by maximizing the NPV and IRR, and also observed different optimal solutions.
In this paper, the origin of the differences between optimal solutions is briefly discussed, as well as the consequences of decision-making based on wrong criteria in terms of the economic, operational and environmental performances of optimal chemical processes. The WAR algorithm (Young et al., 2000) was applied to evaluate the potential environmental impact (PEI) of the case-study processes. It was assumed that process flow sheets involve reaction, separation and recycling sections, and optionally, other subsystems, e.g. heat exchanger network, utility systems, wastewater treatment etc. Mathematical models involve estimation of the capital investment, and the cash flow.

2. The origin of the differences between optimal solutions

It was observed, that some flow sheet optimization models produce substantially different optimal designs when optimized regarding different objectives, while the others produce negligible differences. The latter indicates that only suboptimal solutions can be obtained with such models even when using proper optimization criterion, i.e. the NPV. Our recent work (Kasaš et al., 2009) shows that the main responsibility for the differences is the shape of the cash flow function vs. investment, and the steepness of its derivative curve. The cash flow function can be concave (monotonically increasing) or unimodal (with a maximum). This depends on the quality of trade-offs between the investment, and the benefit obtained. However, the quality of trade-offs in the model depends on the preciseness of the flow sheet model. Simplified models, e.g. stoichiometric reactor, result in unimodal cash flow (F_C) function vs. investment (I) with steep derivative curve (Figure 1a). A precise model, e.g. a kinetic reactor, produces a concave cash flow function whose derivative curve approaches asymptotically to a constant positive value (Figure 1b).

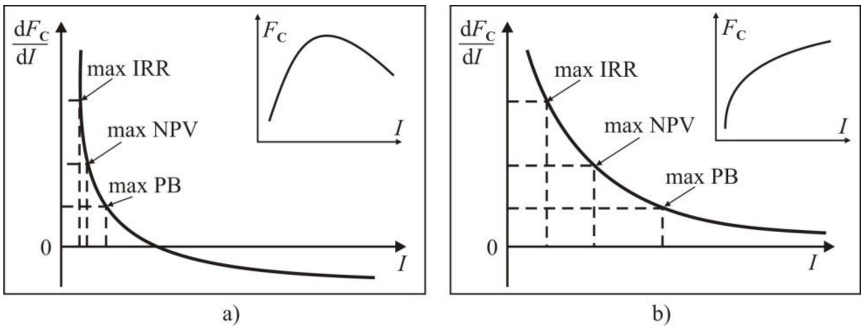

Figure 1: Derivative of unimodal (a) and concave (b) cash flow function.

It can be shown, by deriving stationary conditions for maximum profit, NPV and IRR, that optimal solutions obtained by using these criteria are very similar or equal (Figure 1a) for unimodal cash flow functions, whilst they are significantly different (Figure 1b) for concave cash flow functions. Moreover, the lowest investment level is obtained with the maximization of IRR, higher with the NPV, and the highest with the PB. This indicates that process models have to be formulated at a level of complexity which produces a concave cash flow function because, only in this case, a proper optimal solution can be derived at suitable economic criterion, the NPV.

3. Case-study examples

In the following section, mixed integer nonlinear programming (MINLP) syntheses of dimethyl ether, methanol and hydrodealkylation (HDA) processes were performed, together with simultaneous heat integration. These syntheses were performed by means of an automated MINLP Process Synthesizer MIPSYN (Kravanja, 2010).

3.1 Dimethyl ether process synthesis

A plant produces 50,000 t of dimethyl ether (DME) per year via the catalytic dehydration of methanol over an acid zeolite catalyst. The superstructure of the process (Figure 2) involves topological selections between: (i) two feed streams, one of them being more expensive as it contains less impurities, (ii) two reactors from which more expensive allows for higher conversion, (iii) discharging wastewater or implementing a wastewater treatment plant, and (iv) a steam-boiler or cogeneration unit. The kinetic model is used for the reactors, and the targeting model for heat integration (Duran and Grossmann, 1986). Three economic objective functions are optimized. The more expensive feed stream and reactor are selected in all three optimal solutions, while wastewater treatment unit is ignored. A steam-boiler is selected for steam production when maximizing IRR, and the cogeneration unit when using the PB and NPV criteria.

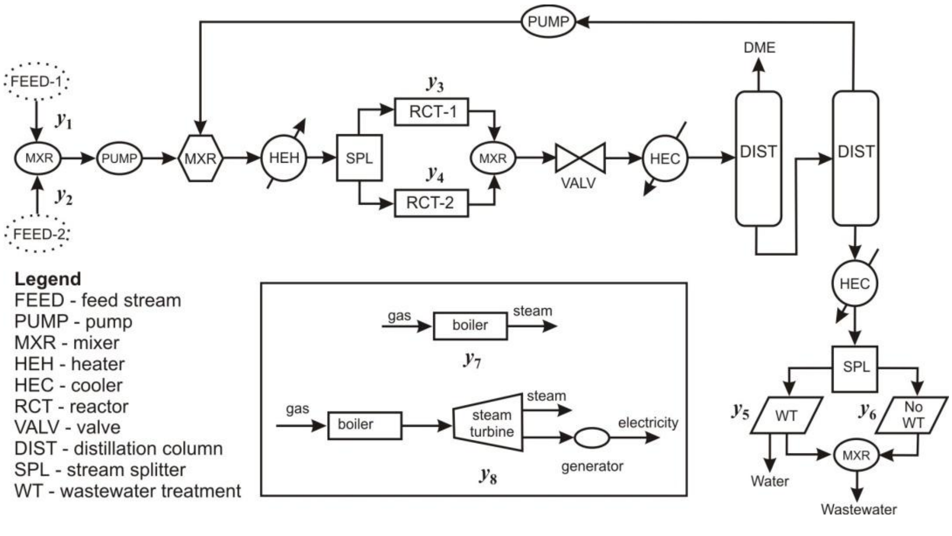

Figure 2: Superstructure of DME process.

The solution obtained using IRR criterion has the lowest investment cost and the lowest cash flow (Table 1). The conversion per pass is the lowest too, while the utility cost, CO_2 emission tax, and PEI value are the highest among the three solutions. Incorrect IRR criterion leads to inefficient utilization of reactant and utilities, and high environmental impact. Moreover, long-term use of IRR leads to suboptimal solutions with respect to the NPV optimization. The solution with maximum PB has good economic and environmental characteristics; however, its profitability (expressed as IRR) is the lowest. Profit is the accounting measure which does not take into account the time value of money, and favours late cash flows. As the solutions obtained with all three criteria are substantially different we can conclude that the model is developed at the sufficient level of the preciseness and the correct solution is obtained using the NPV criterion.

Table 1 Economic, operational and environmental indicators of DME process.

	max IRR	*max NPV*	*max PB*
NPV (kEUR)	6 111	6 303	6 207
PB (kEUR/a)	1 413	1 477	1 487
IRR (%)	33.01	31.91	30.22
Investment (kEUR)	3 953	4 300	4 621
Cash flow (kEUR/a)	1 323	1 394	1 423
Utility cost (kEUR/a)	568	540	526
CO_2 emission tax (kEUR/a)	73.8	33.5	32.6
Conversion per pass	0.95	0.97	0.98
Reactor volume (m^3)	3.81	5.85	8.48
Reboiler power (MW)	2.19	–	–
Cogeneration power (MW)	–	0.28	0.27
Total PEI (10^{-3})	5.88	5.64	5.54

3.2 HDA process synthesis

The HDA process was described by Kocis and Grossmann (1989). During the process toluene and hydrogen are reacted to make benzene. The superstructure (not presented here because of space limitations) involves topological selections between isothermal and adiabatic reactors, and between direct and indirect distillation sequences. The targeting model for minimal utility consumption was applied. Optimal solutions obtained with all three objective functions contain the adiabatic reactor and the distillation sequence where biphenyil is removed as bottoms in the first column, followed by the separation of benzene and toluene in the second column. In this case study, the differences between the solutions obtained with different objectives are small, however the same trends are observed as in the previous case (Table 2). It seems that the level of details in the model is low; the analysis of trade-offs between cash flow and investment is under investigation.

3.3 Methanol process synthesis

This section discusses MINLP synthesis of the methanol process flow sheet from synthesis gas. The example was taken from literature (Kravanja and Grossmann, 1990), whilst the prices were updated.

Table 2 Economic, operational and environmental indicators of HDA process.

	max IRR	*max NPV*	*max PB*
NPV (kEUR)	14 673	14 773	14 690
PB (kEUR/a)	4 715	4 762	4 771
IRR (%)	16.3	16.2	16.1
Investment (kEUR/a)	1 641	1 676	1 694
Cash flow (kEUR/a)	5 189	5 248	5 273
Conversion per pass (%)	40.9	42.6	44.2
Reactor volume (m^3)	18.6	19.7	21.2
Total power (MW)	13.190	13.163	13.161
PEI (10^{-5})	5.33	5.32	5.31

The superstructure of the process involves topological selections between: (i) two feed streams, one of which contains more hydrogen and is more expensive than the other, (ii) one-stage or two-stage compression of the feed stream, (iii) two reactors, one of which is more expensive and allows for higher conversion, and (iv) one-stage or two-stage compression of the recycle stream. The MINLP model (Yee and Grossmann, 1990) was added to the mathematical model of the process superstructure for simultaneous heat integration and heat exchanger network (HEN) synthesis. Three economic objective functions were optimized, as in the previous subsections. A more expensive feed stream was selected for all optimal solutions together with two-stage compression of the feed stream, and one-stage compression of the recycle stream. The cheaper reactor with lower conversion was selected by maximizing IRR and NPV, while a more expensive reactor with higher conversion was obtained by maximizing PB (Table 3).
Similarly as with other two processes, the IRR solution has the lowest conversion per pass, the highest utility cost and environmental impact. The PB solution has good operational and environmental characteristics, but is less profitable, i.e. has a lower IRR value. The correct solution is obtained using the NPV criterion.

Table 3 Economic, operational and environmental indicators of methanol process.

	max IRR	*max NPV*	*max PB*
NPV (MEUR)	180.80	181.98	180.92
PB (MEUR/a)	38.83	39.26	39.41
IRR (%)	41.69	40.97	39.57
Investment (MEUR)	82.63	85.24	89.12
Cash flow (MEUR/a)	34.63	35.13	35.50
Utility cost (MEUR/a)	11.04	10.68	10.43
Conversion per pass (%)	16.20	18.19	19.56
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
Total PEI (10^{-3})	3.75	2.96	2.50

4. Conclusion

From the financial point of view, the profit and internal rate of return are not applicable for investment projects when choosing among mutually exclusive alternatives. Anyway, they are often used in process systems engineering. This paper has discussed the consequences of decision-making based on wrong optimization criteria in terms of the economic, operational, and environmental performances of optimal chemical processes. Solutions with ineffective resource utilization and low sustainability performance are obtained when using IRR. Maximization of profit produces more efficient solutions with lower operating costs, which are achieved by e.g. higher conversion, better separation and/or higher level of heat integration. These solutions are, despite the higher investment level, more sustainable. 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 favours late cash flows. [gNPV is the only correct criterion from the financial viewpoint, while IRR and profit are convenient from a practical but not conceptual viewpoint. NPV establishes a balance between a fast return on investment and long-term steady generation of cash flow with fair environmental performance.

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